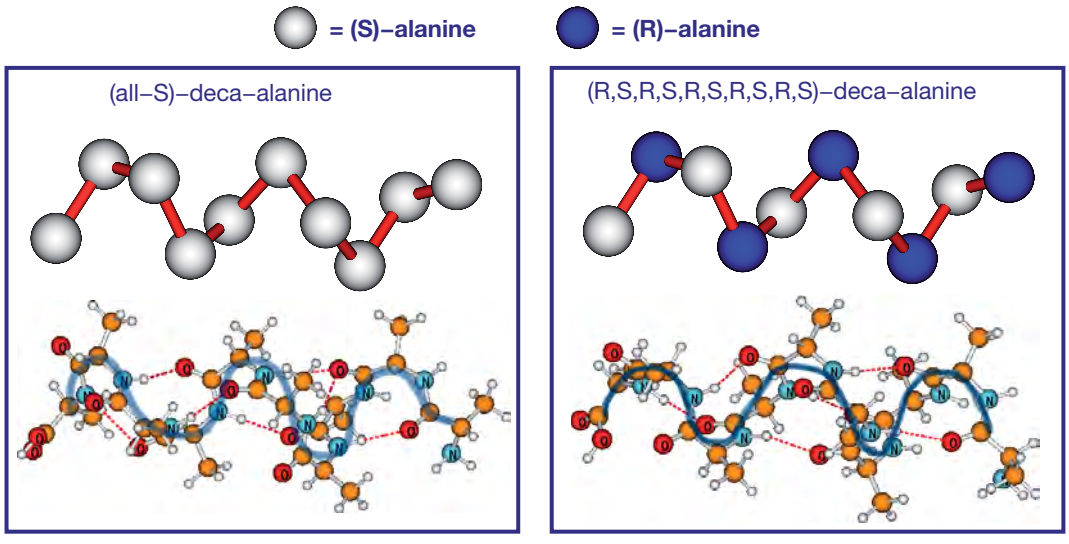
CSE

Computational Science and Engineering

Annual Report 2005/2006



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Swiss Federal Institute of Technology Zurich

CSE

Computational Science and Engineering

Annual Report
2005 / 2006

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Cover:

Optimized structures of helical decaalanine in all-S and alternating-R,S configurations as model structures to probe the selectivity of Raman Optical Activity spectroscopy with respect to axial and central chirality.

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Introduction

This is the sixth Annual Report of Computational Science and Engineering, CSE, at the ETH. It has already become customary that the report is done electronically only. Most of us have become adjusted to the fact that it is much more convenient to obtain information in electronic form. High quality four colour printers are accessible for those who still like to read a hard copy. We started last year with the new Master Program in CSE. Unfortunately, for administrative reasons we could not advertise this Master Program agressively neither last year nor this year. However, this will now change. Therefore, it becomes particularly important to have the report electronically available on the web to attract students not only from within ETH but from all over the world. More and more persons are interested in research and education in CSE, students and 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.

This fall the first students finished their last exams before starting to work on their Master thesis. In spring of 2007 the frist group of students will have finished the whole new Bachelor/ Master cycle. This is the moment to review the program as a whole and therefore we plan for a workshop on CSE, Research and Education, in 2007. As it happens, 2007 will be the 10 anniversary of the CSE curriculum at ETH.

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 Markus Reiher from Physical Chemistry will show in the featured report progress in his field.

I wrote last year that the work on the preparation for the International Congress on Industrial and Applied Mathematics, ICIAM 2007, was already in full swing. However, as of now the work intensity increased incredibly. We have about 3400 persons who indicated that they will participate. A total of 1050 contributed papers have been submitted and there will be more then 300 minisymposia with, up to now about 1500 lectures. There will about three dozens invited lectures. We are looking forward to this event which will be held at the University of Zürich and at ETH, July 16-20. A large portion of the congress will cover CSE.

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

Zürich, November 19, 2006
Rolf Jeltsch, Studiendelegierter und Mitglied des Ausschusses Rechnergestützte Wissenschaften

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Education

In October 2005, 14 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 1 student, Physics 4, Computer Science 2, Mechanical Engineering 2, Electrical Engineering 3; and from Swiss Fachhochschulen in Electrical Engineering 1and in Computer Science 1.

From outside ETH 2 students entered the CSE Master curriculum, 1 from the University of Erlangen-Nürnberg with a Bachelor degree in Computational Engineering, 1 from a German Fachhochschule with a degree in Mechanical Engineering.

In the last academic year the first 13 students earned their Bachelor degree in CSE and will thus be able to continue their studies in the CSE Master Program which started last October. The Master studies will take one and a half years including the five months of the Master thesis and will lead to the degree of a Master of Science ETH in CSE.

In the two and a half years Diploma curriculum in CSE existing since October 1997 and started for the last turn in October 2003, 15 students finished their studies in 2005/2006.

The total number of CSE students enrolled in the academic year 2005/2006 was 46.

The presentation of the CSE Bachelor/Master curricula for ETH students of the second semester of June 7, 2006 was attended by around 50 students. It is hoped that a fair number of them will start with the CSE Bachelor studies this fall.

In the past academic year 28 students have successfully finished a CSE curriculum, Diploma and Bachelor, respectively, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/diploma thesis and, in parentheses, the name and the department/institute of the advisor.

Bachelor Theses

M. Blattmann	Durchführung idealisierter Simulationen im regionalen Klimamodell CHRM mit einem Wasserdampftracer (H. Davies, Atmospheric and Climate Science)
S. Bucheli	Berechnung der Strömung im Gleichgewichtsorgan (L. Kleiser, Fluid Dynamics)
R. Carnecky	2D Plasma Flow past a cylinder (C. Schwab, Applied Mathematics)
L. Gamper	XML Database for Physics Simulations (M. Troyer, Theoretical Physics)

S. Gerster	Simulation and Control of a 2DOF Robot Arm (J. Nelson Bradley, Robotics and Intelligent Systems)
M. Koller	Numerische Simulation einer turbulenten Freistrahlströmung (L. Kleiser, Fluid Dynamics)
M. Müller	Free Energy Calculations on Monosaccharide Isomerizations (P. Hünenberger, Computational Chemistry)
C. Scherrer	Monotone Multigrid Solver for American Put with Stochastic Volatility (C. Schwab, Applied Mathematics)
M. Tobler	Magnetic Micro Robot Steering Using Two Magnets (B. Nelson, Robotics and Intelligent Systems)
C. Tobler	Untersuchung zur Wärmeleitungsgleichung in Terra3D (C. Schär, Atmospheric and Climate Science)
K. Schüpbach	Adaptive FEM (M. Gross, Computer Graphics)
S. Villiger	Optionsbewertung mittels hochdimensionaler numerischer Integration (C. Schwab, Applied Mathematics)
B. Wüthrich	Object-Oriented Numerical Interpolation Component in Eiffel (B. Meyer, Software Engineering)

Diploma Theses

G. Baschera	Automated Image Based Calibration of a Scanning Electron Microscope (J. Nelson Bradley, Robotics and Intelligent Systems)
D. Caviezel	Parallelization of the Multiblock CMFD-Code TransAT-MB (P. Jenny, Fluid Dynamics)
J. Eller	Train Driver Rostering at SBB Cargo (H.-J. Lüthi, Operations Research)
A. Elsener	Statistical Analysis in Ceminformatics (P. Bühlmann, Statistics)
M. Guidon	Continuous Time simulation of dissipative Quantum systems (M. Troyer, Theoretical Physics)

M. Hack	Verbrennungsmodellierung mit einer PDF-Methode (P. Jenny, Fluid Dynamics)
N. Hodler	Numerical Computation of Eigenvalues for a Covariance Operator at Small correlation Length (C. Schwab, Applied Mathematics)
R. Mooser	Wavelet Solution of Elliptic Stochastic PDEs (C. Schwab, Applied Mathematics)
E. Huber	Development and Validation of a Software Algorithm for Inferring Mechanical Properties of Tendon by Analyzing Cell Displacements in Confocal Fluorescence Endomicroscopy (R. Müller, Biomedical Engineering)
T. Oesch	Wavelet Methods for Computation of optimal Investment of an Insurance (C. Schwab, Applied Mathematics)
J. Renggli	Quadtree Techniques for the Construction of Structured Auxiliary Meshes (R. Hiptmair, Applied Mathematics)
P. Rousselot	Dammerosion – Numerische Simulation eines hochinstationären Phänomens (H.-E. Minor, Hydraulics, Hydrology and Glaciology (VAW))
D. Sydler	Nutzung von Vorwissen und Tracerexperimenten zur optimalen Diagnose von Leckagen in abwasserkanälen (W. Gujer, Urban Water Management)
M. Uhr	Optimal Operation of a Hydroelectric Power System Subject to Stochastic Inflows and Load (M. Morari, Automatic Control)
M. Wittberger	Finite-Element-Time-Domain (FETD) Simulation of charged Particles in a Cavity (Rolf Jeltsch, Applied Mathematics)Rolf Jeltsch

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

Term Papers

G.-M. Baschera	Flow Simulation and Visualization using unstructure meshes (D. Szczerba, Computer Vision Laboratory)

L. Blaser	Mass Transport in Haemodynamics (A. Quarteroni, CMCS, EPF Lausanne)
C. Bosshard	Solving the Train Routing Problem with a Multicommodity Flow Formulation (H.-J. Lüthi, Operations Research)
S. Bucheli	Constraint-based Rigid Body Simulation with Constant Time Stepping Schemes (M. Gross, Computer Graphics Lab)
D. Caviezel	Parallel Solver for the Heat Equation with Compact Finite Difference Schemes (L. Kleiser, Fluid Dynamics)
A. Elsener	MD Simulation for a Coarse grained Model (W. van Gunsteren, Computational Chemistry)
N. Hodler	Das Stäbchenspiel (M. Troyer, Theoretical Physics)
E. Huber	Parallelization of a Particle Simulation in Costal Waters Using Forward and Reverse Time Diffusion (A. W. Heemink, Applied Mathematical Analysis, TU Delft)
R. Mooser	Wavelet FEM für PDEs mit stochastischen Daten (C. Schwab, Applied Mathematics)
M. Müller	Blocking prediction in the ECMWF ensemble forecasting system (E. Källén, Physics of the Atmosphere, Stockholms Universitetet)
J. Nart	Adaptive Agents, Natural Resources, and Civil War (R. Riolo, Complex Systems, University of Michigan)
J. Renggli	Sparsification of FFT (C. Schwab / W. Petersen, Applied Mathematics)
S. Riva	An algorithm to Reduce Point Data Sets by Binary Merging of Nearest Neighbours (B. Moore / J. Stadel, Astrophysics, University of Zurich)
K. Schüpbach	Hierarchical Algorithms for Simulation of Deformable Objects, (M. Gross, Computer Graphics Lab)
M. Uhr	A Java Simulation Framework for Testing Embedded (R. Riener, Automatic Control)

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 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 diploma theses (if there are free time slots).

Zürich, September 26, 2006
Kaspar Nipp,
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 WS05/06

03.11.05	O. Sterz, CST GmbH, Darmstadt Simulation for Today's Engineering Electromagnetics
17.11.05	F. Ihlenburg, Hochschule für Angewandte Wissenschaften (HAW), Hamburg Vibroakustische Simulation in der Automobilentwicklung
24.11.05	M. Mascagni, Angewandte Mathematik Random Number Generation: The Engine of Monte Carlo Methods
01.12.05	A. Curioni, IBM Rüschlikon Large Scale Molecular Dynamics simulations on BlueGene: Towards In-silico Material Design
12.01.06	P. Bartelt, Schnee- und Lawinenforschung, Davos The Role of Numerical Simulation in Natural Hazard Prevention with Examples from Snow Avalanches, Debris Flows and Rock Falls
19.01.06	S. Bonhoeffer, Theoretische Biologie Mathematische Modellierung von Virus-Infektionen
26.01.06	G. Lake, CSE Uni Zürich Gravity for Planets to Cosmology

Case Studies Seminar SS06

20.04.06	D. Bresch / S. Wunderlich, Swiss Re Natural Catastrophe Modelling at Swiss Re
04.05.06	H. J. Herrmann, Baustoffe Simulations of Granular Materials
11.05.06	W. Wiechert, Uni Siegen Simulation and Design of a High Energy Ball Mill
18.05.06	A. Kruzhin, Rofin-Sinar Laser GmbH, München Certain Mathematical Problems Arising in Laser Marking
01.06.06	M. Reiher, Theoretische Chemie Algorithms in Quantum Chemistry
08.06.06	W. van Gunsteren, Informatikgestützte Chemie Computer Simulation of Biomolecular Systems – Achievements and Perspectives
15.06.06	P. Jenny, Fluiddynamik Multi-Scale Finite-Volume Method for Elliptic and Parabolic PDEs
22.06.06	R. Müller, Bioengineering Computer Simulations in Orthopedics - From Macro to Nano

4

Computational Highlight

Finding a Needle in a Haystack: Smart Calculation of Characteristic Vibrations in Large Molecules

Carmen Herrmann, Johannes Neugebauer, and Markus Reiher

Laboratorium für Physikalische Chemie, ETH Zürich, Hönggerberg Campus HCI, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland

Abstract

Vibrational spectroscopy is a powerful tool to investigate the structure and dynamics of molecular systems. When large molecules are studied, quantum chemical calculations help to interpret the spectra. In many cases, experimental questions are related to specific regions of a vibrational spectrum, so that an assignment is only required for a subset of vibrations. This holds true in particular for biomolecules, inorganic compounds which are stabilized by many bulky ligands, or other extended systems. In standard quantum chemical calculations of the vibrational spectrum, all normal modes and frequencies of the molecule under study are determined. However, the selective calculation of the relevant information only can be made much more efficient by using mode-selective techniques such as the mode-tracking algorithm. A critical point for the performance of the mode-tracking scheme is the preparation of a guess vibration, which is then iteratively refined. This guess defines the scientific problem which is to be studied. As examples, we review the calculation of adsorbate modes of a flexible thiophenolate anion attached to a rigid silver cluster modeling an extended silver surface. It reveals that mode-tracking works very well for such systems and results in a considerable gain of computational efficiency. The second example is the mode-selective calculation of Raman Optical Activity intensity differences for the breathing modes of two different diastereomers of a right-handed deca-alanine helix.

1 Introduction

A large variety of experimental techniques has been developed in order to investigate the structure and dynamics of molecules, which yield valuable and often complementary information. In addition to Nuclear Magnetic Resonance and X-Ray spectroscopy, vibrational spectroscopy is a very powerful tool to obtain such information. Because of the large number of special vibrational spectro-

scopic techniques such as Resonance Raman, Raman Optical Activity or Difference IR spectroscopy, and the size of many interesting molecules (like e.g. large biomolecules) under study, it is often difficult to interpret recorded spectra based on experience and empirical rules of thumb alone, and it may be impossible to assign important vibrational peaks uniquely. In such cases, quantum chemical or molecular dynamics calculations of vibrational spectra can help to make reliable connections between molecular structure and spectra. In our group, we concentrate on the calculation of vibrational spectra with means of static quantum chemistry.

The basis of the quantum chemical description of molecular vibrations of molecules with more than a few atoms is the Born–Oppenheimer approximation [1], which allows for a separate description of the movements of the atomic nuclei and the electrons. These are coupled in the time-independent nonrelativistic Schrödinger equation

$$\hat{H}_{\mathrm{mol}}\Psi_I = [\hat{T}_{\mathrm{K}} + \hat{T}_{\mathrm{e}} + \hat{V}_{\mathrm{nuc,nuc}} + \hat{V}_{\mathrm{nuc,e}} + \hat{V}_{\mathrm{e,e}}]\Psi_I = E_I\Psi_I, \tag{1}$$

(where I labels the state of the system) by the electron-nucleus-interaction Hamiltonian $\hat{V}_{\mathrm{nuc,e}}$, whereas the contributions to the total molecular Hamiltonian $\hat{H}_{\mathrm{mol}}$ which describe the kinetic energy of the nuclei ($\hat{T}_{\mathrm{K}}$), the kinetic energy of the electrons ($\hat{T}_{\mathrm{e}}$), the interaction of the nuclei ($\hat{V}_{\mathrm{nuc,nuc}}$), and the interaction of the electrons ($\hat{V}_{\mathrm{e,e}}$) refer to either nuclear or electronic coordinates only and thus do not prevent a separation of the Schrödinger equation into a nuclear and an electronic part. The Born–Oppenheimer approximation is based on the adiabatic approximation, in which the wave function $\Psi_I(\mathbf{R}, \mathbf{r})$ is separated into an electronic and a nuclear part. The nuclear part $\chi_a(\mathbf{R})$[1] depends on the $3M$ coordinates $\mathbf{R}_A$ of all M nuclei collected in the vector $\mathbf{R}$, and the electronic part $\Psi_{e,i}(\mathbf{r}, \tilde{\mathbf{R}})$ depends explicitly on the $3N$ coordinates $\mathbf{r}_i$ of all N electrons (summarized as the vector $\mathbf{r}$), and parametrically on the nuclear coordinates [2] (which is expressed by the tilde),

$$\Psi_I(\mathbf{R}, \mathbf{r}) = \chi_a(\mathbf{R}) \cdot \Psi_{e,i}(\mathbf{r}, \tilde{\mathbf{R}}). \tag{2}$$

The indices a and i label nuclear and electronic energy levels, respectively, and are defined by the composite total index I. By neglecting the action of the nuclear

[1] As far as the notation is concerned, vectors are printed in bold-face and small letters, matrices in bold-face and capitals. As an exception, nuclear coordinates are indicated by bold-face capitals, $\mathbf{R}$ referring to cartesian and $\mathbf{Q}$ to normal coordinates. If not mentioned otherwise, all nuclear coordinates are mass-weighted ones, which are related to non-mass-weighted ones as $\mathbf{R}_A^{(m.w.)} = M_A^{1/2} \cdot \mathbf{R}_A$, where A refers to the x, y or z coordinate of nucleus A and M_A is its mass. For the sake of simplicity, the superscript $(m.w.)$ is left out in the text.

[2] Parametrical dependence of the electronic wave function on the nuclear coordinates means that these coordinates enter the electronic Schrödinger equation as constant values. Different electronic wave functions are thus obtained for different sets of nuclear coordinates, i.e. for different molecular structures.

kinetic energy operator onto the electronic wave function, the adiabatic approximation turns into the Born–Oppenheimer equation. As a result, after inserting Eq. (2) into Eq. (1), multiplying from the left with $\Psi^{\star}_{e,i}(\mathbf{r},\tilde{\mathbf{R}})$ and integrating over all electronic coordinates, the nuclear Schrödinger equation,

$$\left[\hat{T}_K + E_{e,i}(\mathbf{R})\right] \chi_a(\mathbf{R}) = E_{tot}\chi_a(\mathbf{R}), \tag{3}$$

is obtained, which describes the nuclei as moving on the potential energy surface (PES) defined by $E_{e,i}(\mathbf{R})$ of the electronic state i. The PES may be obtained pointwise by solving the electronic Schrödinger equation,

$$[\hat{T}_e + \hat{V}_{nuc,nuc} + \hat{V}_{nuc,e} + \hat{V}_{e,e}]\Psi_{e,i}(\mathbf{r},\tilde{\mathbf{R}}) = E_{e,i}(\mathbf{R})\Psi_{e,i}(\mathbf{r},\tilde{\mathbf{R}}), \tag{4}$$

for different positions of the nuclei. This provides the potential in which the nuclei are moving. As far as the nuclear Schrödinger equation is concerned, it is sufficient to know that it is possible to calculate the electronic PES and its derivatives pointwise.
At present, the most popular way to describe the electronic structure $E_{e,i}(\mathbf{R})$ of large molecules with means of first-principles quantum chemistry is density functional theory (DFT) [2–4]. This method relies on regarding the ground-state electron density instead of the electronic wave function as the central quantity which contains all information on the molecule. Since the exact universal density functional is not known, approximate density functionals such as BP86 [5,6] and B3LYP [7, 8] are employed in actual calculations. Furthermore, the molecular electronic structure is usually expressed using a set of atomic-orbital-like basis functions. A variety of standard basis sets of different size such as SVP and TZVP [9] has been developed.

The most simple expression for the nuclear wave function $\chi_a(\mathbf{R})$ is a product of functions which each only depend on one nuclear coordinate. This product will be an exact ansatz for the solution of Eq. (3) if the individual coordinates are not coupled through the terms in the Hamiltonian operator in Eq. (3). The first step to achieve such a decoupling is to express the dependence of the PES on Cartesian nuclear coordinates as a Taylor series around the nuclear equilibrium structure $\mathbf{R} = \mathbf{0}$,

$$\begin{aligned} E_{e,i}(\mathbf{R}) &= E_{e,i}(\mathbf{0}) + \sum_{A=1}^{3M} \left(\frac{\partial E_{e,i}}{\partial R_A}\right)_0 R_A \\ &+ \frac{1}{2}\sum_{A=1}^{3M}\sum_{B=1}^{3M} \left(\frac{\partial^2 E_{e,i}}{\partial R_A \partial R_B}\right)_0 R_A R_B + \ldots, \end{aligned} \tag{5}$$

and to truncate it after the second-order term (harmonic approximation). Then, considering that the energy gradients are zero at the equilibrium (= minimum) structure, choosing the equilibrium energy as zero and transforming it to a set of

$3M$ mass-weighted normal coordinates $\mathbf{Q}_A$ which makes all mixed second derivatives of the electronic energy $(\partial^2 E_{e,i}/\partial \mathbf{Q}_A \partial \mathbf{Q}_B)_{A \neq B}$ vanish, a decoupled description is possible. Thus, in practice, a quantum chemical vibrational analysis is carried out by calculating and diagonalizing the Hessian $\mathbf{H} = (\partial^2 E_{e,i}/\partial R_A \partial R_B)$,

$$\mathbf{Q}^T \mathbf{H} \mathbf{Q} = \mathbf{H}^Q. \tag{6}$$

The columns of the matrix $\mathbf{Q}$ which diagonalizes $\mathbf{H}$ are the normal mode vectors. 6 of them (or 5, for linear molecules) correspond to translational and rotational motions, while the remaining $3M - 6$ (or $3M - 5$ in the case of linear molecules) ones describe the vibrational motions of the molecules.

The nuclear kinetic energy operator $\hat{T}_K = \sum_A \partial^2/\partial \mathbf{Q}_A^2$, is also diagonal with respect to these coordinates, so that the product

$$\chi_a(\{\mathbf{Q}_I\}) = \psi_1(\mathbf{Q}_1) \cdot \psi_2(\mathbf{Q}_2) \cdot \cdots \cdot \psi_M(\mathbf{Q}_M) \tag{7}$$

is an exact solution of the nuclear Schrödinger equation in harmonic approximation, which is now separable into $3M$ independent equations of harmonic oscillator form with a mass equal to unity (since mass-weighted coordinates are employed). The vibrations of the molecule are thus described as a system of decoupled harmonic oscillators. The eigenfunctions of harmonic oscillator equations are known, and their eigenvalues (the angular frequencies ω_I) are equal to the square root of the second energy derivatives. Of course, since $\omega = 2\pi\nu$ and $\tilde{\nu} = \nu/c$, vibrational frequencies ν and wavenumbers $\tilde{\nu}$ can be easily calculated from the angular frequencies.

Truncating the Taylor expansion of the PES in Eq. (5) after the second term is mandatory for molecules with about 5 atoms or more for reasons of computational feasibility. For smaller molecules, the Taylor expansion can be circumvented by calculating the PES explicitely pointwise. If, for example, the PES of a triatomic molecule is calculated using 10 points along 3 internal coordinates, the total molecular energy needs to be evaluated at $10^3 = 1000$ different nuclear structures (= points on the PES). By adding only one atom, the dimensionality of the problem rises by a factor of 1000, since the system now has 6 independent internal coordinates, so $10^6 = 1000000$ points would have to be evaluated. This shows why medium-sized and large molecules need to be treated within the harmonic approximation. For medium-sized molecules, the deviations of the harmonic approximation from the true PES may be captured partly by calculating anharmonic corrections in a second step. For an overview of typical molecular size classifications and the capabilities of present-day quantum chemical methods to describe their vibrational spectra see Fig. 1.

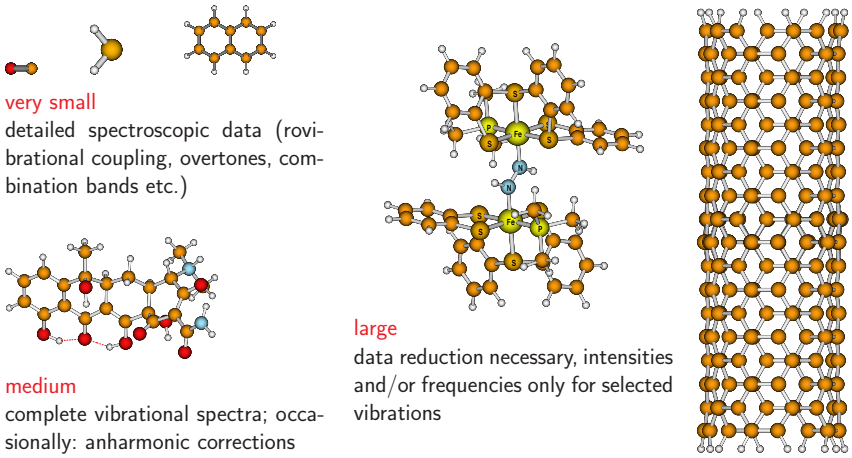


Figure 1: Overview of molecule size classifications and the performance of present-day quantum chemical methods to calculate their spectra.

Especially when large molecules are investigated, the interesting parts of the vibrational spectrum may be localized on a certain fragment of the molecule. Conventional quantum chemical calculations of vibrational spectra, however, yield all vibrational modes of the molecule. When first-principles quantum chemical methods such as density functional theory with sufficiently large basis sets shall be employed, the calculation of the Hessian for systems with 100 atoms or more requires enormous computational resources or even becomes unfeasible. Fig. 2 shows an example of a large molecule with bulky substituents and its calculated IR spectrum. The molecules contains 182 atoms, which corresponds to 546 degrees of freedom with 540 vibrational modes. Bulky substituents are often ignored in quantum chemical calculations, though their effect on vibrational spectra may be significant.

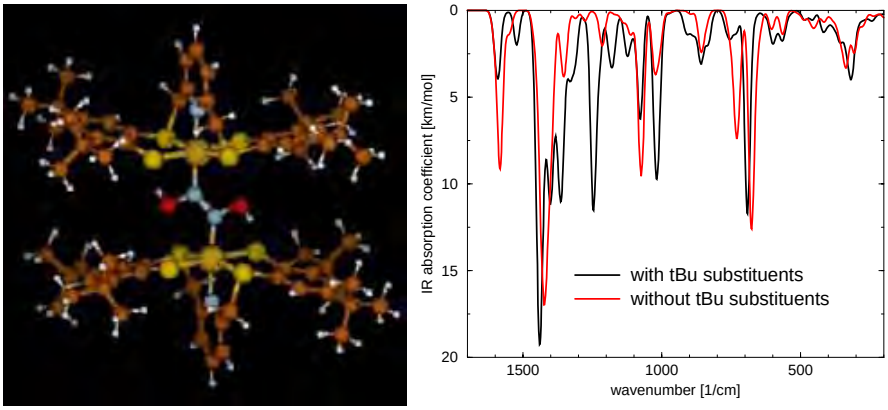


Figure 2: Calculated IR spectrum of a $(NOH)_2$ transition metal complex, calculated with and without inclusion of the bulky *t*-butyl substituents (BP86/RI/SVP).

If only those parts of the vibrational spectrum are calculated with mode-selective techniques which are really of interest, the effort will be greatly reduced and even larger molecules will become accessible to first-principles methods. Aiming at a target-oriented solution of problems, it actually seems unreasonable first to calculate much more information than necessary with a huge computational effort just to discard the major part of the data in a second step. Moreover, the latter step may require to find "a needle in a haystack", i.e., a particular vibration among hundreds of others by visual inspection of the results. In contrast to this, mode-specific techniques yield "the needle without the haystack". In order not to loose accuracy in such mode-specific approaches, a necessary condition is that no (or only well-controlled) approximations in addition to those already made in the calculation of full vibrational spectra are introduced. "Well-controlled" means that the approximate size of the introduced error is known. For the normal modes, all of this can be achieved by using the mode-tracking protocol [10], which makes the selected calculation of exact (harmonic) normal modes possible based on preconstructed initial guess vibrations [11–17]. Various applications of mode-tracking are documented in Refs. [11,12,14–19], while the stability and efficiency of the algorithm has been analyzed in Ref. [13]. The principle of data reduction by mode-tracking is visualized in Fig. 3

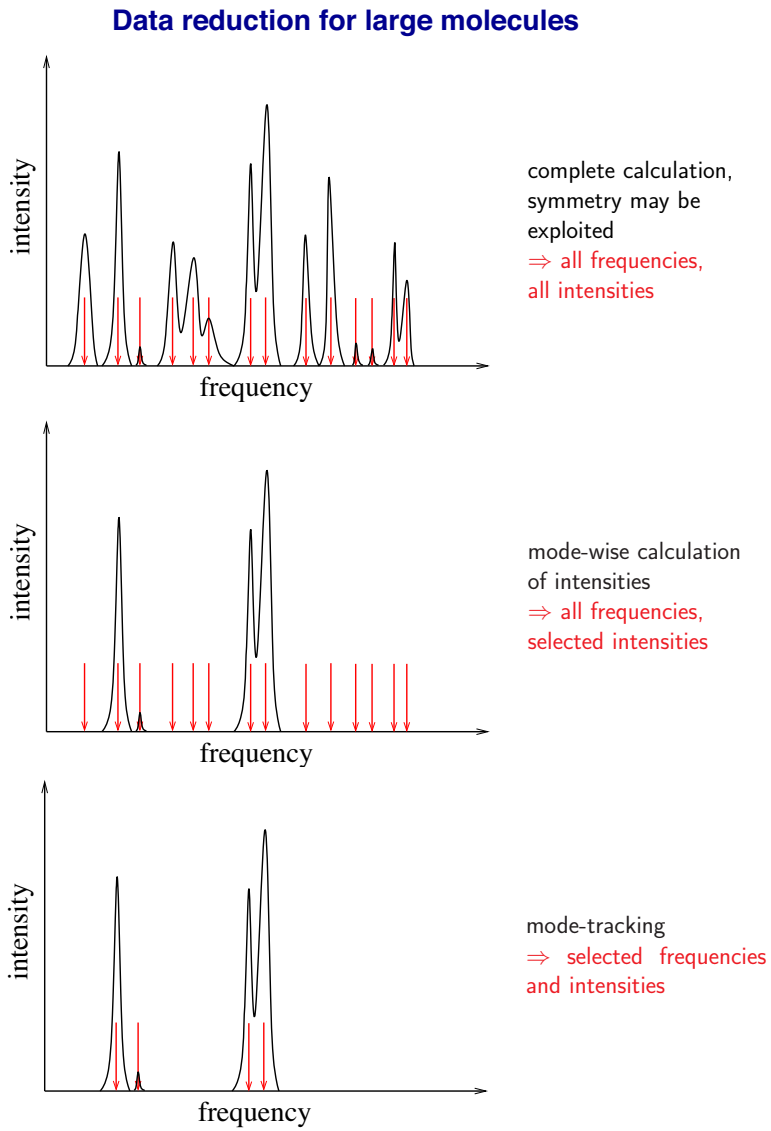


Figure 3: Illustration of the central goal of mode-tracking compared to standard techniques: Calculate only the relevant information, i.e., only selected vibrational frequencies and intensities.

Mode-tracking has been shown to work for various types of local subsystems — for a flexible adsorbate on a rigid metal cluster [17] (see middle right panel of Fig.

4), for carbon chains in dinuclear polyynediyl rhenium complexes [11] (lower left panel), for OH fragments in weakly interacting oligomers [19] (lower right panel), as well as for calculating the effects of the periphery of a large transition metal complex on local vibrations [12] (middle left panel). It has also been successfully applied to the selective calculation of vibrations which involve atoms in the whole system, and which are characterized by, e.g., a certain symmetry, or by breathing motions (see upper right panel of Fig. 4).

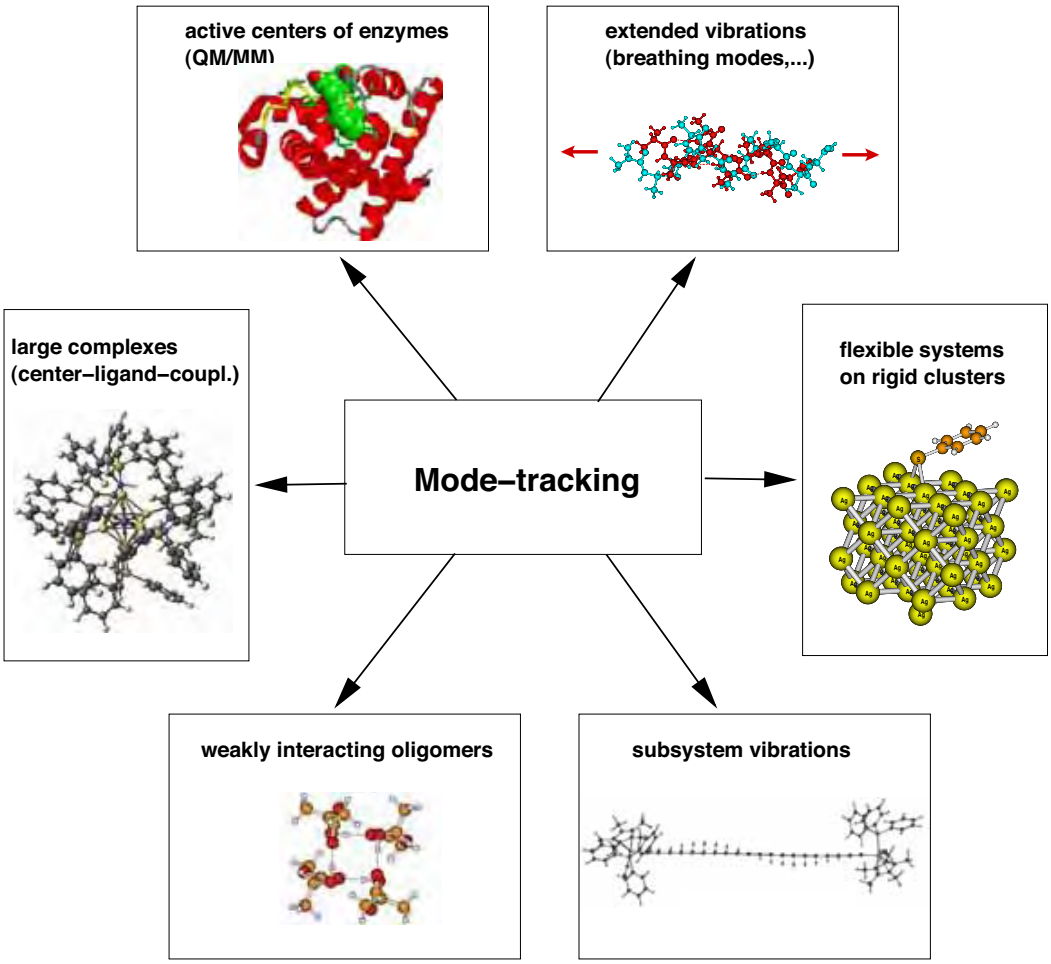


Figure 4: Some examples of the range of applicability of the mode-tracking scheme.

Two of these examples, a thiophenolate adsorbate on a silver cluster (middle right panel) and helical deca-alanine (upper right panel) will be reviewed in further de-

tail after discussing some algorithmic and practical aspects of the mode-tracking scheme.

2 A closer look at the mode-tracking algorithm

The mode-tracking protocol allows for the selective calculation of vibrational frequencies and normal modes from eigenpairs of the Hessian through subspace iteration [10, 13]. It can be outlined as follows (see also Fig. 5):

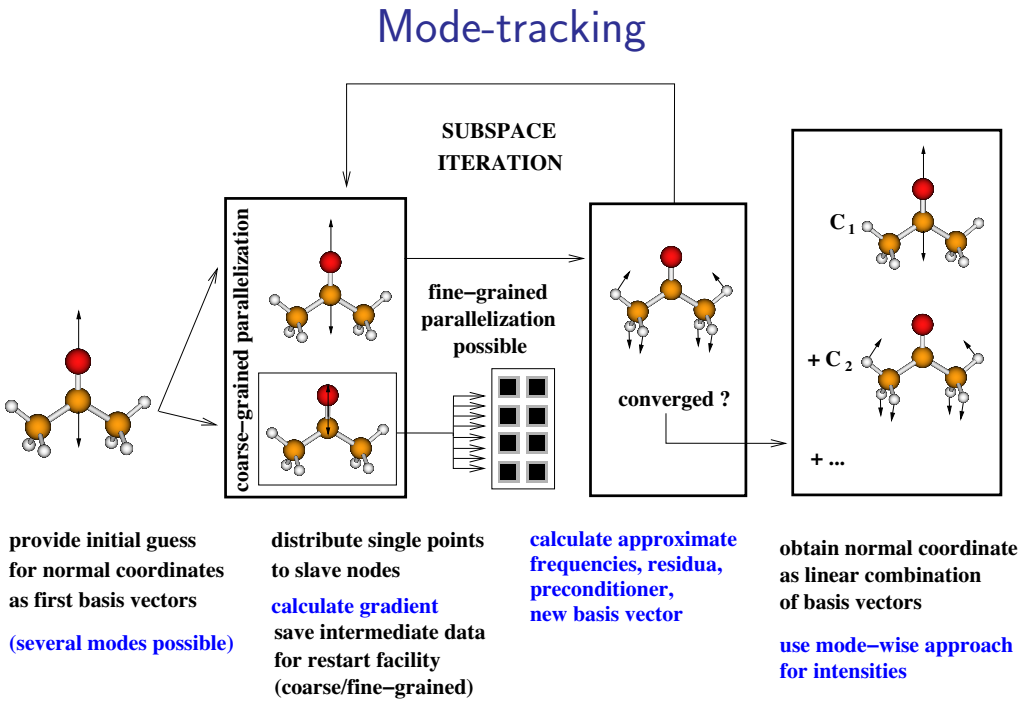


Figure 5: The mode-tracking protocol.

1. Guess a vibration $\mathbf{Q}_\mu^{(0)}$, which may be chosen based on chemical intuition or on a precedent vibrational analysis with a lower level of accuracy.

2. Use this guessed vibration as a first basis vector $\mathbf{b}_1$ in a Davidson-like algorithm [20]: $\mathbf{b}_1 = \mathbf{Q}_\mu^{(0)}$.

3. Construct the small Davidson matrix $\tilde{\mathbf{H}}^{(i)}$ from the Hessian $\mathbf{H}$ and the matrix $\mathbf{B}^{(i)}$ which contains all basis vectors of iteration i as columns, $\tilde{\mathbf{H}}^{(i)} = \mathbf{B}^{(i)T}\mathbf{H}\mathbf{B}^{(i)}$, and diagonalize it: $\tilde{\mathbf{H}}^{(i)}\mathbf{c}_\mu^{(i)} = \lambda_\mu^{(i)}\mathbf{c}_\mu^{(i)}$.

4. Calculate the approximate eigenvectors $\mathbf{Q}_\mu^{(i)}$ of the Hessian from $\mathbf{c}_\mu^{(i)}$ and $\mathbf{B}^{(i)}$: $\mathbf{Q}_\mu^{(i)} = \sum_{j=1}^{i} c_{\mu,j}^{(i)} \mathbf{b}_j$.

5. Check for convergence.

6. If the convergence criteria are not satisfied, create one new basis vector per tracked normal mode $\mathbf{Q}_\mu^{(i)}$ from the corresponding residuum vector $\mathbf{r}_\mu^{(i)}$, $\mathbf{r}_\mu^{(i)} = \sum_{j=1}^{i} c_{\mu,j}^{(i)} \left[\mathbf{H}\mathbf{b}_j - \lambda_\mu^{(i)} \mathbf{b}_j\right]$ and go back to step 3. For details on convergence criteria and creating new basis vectors using a preconditioner we refer to Refs. [10] and [13].

In order to calculate the matrix product $\mathbf{B}^{(i)T}\mathbf{H}\mathbf{B}^{(i)}$ without computing the Hessian $\mathbf{H}$, a matrix $\mathbf{\Sigma}^{(i)} = \mathbf{H}\mathbf{B}^{(i)}$ is defined. The elements ${\Sigma_{jI}}^{(i)}$ are evaluated by applying the chain rule for differentiation,

$$\Sigma_{jI}^{(i)} = \sum_J \left(\frac{\partial^2 E}{\partial \mathbf{R}_I \partial \mathbf{R}_J}\right)_0 B_{jJ}^{(i)} \quad = \quad \left(\frac{\partial^2 E}{\partial \mathbf{R}_I \partial \mathbf{b}_j}\right)_0 = \left[\frac{\partial}{\partial \mathbf{b}_j}\left(\frac{\partial E}{\partial \mathbf{R}_I}\right)\right]_0, \qquad (8)$$

where the $B_{jJ}^{(i)}$ are the coefficients for the Cartesian basis vector $\mathbf{R}_J$ in the basis vectors $\mathbf{b}_j$ and E denotes the total molecular energy. The components of $\mathbf{\Sigma}^{(i)}$ can thus be calculated numerically as directional derivatives of the gradient components along the basis vectors $\boldsymbol{b}_j$. Several normal modes may be optimized simultaneously using the Davidson–Liu (also known as block-Davidson) method [21, 22].

In contrast to the Partial Hessian Vibrational Analysis technique [23], where the problem is simplified by diagonalizing only a subsystem block of the Hessian while discarding couplings to the remaining degrees of freedom, the mode-tracking technique converges a set of initial guess vectors to *exact* eigenvectors of the full Hessian provided the convergence criteria are chosen sufficiently tight.

3 Algorithmic program design

The mode-tracking algorithm is implemented in the program AKIRA [10]. AKIRA is a meta-program which may be connected to any quantum chemistry program package providing energy gradients. At the moment, interfaces to TURBOMOLE [24], DALTON [25], ADF [26, 27], and GAUSSIAN [28] are available for the raw data calculation (see Fig. 6).

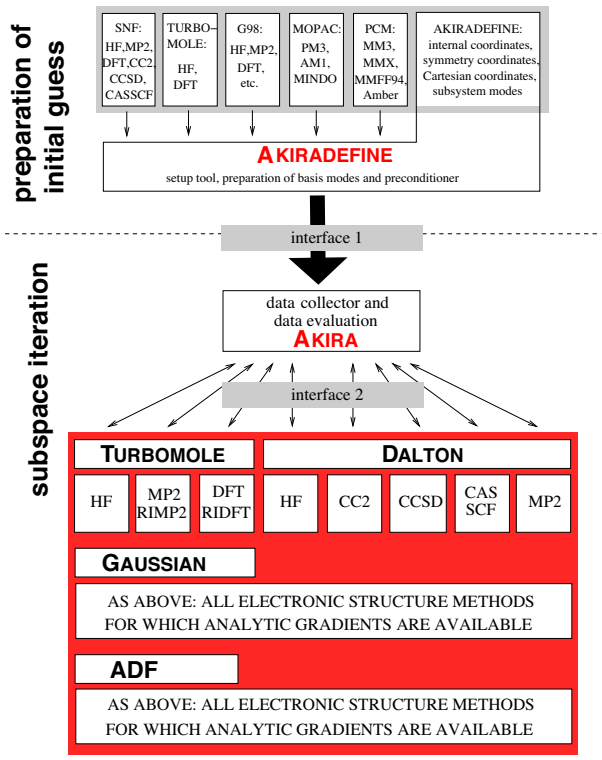


Figure 6: Hierarchical structure of the mode-tracking program AKIRA [10]; http://www.theochem.ethz.ch/software/akira.

In the context of mode-tracking, the term "raw data" denotes molecular gradients, which are calculated analytically by the quantum chemistry program packages mentioned above and differentiated numerically along basis vectors by AKIRA. The advantages of such a semi-numerical implementation of the algorithm are the following:

- Raw data available from almost every quantum chemical program — and thus from any method — can be used,
- coarse- and fine-grained parallelization possible,
- easy and efficient restart facilities available,
- easy implementation of point-group symmetry,
- control of numerical error by number of grid points, Richardson extrapolation,

⇒ various existing program packages can be docked and driven,

⇒ calculations are possible for any molecular size for which a partial structure optimization is feasible.

4 How to guess a normal mode

Initial guess modes for the mode-tracking algorithm may be obtained in various ways, e.g., by specifying certain internal coordinates like the stretching of a bond, by starting with all possible displacements of a certain atom along Cartesian coordinates, or by performing a full frequency calculation with a method of low computational cost. The Hessian obtained from such a calculation may also be employed as a guess for the exact Hessian for preconditioning (see Ref. [13] for more details). In order to demonstrate the convergence characteristics of initial guesses from *different* types of force-field calculations, we studied the C=O stretching mode of cyclohexanone and compared the mode-tracking results to a full force-field calculation [13]. For this analysis, we used preconditioners and initial normal mode guesses from the semi-empirical MINDO, AM1, and PM3 methods implemented in MOPAC [29], as well as from the classical[3] MMX force field implemented in PCMODEL [30]. We also applied an initial guess from a full BP86/RI[4] /SV(P) force-field calculation with Ahlrichs' small SV(P) basis set [9] as well as a "guess" from a BP86/RI/TZVP calculation using our vibrational program package SNF [33], which represents the exact normal mode (and Hessian). As expected, the latter normal mode led to a one-step convergence, as should be the case for an exact eigenvector. Due to numerical inaccuracies, the AKIRA-wavenumber of 1719.1 cm^{-1} was about 0.9 cm^{-1} higher than that from the full force-field calculation. To get an idea of the change of the frequencies and of the role of the convergence criteria, we examined the wavenumbers and maximum components of the residuum vectors, which are shown in Fig. 7 for

[3]Classical methods describe molecules as composed from atoms as elementary particles, whose interaction is evaluated based on a range of parameters fitted to experimental data. In first-principles methods, on the other hand, the elementary particles are the atomic nuclei and electrons. Semi-empirical methods may be considered as a hybrid between both. As far as experimental data needed for first-principles calculations are concerned, either only natural constants (in pure ab-initio methods) enter the calculation, or the fitting to experimental data is of a very general form. The latter applies to DFT, where approximate density functionals may be obtained from fitting to experimental data. In contrast to genuine semi-empirical methods, however, the obtained density functionals yield high-quality results for molecules which are structurally very different from the ones which have been used for fitting. The quality of the results and the computational cost increase in the order empirical < semi-empirical < first-principles methods.

[4]RI ("resolution of the identity", also called "density fitting") is a technique to accelerate DFT calculations considerably by expressing the density using a set of auxiliary basis functions [31, 32].

calculations with Hessian and start vector from the guess model.

As can be seen in Fig. 7, the lowest initial residual and the best convergence characteristics were obtained when using the SNF results obtained with the small SV(P) basis set, followed by the semi-empirical models, in particular PM3 and AM1. The convergence behavior of the semi-empirical models was better than for a guess from the classical MMX forcefield, although a purely classical calculation using MMX yielded quite accurate vibrational frequencies for this molecule. This indicates that the MMX normal modes and Hessians were not as well suited as initial guesses from PM3 and AM1. It should be noted that in case of the BP86/RI/SV(P) guess the wavenumber in the first iteration was 1719.0 cm^{-1} and thus very close to the converged TZVP frequency. This shows that the normal mode from the calculation using the small SV(P) basis set was quite similar to that obtained with the larger TZVP basis set, while the wavenumber obtained in the BP86/RI/SV(P) calculation (1771.8 cm^{-1}) was not. Therefore, a high-quality result for the BP86/RI/TZVP wavenumber may be obtained by numerical differentiation of the gradients along the BP86/RI/SV(P) normal coordinate.

All converged wavenumbers were in good agreement with the result of the full SNF calculation; small deviations up to 0.9 cm^{-1} of the AKIRA results from the full calculation were due to slight numerical inaccuracies originating from the different basis vectors used in the different calculations. Note that with the AM1, PM3, or SNF guesses only four single-point calculations for distorted structures (two per iteration) were necessary, while a complete force-field calculation exploiting the C_s symmetry would have required 61 single-point calculations for this small test molecule.

5 Flexible subsystems in rigid environments: Direct targeting of subsystem vibrations

Mode-tracking is ideally suited for calculating the vibrational frequencies and normal modes of a flexible subsystem selectively which is attached to an environment which may be considered as rigid. For such systems, there will be many vibrations which involve mainly the atoms of the flexible subsystem, so that the calculated normal modes of the free subsystem provide a high-quality initial guess for the composite system. One important example is an adsorbate molecule attached to a metal cluster. Such systems are of considerable practical relevance, since the vibrational analysis of adsorbates on surfaces is an important analytical technique in surface science [34–37].

We investigated whether the mode-tracking protocol can be selectively applied to the adsorbate vibrations only, whether it reproduces the results of a complete

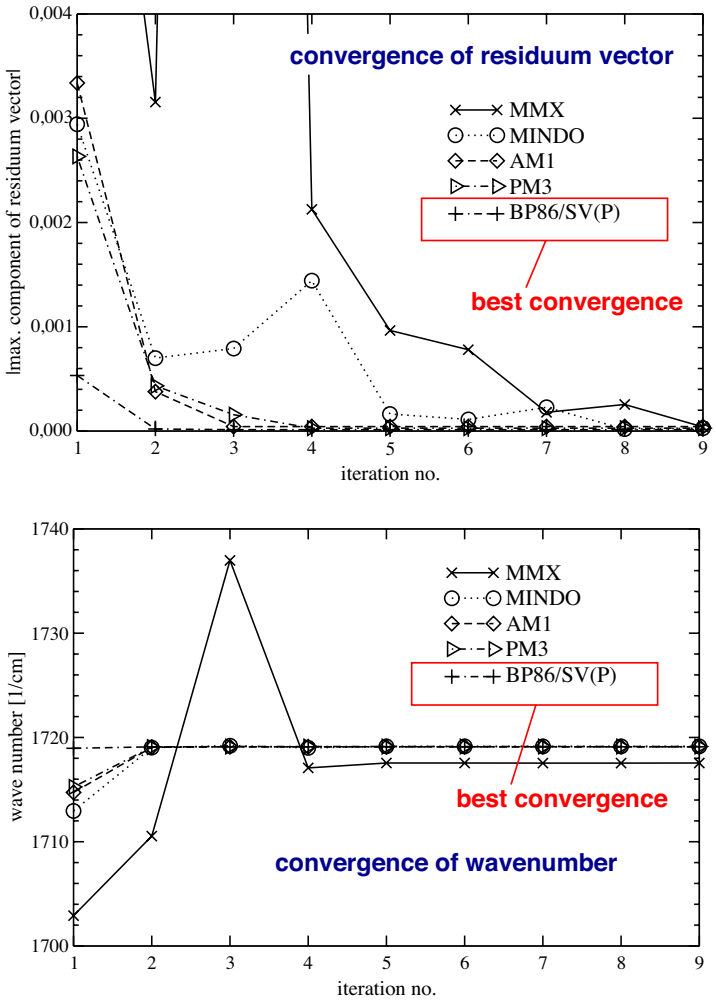


Figure 7: Change of the maximum component of the residuum vector $\mathbf{r}_\mu^{(i)}$ (top) and the wavenumber (bottom) in the subspace iteration process (BP86/RI/TZVP) for the C=O stretching vibration in cyclohexanone. Note that one basis vector is added in each iteration step (see Ref. [13] for details).

calculation of all vibrational modes, and how vibrational calculations for partially optimized structures compare to those for fully optimized structures [17]. We studied three variants of thiophenolate attached to a Ag_{51} cluster:

- a fully optimized thiophenolate–Ag_{51} cluster (structure **1** in Table 1), for which the harmonic approximation is valid,
- a partially relaxed adsorbate–metal cluster system where the silver cluster was frozen during the structure optimization of the adsorbate (structure **2** in Table 1), and
- a thiophenolate anion which was optimized in its isolated form, placed on an unrelaxed Ag(111) surface fragment without further optimization (structure **3** in Table 1).

The frozen clusters in structures **2** and **3** were constructed as a fragment of an Ag(111) surface using the experimental parameters of elemental silver. The metal fragment in the completely relaxed model **1** lost its regular structure after optimization. The three structures do not differ much with respect to the orientation of the adsorbate on the surface. Potential differences in their vibrational spectra will therefore most likely be explained by the influence of the structural changes in the metal cluster (when comparing **1** and **2**) or by the nonzero adsorbate gradient components (when comparing **2** and **3**).

In principle, the calculation of vibrational frequencies and normal modes within the harmonic approximation requires that the molecule under study is in an energy minimum with respect to all nuclear degrees of freedom. However, a structure optimization of the whole system might lead to a metal cluster structure which is far away from the one of an extended crystal surface. A partial optimization of the molecular structure reproduces the experimental arrangement of the atoms better than a fully relaxed surface. It can be shown that the harmonic approximation is justified for partly optimized structures if only those modes are interpreted which are centered on the optimized molecular subsystem [17].

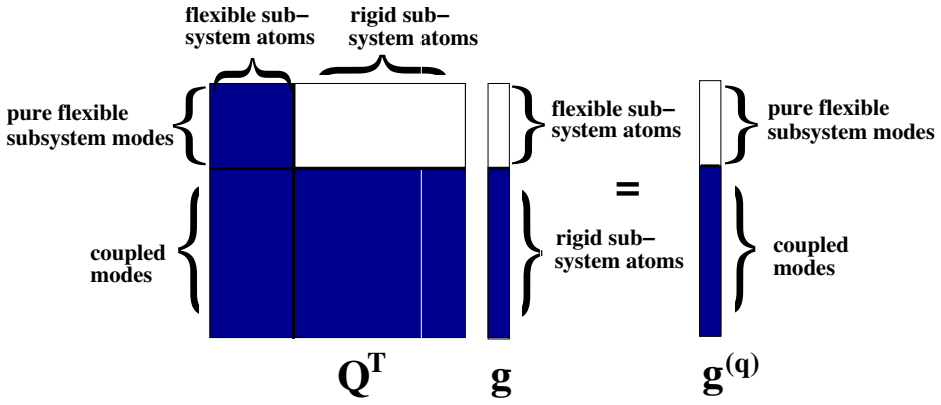
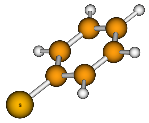
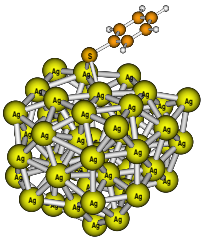
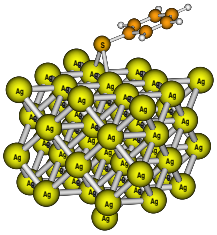
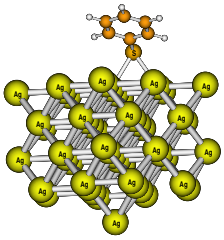


Figure 8: Schematic representation of the transformation of the (mass-weighted) Cartesian gradient vector $\mathbf{g}$ from a Cartesian to a normal mode basis ($\mathbf{g}^{(q)}$) by the transpose of the normal mode matrix $\mathbf{Q}$. The white areas denote vanishing vector and matrix entries, the grey areas non-vanishing ones. Whether the "coupled modes" are located on the rigid subsystem (in which case the lower left part of $\mathbf{Q}$ would also be white) or delocalized, does not affect our reasoning (for more details, see Ref. [17]).

This is because for those normal modes which involve solely motions of the relaxed subsystem, only the gradient components involving coordinates of the subsystem atoms need to be zero in order to preserve the validity of the harmonic approximation (see Fig. 8 and Ref. [17]). In practical applications, e.g. in the case of an adsorbed molecule on a metal cluster under study here, normal modes which only involve the optimized adsorbate do not necessarily exist. If the coupling of the adsorbate vibrations to the surface is weak, however, the considerations made above will nonetheless be of practical relevance. Indeed, except for the 5 lowest thiophenolate modes, the block of the matrix shown in white in Fig. 8 contained only elements close to zero for the actually calculated transpose of the normal mode matrix, $\mathbf{Q}^T$, so that the 25 highest-wavenumber vibrational modes of the adsorbed thiophenolate can be interpreted within the harmonic approximation in all three cases.

As initial guess for the mode-tracking algorithm, the 36 vibrational, rotational and translational normal modes obtained with SNF [38] for the small free (isolated) thiophenolate anion were chosen. The vibrational frequencies of 4 of the 30 highest-frequency vibrational modes, which are mainly located on the the thiophenolate adsorbate, are reported in Table 1 and compared to a full frequency calculation for the fully relaxed system. As a reference, the vibrational frequencies of free thiophenolate are also given.

Table 1: Selected vibrational frequencies for thiophenolate in its free form and attached to an Ag_{51} cluster, calculated by a full vibrational analysis or by mode-tracking. Structure optimizations carried out with DFT – BP86/RI, SV(P) (Ag) / TZVP (else); see Ref. [17] for details.

					
	free	fully optimized **1**		partially optimized **2**	non-optimized **3**
mode	full	full	mode-tracking	mode-tracking	mode-tracking
1	160	241	241	225	215
11	802	858	858	857	857
27	3046	3100	3102	3099	3091

The wavenumber shifts with respect to the free thiophenolate were within 20 to 50 cm^{-1} for 12 of the 30 modes (where the partially optimized structure **2** was taken for comparison). The mode-tracking vibrational analysis of **1** (column 4 in Table 1) yielded frequencies very close to those of the full calculation of the vibrational spectrum (column 3) for most normal modes. The difference usually did not exceed 3 cm^{-1}. Modes 11 and 27 are excellent examples for this and illustrate in addition that the differences between the three different structures was far below the wavenumber shifts of the thiophenolate modes induced by the presence of the silver cluster. At very low wavenumbers, the influence of the model (**1**, **2** or **3**) was larger, but still sufficiently below the induced wavenumber shifts. Altogether, this suggested that for the surface–adsorbate cluster under study here, with a given adsorbate binding site and structure, the structure of the surface did not necessarily have to reproduce the experimental one exactly in order to describe the effects of adsorption on a metal surface within the harmonic approximation. Furthermore, the error introduced by the lack of structure optimization of the adsorbate in structure **3** was not crucial in this case.

In all three cases, the use of the mode-tracking algorithm led to a significant reduction of the computational cost [17]. For example, convergence was achieved within 3 iterations with 78 single-point calculations for the partially optimized

structure **2**, and within one iteration, which corresponds to 72 single-point calculations, for the unrelaxed structure **3**. Convergence within one iteration as in the latter case indicates that the guess normal modes of the free subsystem are already very close to the exact ones. Compared to the full frequency calculation, which required 378 single-point calculations, mode-tracking reduced the computational effort to between one third and one fifth, with a very moderate loss of accuracy. This gain in efficiency corresponds to the minimum which could be achieved by a straightforward targeting of the whole adsorbate spectrum. It would have been larger if the ratio of adsorbate atoms to cluster atoms, which is close to 1:4 here, had been further reduced, if the parameters of the mode-tracking algorithm (like the choice of the preconditioner, the root-homing scheme and the step-size in the numerical differentiation) had been further optimized, or if only a few characteristic adsorbate modes had been tracked whose frequencies were expected to be shifted most after adsorption to a surface.

The vibrational analysis of all three models yielded very similar normal modes. Furthermore, the vibrational normal modes of the thiophenolate, except modes 7, 11, and 28, were not changed qualitatively by the adsorption. As an example, the modes 12 and 27, whose frequencies changed by more than 50 cm^{-1} after adsorption when taking the partially optimized structure **2** for comparison, are depicted in Fig. 9 for the free thiophenolate as well as for structure **2**.

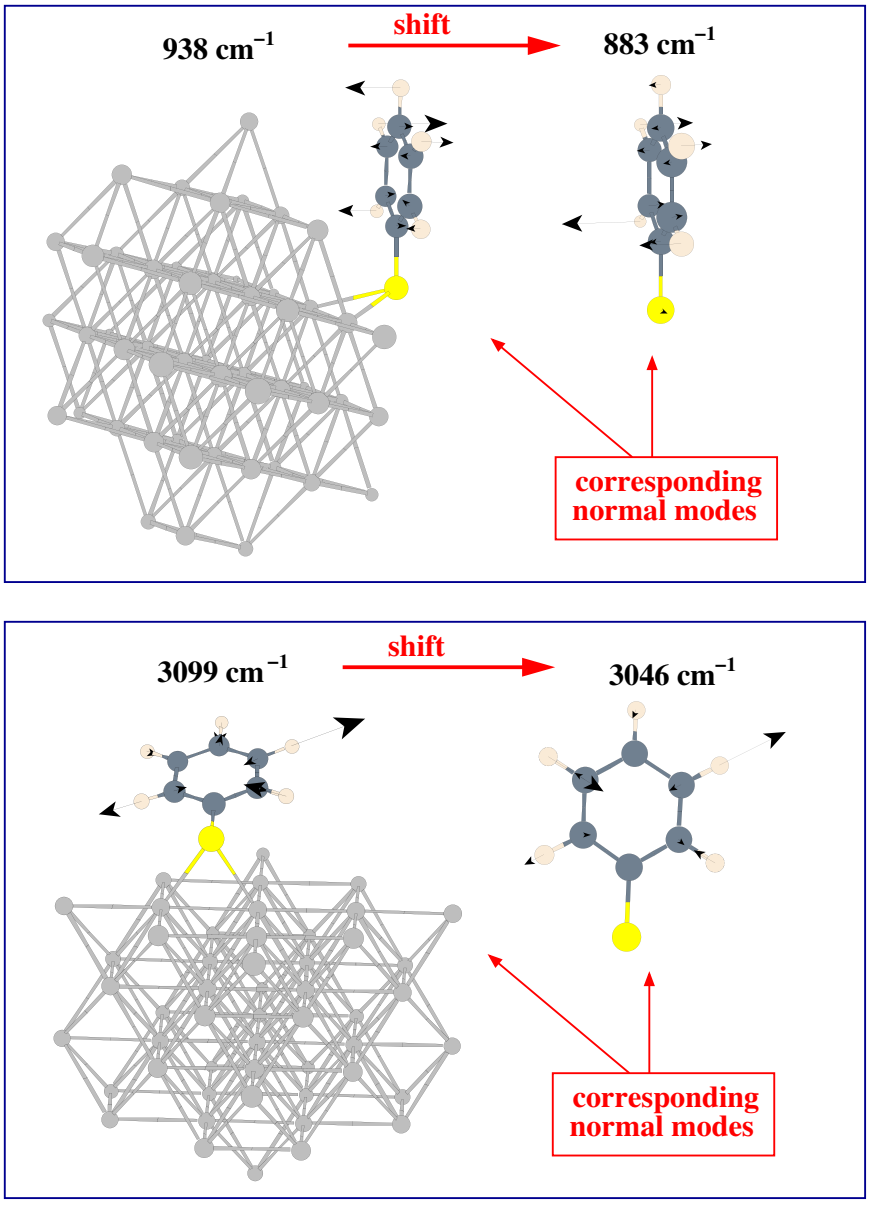


Figure 9: Normal modes 12 and 27 of the free thiophenolate and of the partially optimized structure **2** (for more details, see also Ref. [17]).

To summarize, mode-tracking reproduced the results of the full calculation for model (**1**) reliably. The discrepancies between the normal modes and frequencies for the three models under study were negligible compared to the differences between the free and the adsorbed thiophenolate. Furthermore, coupling between

adsorbate and cluster modes was only observed for the 5 lowest adsorbate modes. Thus, the results of a harmonic vibrational analysis were meaningful for all three models, despite the fact that the structures of two of them were not fully relaxed, and that a quantum chemical vibrational analysis normally requires fully relaxed molecular structures with a total molecular gradient of zero (see discussion in the introduction). The calculation of thermodynamic quantities of similar flexible systems on a rigid cluster, however, for which the lower-frequency modes are important, will require a careful setup of the model.

6 Low-frequency helical breathing modes in deca-alanine

Vibrational Raman Optical Activity (ROA) is the chiral analogue to Raman spectroscopy. Instead of an unpolarized incident light beam, right and left circularly polarized light is used, and the scattering intensity *differences* between both are plotted in the spectra. For achiral molecules, these differences are zero, but for chiral molecules, they appear as positive or negative peaks in the spectrum.

ROA is especially valuable for the investigation of peptides, since as a Raman technique, it allows for measurements in the natural environment of most peptides, i.e., in aqueous media. Furthermore, from experimental evidence it is known that ROA is especially sensitive to the peptide secondary structure. In order to test the limits of this sensitivity, we investigated whether the ROA patterns associated with a certain backbone conformation are retained regardless of the local chirality of the individual amino acids [18]. This comparison was carried out for two right-handed helical deca-alanines with different local configurations of the amino acid building blocks. The helices under study were (all-*S*)-deca-alanine (see Fig. 10; the label *S* is chosen according to the Cahn–Ingold–Prelog notation and corresponds to the biologically relevant L configuration) and (*R,S,R,S,R,S,R,S,R,S*)-deca-alanine.

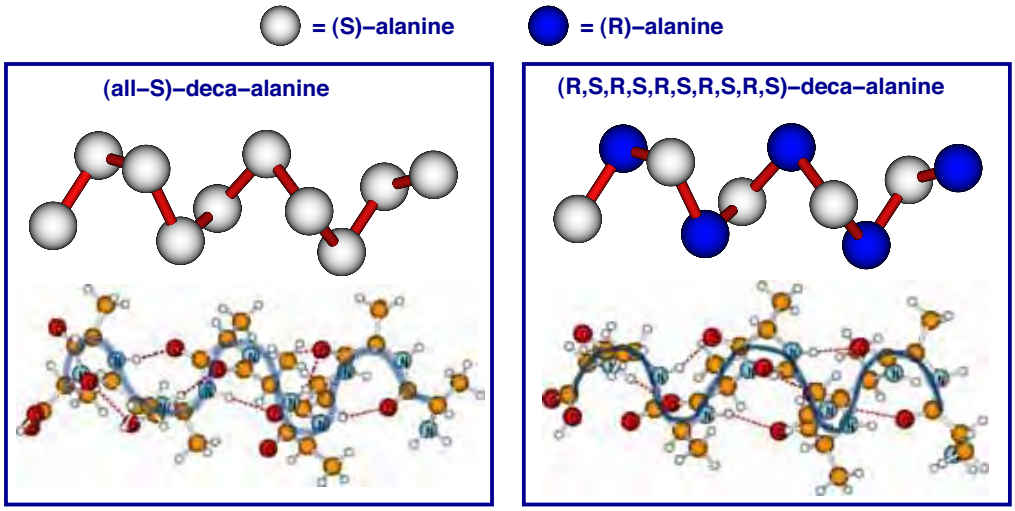


Figure 10: Symbolical and ball-and-sticks-representation of both diastereomers of deca-alanine (see Ref. [18] for details).

The calculation of ROA spectra of molecules with 50-100 atoms or more is still a computational challenge. Deca-alanine, which consists of 103 atoms, is the largest molecule for which quantum chemical ROA studies have been carried out at present. A calculation of an extended wavenumber range pushes current computational resources to their limit, so that massive parallelization was required to calculate the necessary property tensors and their derivatives. This, as well as the necessary good restart facilities, is provided by a combination of our SNF program [38] and the parallel version of the DALTON [25] quantum chemical program package. For the calculation of vibrational normal modes and frequencies, second derivatives of the electronic energy w.r.t. nuclear coordinates are needed, and for the ROA intensities, first derivatives w.r.t. nuclear coordinates of three generalized molecular polarizability tensors are required. These are the electric dipole–electric dipole polarizability (which is also needed for the calculation of conventional Raman spectra), the electric dipole–magnetic dipole polarizability, and the electric dipole–electric quadrupole polarizability. SNF was used to calculate numerical derivatives of these molecular properties, which were provided by DALTON [39, 40]. Molecular gradients were supplied by the TURBOMOLE [24].

Just as the amide modes, for which calculated ROA intensities have been reported in Ref. [18], the low-frequency breathing modes of the helical (all-*S*) and (*R,S,R,S,R,S,R,S,R,S*) diastereomers of deca-alanine were expected to reflect the global chirality of the two right-handed helices rather than the local chirality of the individual amino acids. As can be seen in Fig. 11, these modes solely consist

of helix backbone motions. Breathing modes of helical peptides have not been recorded (or rather assigned) experimentally yet.

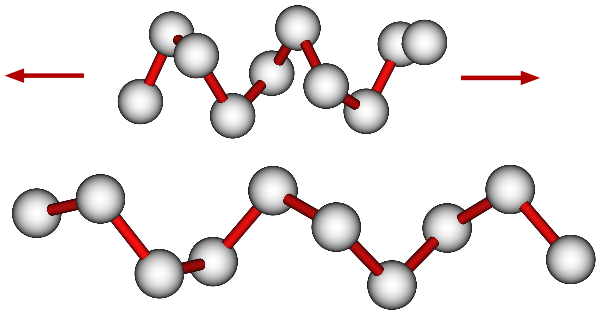


Figure 11: Schematic representation of the helical breathing mode of (all-*S*)-deca-alanine (see Ref. [18] for more details).

Since these lower-frequency regions of peptides largely couple because of near-degeneracies of vibrational states, these modes were not obtained by a standard full vibrational analysis, but were calculated using the mode-tracking technique [10, 13]. The relation between the breathing modes obtained by mode-tracking and the normal modes calculated in the standard way, which can be subject to a mixture with (near-) degenerate vibrations, can be checked via evaluation of the square of the scalar product of the corresponding mass-weighted normal modes. We found, for instance, in the case of (all-*S*)-deca-alanine, that the breathing mode contributed to 49.5 % to a vibration found at lower wavenumber in a full vibrational analysis, whereas this was reduced to 28.3 % in the corresponding (*R,S,R,S,R,S,R,S,R,S*) case [18].

Indeed, the two breathing modes, which are predicted to show up at 65 and 120 cm^{-1} for the (all-*S*) and the (*R,S,R,S,R,S,R,S,R,S*), configurations, respectively, show backscattering intensity differences of $1.31 \cdot 10^{-2}$ and $3.99 \cdot 10^{-2}$ $Å^4$ a.m.u.$^{-1}$, respectively, at an excitation wavelength of 488.88 nm. These intensity differences are small compared to those of the amide modes, because the Raman scattering intensity of this mode is small. If circular intensity differences (CIDs) $I^R - I^L/I^R + I^L$ are calculated, however, the CIDs of the breathing modes ($4.32{\cdot}10^{-3}$ and $2.55{\cdot}10^{-3}$) would be comparable in magnitude to those of the amide modes (ranging from $-5.87{\cdot}10^{-3}$ to $4.40{\cdot}10^{-3}$ and from $-9.33{\cdot}10^{-3}$ to $7.78{\cdot}10^{-3}$, respectively). Despite the different individual amino acid configurations, the intensity differences of both modes have the same sign, and a magnitude which is not too different from each other in view of the range of $-22.47 \cdot 10^{-2}$ to $54.30 \cdot 10^{-2}$ covered by the intensity differences associated with the amide vibrational modes. The breathing mode ROA signal is therefore apparently dominated

by the axial chirality of the helix.

7 Perspective and Outlook

Questions which may be answered by investigating the properties of certain subsystems of molecules or molecular aggregates occur quite frequently in chemistry [41, 42]. Such subsystems may be, e.g., solute molecules, the central region of a metal complex with bulky ligands, or the active centers of enzymes. The selective calculation of information on the relevant subsystem only instead of all information on the whole system poses a challenge for quantum chemistry. Nonetheless, developing algorithms for such selective calculations is more than worth the effort, since given a system of certain size, this may reduce the computer-time considerably, and for given computational resources and computer time, it may make much larger systems accessible to calculations. Such selective procedures are also appealing from an intellectual point of view, as they turn the conventional procedure of first calculating all data and then selecting the important ones upside down. The mode-tracking algorithm [10] is an excellent means to deal with molecular subsystems in the context of vibrational spectroscopy. In the future, the range of applications will be extended, among others, to the binding of substrates to the active sites of enzymes. A new interface has been established which connects the mode-tracking program AKIRA to the Quantum Mechanics / Molecular Mechanics (QM/MM) module of the ADF [26, 27] quantum chemistry program package. It will be used to demonstrate the influence of the myoglobine enzyme surroundings onto carbonmonooxide binding to its iron-porphyrin active site [43].

8 Acknowledgements

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5

CSE Research Projects

Title: Cellular structures in hydrogen jet diffusion flames using detailed chemistry

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
[3]Institute of Fluid Dynamics.

Description:

Experimental investigations of CO_2-diluted H_2 jet diffusion flames have reported the formation of cellular structures, which occur near the extinction limit (D. Lo Jacono, PhD Thesis, EPFL, 2005). It was found that a variety of different cellular patterns can form (rotating single-cell, 2-cell, and 3-cell states as well as stationary 4-cell, 5-cell, and 6-cell states), and the appearances of particular cellular states depend significantly on the initial mixture strength, the proximity to the extinction limit, and fuel jet velocity. For given fuel and oxidizer compositions, several preferred states were found to co-exist, and the particular state realized was determined by the initial conditions. The number of cells in the preferred states was found to decrease with decreasing oxygen concentration in the co-flow.

Extending our previous work with simple chemistry and transport (C.E. Frouzakis et al., *Proc. Comb. Inst.*, 30: 185-192, 2005), simulations with detailed kinetics and mixture-averaged transport properties were performed with our spectral-element based code that solves the conservation equations of mass, momentum, species and energy in the low Mach number limit. For a fixed hydrogen concentration in the fuel stream, the three-dimensional simulations show that cellular flames with different number of cells can be obtained by varying the fuel-jet velocity, in quantitative agreement with the experiments. The cellular flames were found to be associated with a large leakage of reactants through the reaction zone, and exhibit a triple flame structure at the flame base near the jet exit.

References: Presented in the work-in-progress session at the 31^{st} International Symposium on Combustion (August 6-11, 2006, Heidelberg, Germany).

Title: Pulsating jet diffusion flames

Researchers: Christos E. Frouzakis[1], Ananias G. Tomboulides[2], Paul Papas[3], Lambros Kaiktsis[4],Konstantinos Boulouchos[1]

Institute/ Group: [1]Aerothermochemistry and Combustion Systems Laboratory
[2]University of Western Macedonia, Kozani, Greece
[3]Colorado School of Mines, Golden, U.S.A.
[4]Laboratory of Marine Engineering, National Technical University of Athens, Greece

Description:

Flame oscillations near extinction have been observed in diluted propane-oxygen jet diffusion flame experiments (M. Füri, P. Papas, P. A. Monkewitz *Proc. Combust. Inst.* 28:831–838, 2000), where the anchoring flame base oscillated in the streamwise direction while the flame tip oscillated at a comparable amplitude with a phase shift of 180^o relative to the flame edge, resulting in a periodic extension and contraction of the flame length.

The pulsations may be driven by several factors: hydrodynamic instabilities, imbalance of mass and heat diffusion at the flame base (thermo-diffusive instabilities), and gravity. Numerical simulations of the experimental setup were performed, using our MPI-based parallel, spectral element code to solve the conservation equations of mass, momentum, species and energy in the low Mach number limit. As in the experiment, the simulations show the appearance of pulsating flames in a small range of oxygen mass fraction in the oxidizer stream, Y_{O_2}, close to extinction, the growth of the pulsation amplitude as Y_{O_2} is decreased, and the eventual *dynamic* extinction of the flame when the pulsation amplitude becomes too large. It was found that the pulsations appear after a subcritical Hopf bifurcation, resulting in a small range of Y_{O_2} where both the lifted and the pulsating flame can be stabilized.

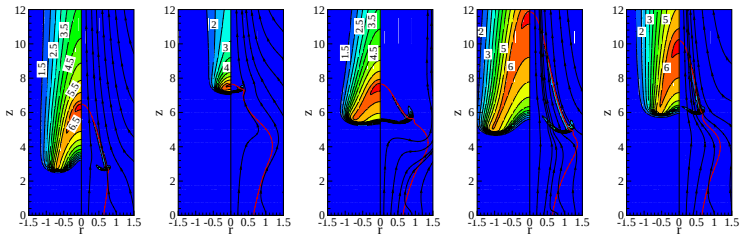


Figure 1: Isocontours of temperature (normalized by 300K, left half) and reaction rate (right half) of (a) steady lifted flame (Y_{O_2}=0.2280), and (b)-(e) four time instants during one period of the pulsating flame for Y_{O_2}=0.205. The red line shows the stoichiometric mixture fraction isoline.

References: Presented in the work-in-progress session at the 31^{st} International Symposium on Combustion (August 6-11, 2006, Heidelberg, Germany). Manuscript in preparation.

Title: Consistent lattice Boltzmann method

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

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

Description: Lack of energy conservation in lattice Boltzmann models leads to unrealistically high values of the bulk viscosity. For this reason, the lattice Boltzmann method remains a computational tool rather than a model of a fluid. A novel lattice Boltzmann model with energy conservation is derived from Boltzmann's kinetic theory. Simulations demonstrate that the new lattice Boltzmann model is the valid approximation of the Boltzmann equation for weakly compressible flows and micro-flows.

References: Phys. Rev. Letters **95**, 260605 (2005)

Title: Thermodynamic theory of incompressible hydrodynamics

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

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

Description:

The grand potential for open systems describes thermodynamics of fluid flows at low Mach numbers. A new system of reduced equations for the grand potential and the fluid momentum is derived from the compressible Navier-Stokes equations. The incompressible Navier-Stokes equations are the quasi-stationary solution to the new system. It is argued that the grand canonical ensemble is the unifying concept for the derivation of models and numerical methods for incompressible fluids, illustrated here with a simulation of a minimal Boltzmann model in a microflow setup.

References: Phys. Rev. Letters **94 (8)**, 80602 (2005).

Title: Entropic lattice Boltzmann method for microflows

Researchers: S. Ansumali[1], I. V. Karlin[2], Ch. E. Frouzakis[2], K. B. Boulouchos[2]

Institute/ Group: [1] Nanyang Institute of Technology, Singapore
[2]Aerothermochemistry and Combustion Systems Laboratory

Description:

A new method for the computation of flows at the micrometer scale is presented. It is based on the recently introduced minimal entropic kinetic models. Both the thermal and isothermal families of minimal models are presented, and the simplest isothermal entropic lattice BhatnagarGrossKrook (ELBGK) is studied in detail in order to quantify its relevance for microflow simulations. ELBGK is equipped with boundary conditions which are derived from molecular models (diffusive wall). A map of three-dimensional kinetic equations onto twodimensional models is established which enables two-dimensional simulations of quasi-twodimensional flows. The ELBGK model is studied extensively in the simulation of the twodimensional Poiseuille channel flow. Results are compared to known analytical and numerical studies of this flow in the setting of the BhatnagarGrossKrook model. The ELBGK is in quantitative agreement with analytical results in the domain of weak rarefaction (characterized by Knudsen number Kn, the ratio of mean free path to the hydrodynamic scale), up to Kn 0:01, which is the domain of many practical microflows. Moreover, the results qualitatively agree throughout the entire Knudsen number range, demonstrating Knudsens minimum for the mass flow rate at moderate values of Kn, as well as the logarithmic scaling at large Kn. The present results indicate that ELBM can complement or even replace computationally expensive microscopic simulation techniques such as kinetic

References: Physica A **359**, 289–305 (2006).

Title: Quasi-equilibrium closure hierarchies for the Boltzmann equation

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

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

Description:

In this paper,explicit method of constructing approximations (the triangle entropy method) is developed for nonequilibrium problems. This method enables one to treat any complicated nonlinear functionals that fit best the physics of a problem (such as,for example,rates of processes) as new independent variables. The work of the method is demonstrated on the Boltzmanns-type kinetics. New macroscopic variables are introduced (moments of the Boltzmann collision integral,or scattering rates). They are treated as independent variables rather than as infinite moment series. This approach gives the complete account of rates of scattering processes. Transport equations for scattering rates are obtained (the second hydrodynamic chain),similar to the usual moment chain (the first hydrodynamic chain). Various examples of the closure of the first,of the second,and of the mixed hydrodynamic chains are considered for the hard sphere model. It is shown,in particular,that the complete account of scattering processes leads to a renormalization of transport coefficients. The method gives the explicit solution for the closure problem,provides thermodynamic properties of reduced models,and can be applied to any kinetic equation with a thermodynamic Lyapunov function.

References: Physica A **360**, 325–364 (2006).

Title: Grad's approximation for missing data in lattice Boltzmann simulations

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

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory
[2] Nanyang Institute of Technology, Singapore

Description:

Engineering applications of computational fluid dynamics typically require specification of the boundary conditions at the inlet and at the outlet. This issue remains unresolved for kinetic-theory based approaches such as the lattice Boltzmann method. Empirically it is known that the accuracy and stability of simulations is greatly influenced by the boundary conditions even at moderate Reynolds numbers. In this paper, we derive a novel outflow boundary condition for the lattice Boltzmann simulations from non-equilibrium thermodynamics and Grad's moment closure. The proposed boundary condition is validated with a three-dimensional simulation of flow over a backward facing step. Results demonstrate that the new outlet condition significantly extends simulation capacity of the lattice Boltzmann method.

References: Europhys. Letters, 74(2), 215-221 (2006).

Title: Entropic Lattice Boltzmann Models for Hydrodynamics in Three Dimensions

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

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory
[2] Nanyang Institute of Technology, Singapore

Description:

Nonlinearly stable entropic lattice Boltzmann models for isothermal incompressible fluid dynamics simulation are derived for the commonly used three-dimensional discrete velocity sets. A new method of fast evaluation of equilibria to machine precision, together with a new asymptotic expansion of the entropy condition enable efficient simulations with this new scheme. Validation with the backward facing step flow is presented.

References: Phys. Rev. Letters **97**, 010201 (2006).

Title: Kinetically reduced local Navier-Stokes equations: An alternative approach to hydrodynamics

Researchers: I. V. Karlin[1], A. G. Tomboulides[2], C. E. Frouzakis[1], S. Ansumali[3]

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

Description:

An alternative approach, the kinetically reduced local Navier-Stokes (KRLNS) equations for the grand potential and the momentum, is proposed for the simulation of low Mach number flows. The Taylor-Green vortex flow is considered in the KRLNS framework, and compared to the results of the direct numerical simulation of the incompressible Navier-Stokes equations. The excellent agreement between the KRLNS equations and the incompressible non-local Navier-Stokes equations for this nontrivial time-dependent flow indicates that the former is a viable alternative for computational fluid dynamics at low Mach numbers.

References: Phys. Rev. E **74**, Rapid Communication, to appear (2006).

Title: Entropic lattice Boltzmann method for simulation of thermal flows

Researchers: N. I. Prasianakis[1], S. S. Chikatamarla[1], I. V. Karlin[1], S. Ansumali[2], K. B. Boulouchos[1]

Institute/ Group: [1] Aerothermochemistry and Combustion Systems Laboratory
[2] Nanyang Institute of Technology, Singapore

Description:

A new thermal entropic lattice Boltzmann model on the standard two-dimensional nine-velocity lattice is introduced for simulation of weakly compressible flows. The new model covers a wider range of flows than the standard isothermal model on the same lattice, and is computationally efficient and stable.

References: Mathematics and Computers in Simulation **72**, 179–183 (2006).

Title: Entropic lattice Boltzmann method for simulation of binary mixtures

Researchers: S. Arcidiacono[1], S. Ansumali[2], I. V. Karlin[3], J. Mantzaras[1], K. B. Boulouchos[3]

Institute/ Group: [1]Paul Scherrer Institute, Combustion Research
[2] Nanyang Institute of Technology, Singapore
[3] Aerothermochemistry and Combustion Systems Laboratory

Description:

A new thermal entropic lattice Boltzmann model on the standard two-dimensional nine-velocity lattice is introduced for simulation of weakly compressible flows. The new model covers a wider range of flows than the standard isothermal model on the same lattice, and is computationally efficient and stable.

References: Mathematics and Computers in Simulation **72**, 79–83 (2006).

Title: Invariant manifolds for physical and chemical kinetics

Researchers: A. N. Gorban I. V. Karlin

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

Description:

The concept of the slow invariant manifold is recognized as the central idea underpinning a transition from micro to macro and model reduction in kinetic theories. We present the constructive methods of invariant manifolds for model reduction in physical and chemical kinetics, developed during last two decades. The physical problem of reduced description is studied in the most general form as a problem of constructing the slow invariant manifold. The invariance conditions are formulated as the differential equation for a manifold immersed in the phase space (*the invariance equation*). The equation of motion for immersed manifolds is obtained (*the film extension of the dynamics*). Invariant manifolds are fixed points for this equation, and slow invariant manifolds are Lyapunov stable fixed points, thus *slowness is presented as stability*.

A collection of methods to derive analytically and to compute numerically the slow invariant manifolds is presented. Among them, iteration methods based on incomplete linearization, relaxation method and the method of invariant grids are developed. The systematic use of thermodynamic structures and of the quasi-chemical representation allows us to construct approximations which are in concordance with physical restrictions.

The following examples of applications are presented: Nonperturbative derivation of physically consistent hydrodynamics from the Boltzmann equation and from the reversible dynamics, for Knudsen numbers Kn of the order 1; construction of the moment equations for nonequilibrium media and their dynamical correction (instead of extension of the list of variables) in order to gain more accuracy in description of highly nonequilibrium flows; kinetic theory of phonons; model reduction in chemical kinetics; derivation and numerical implementation of constitutive equations for polymeric fluids; the limits of macroscopic description for polymer molecules, cell division kinetics.

Keywords: Model Reduction; Invariant Manifold; Entropy; Kinetics; Boltzmann Equation; Fokker–Planck Equation; Navier-Stokes Equation; Burnett Equation; Quasi-chemical Approximation; Oldroyd Equation; Polymer Dynamics; Molecular Individualism; Accuracy Estimation; Post-processing.

References: A. N. Gorban and I. V. Karlin, Invariant Manifolds for Physical and Chemical Kinetics, Lecture Notes in Physics 660, (Springer, Berlin, 2005).

Title: Computational Solid State Electronics

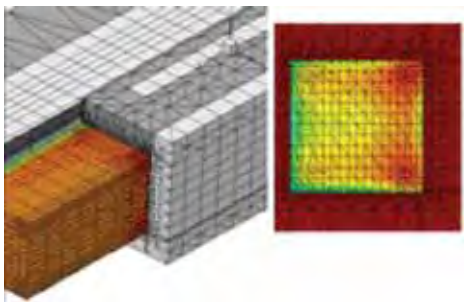
Researchers: Wolfgang Fichtner
Andreas Schenk
Bernhard Schmithüsen
Stefan Röllin
Christoph Müller
Dölf Aemmer

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

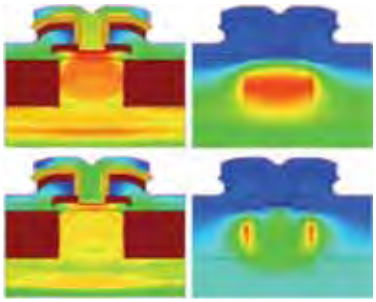
Description:

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.

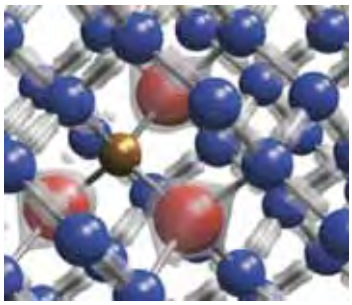
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulation tools for molecular dynamics studies in material diffusion, novel devices such as nanowire transistors, and quantum devices. 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 compute-servers of our laboratory and we also use the IBM SP4 and Cray XT3 systems at CSCS Manno in a *Large User Project*. The following pictures illustrate some of our activities:



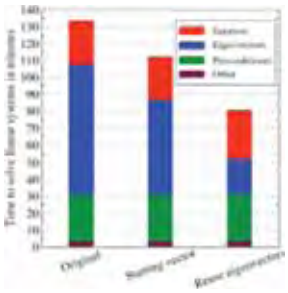
Simulation of post-CMOS devices: 3D mesh for a triple-gate silicon nanowire transistor and quantum-mechanical electron density in a cross section.



Harmonic Balance simulation of a bipolar transistor: 1st and 2nd harmonic magnitudes (top/bottom), and electron density resp. electrostatic potential (left/right).



Ab initio simulation of dopant atoms and vacancy clusters in heavily doped silicon.



Performance issues of spectral preconditioners in device simulation and reduction of simulation time.

Title: Jacobi–Davidson algorithms for the complex symmetric eigenvalue problem

Researchers: Oscar Chinellato
Peter Arbenz

Institute/ Group: Institute of Computational Science, ETH Zürich

Description:

The development and optimization of modern optoelectronic semiconductor lasers, such as vertically-cavity surface-emitting lasers (VCSELs) require the solution of the three-dimensional homogeneous Maxwell equations describing the optical field. Their numerical discretization by finite element methods (of Nédélec type) lead to large sparse generalized complex-symmetric matrix eigenvalue problems.

The stable and accurate computation of these matrices is investigated. Variants of the Jacobi–Davidson method are derived and implemented that can exploit their complex-symmetric structure. The correction equations are solved by conjugate-gradient-type algorithms preconditioned by a combination of hierarchical basis and domain decomposition preconditioners.

References:

O. Chinellato, P. Arbenz, M. Streiff, and A. Witzig: *Computation of Optical Modes Inside Axisymmetric Open Cavity Resonators.* Future Generation Computer Systems 21 (8): 1263-1274 (2005).

P. Arbenz and M. Hochstenbach: *Jacobi–Davidson Method for Solving Complex-Symmetric Eigenvalue Problems.* SIAM J. Sci. Comput. 25 (5): 1655-1673 (2004).

O. Chinellato: *Stabilized Linear Modification Algorithms.* Technical Report 468, Institute of Computational Science, ETH Zürich, January 2005.

O. Chinellato: *The Complex-Symmetric Jacobi-Davidson Algorithm and its Application to the Computation of some Resonance Frequencies of Anisotropic Lossy Axisymmetric Cavities.* PhD Thesis ETH No. 16243, 2005.

F. Römer, O. Chinellato, L. Balet, A. Fiore, and B. Witzigmann: *Modelling Photonic Crystal Microcavities with a 3D FEM Maxwell Solver.* To appear in Proceedings of the International Workshop on Phys. Photonic Crystals Metamaterials, June 2006

P. Arbenz, O. Chinellato: *On solving complex-symmetric eigenvalue problems arising in the design of axisymmetric VCSEL devices.* To appear in Appl. Numer. Math., 2006

F. Römer, O. Chinellato, P. Arbenz, and B. Witzigmann: *Investigation of the Purcell Effect in Photonic Crystal Cavities with a 3D Finite Element Maxwell Solver.* Submitted to J. Opt. Quantum Electron.

F. Römer, L. Balet, O. Chinellato, L. Li, N. Le Thomas, R. Houdré, M. Francardi, A. Gerardino, A. Fiore, B. Witzigmann: *Investigation of the optical farfield of photonic crystal microcavities.* To be published in Proc. SPIE, 6480-47.

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

Researchers: Peter Arbenz[⋆]
G. Harry van Lenthe[†]
Uche Mennel[⋆]
Ralph Müller[†]
Marzio Sala[⋆]

Institute/ Group: [⋆]Institute of Computational Science, ETH Zürich
[†]Institute for Biomedical Engineering,
University and 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*. To appear in Proceedings of PARA'06: Workshop on the State-of-the-Art in Scientific Computing.

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*. Submitted to Internat. J. Numer. Methods Engrg.

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

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

Institute/Group: *Institute of Polymers, Department of Materials, ETH Zürich
**Institute of Energy Technology, Department of Mechanical and Process Engineering, ETH Zürich

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:

A. Bardow, I.V. Karlin, A.A. Gusev, General characteristic-based algorithm for off-lattice Boltzmann simulations. *Europhys. Lett.* **75** (2006) 434-440.

Title: Micromechanical mechanism of reinforcement and losses in filled rubbers

Researchers: Andrei A. Gusev

Institute/Group: Institute of Polymers, Department of Materials, ETH Zürich

Description:

Using the finite element method, we show that the relationship between the reinforcement and the losses observed in carbon black or silica filled rubbers can be explained micromechanically, by taking into account that the networking filler particles are joined by coating layers of immobilized glassy polymer and realizing that both storage and dissipation energies are strongly localized in these coating layers.

References:

A.A. Gusev, Micromechanical mechanism of reinforcement and losses in filled rubbers. *Macromolecules* **39** (2006) 5960-5962.

Title: Finite element mapping for spring network representations of the mechanics of solids

Researchers: Andrei A. Gusev

Institute/Group: Institute of Polymers, Department of Materials, ETH Zürich

Description:

We present a general finite element mapping procedure for defining spring network representations of solid mechanics. The procedure is rigorous and equally suitable for setting regular and unstructured spring network models of generally anisotropic solids. We use the procedure to define close-packed triangular and simple cubic lattice spring models of isotropic 2D and 3D elastic media, respectively. We extend the study to heterogeneous solids and show that the mapped spring network approach constitutes an appealing route for incorporating subelement level constitutive equations.

References:

A.A. Gusev, Comment on "finite element mapping for spring network representations of the mechanics of solids" – Reply. *Phys. Rev. Lett.* **96** (2006) 199402.

A.A. Gusev, Finite element mapping for spring network representations of the mechanics of solids. *Phys. Rev. Lett.* **93** (2004) 034302.

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Title: Stress relaxation behavior of thermoplastic elastomers

Researchers: Stephan A. Baeurli*,**
Atsushi Hotta*
Andrei A. Gusev**

Institute/Group: *Department of Chemical Engineering and Materials, University of California, MRL Building, Santa Barbara, CA 93106, USA
**Institute of Polymers, Department of Materials, ETH Zürich

Description:

We present a new semi-phenomenological approach to predict the stress relaxation behavior of thermoplastic elastomers at long times. This approach relies on the method of Gurtovenko and Gotlib [J Chem Phys 115 (2001) 6785], which has originally been conceived to describe the relaxation dynamics of inhomogeneously crosslinked polymers forming agglomerations of crosslinks. We demonstrate that the method can be extended to predict the stretched exponential stress decay of homogeneously crosslinked thermoplastic elastomers, which are subjected to an extensional strain pertaining to the nonlinear regime of mechanical properties. In our approach thermal fluctuations induce fluctuations in size of domains of crosslinks via a chain-pullout mechanism. We compare our theoretical predictions to the experimental measurements of Hotta et al. [Macromolecules 35 (2002) 271] performed on poly(styrene-isoprene-styrene) triblock copolymers, which are composed of hard domains of polystyrene embedded in a rubbery polyisoprene matrix. Our study confirm the importance of the chain-pullout mechanism in the stress relaxation process and demonstrates the involvement of multiple time- and structural-length-scales.

References:

S.A. Baeurle, A. Hotta, A.A. Gusev, A new semi-phenomenological approach to predict the stress relaxation behavior of thermoplastic elastomers. *Polymer* **46** (2005) 4344-4354.

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

Researchers: Andrei A. Gusev

Institute/Group: Institute of Polymers, Department of Materials, ETH Zürich

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:

A.A. Gusev, Physically admissible rules of evolution for discrete representations ofcontinuous media. *J. Non-Cryst. Solids* (2006) in press.

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

Researchers: Andrei A. Gusev*
Olga Guseva**

Institute/Group: *Institute of Polymers, Department of Materials, ETH Zürich
** a) Materials Simulation GmbH, Bluntschlisteig 1, P. O. Box 624, 8027 Zürich; b) Empa, Swiss Federal Laboratories for Materials Testing and Research, Laboratory for Corrosion and Materials Integrity, Überlandstrasse 129, 8600 Dübendorf

Description:

A new, coupled-form finite element approach was introduced to estimate the permeability performance of mixed matrix nanotube/polymer membranes. Based on direct finite element predictions, we developed a set of simple design equations and demonstrated that mixed matrix nanotube/polymer membranes can favorably combine the high-flux performance of nanotubes with the intrinsic selectivity of polymer matrix.

References:

A.A. Gusev, O. Guseva, Rapid mass transport in mixed matrix nanotube/polymer membranes. *Adv. Mater.* (submitted).

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

Researchers: Andrei A. Gusev

Institute/Group: Institute of Polymers, Department of Materials, ETH Zürich

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. 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:

A.A. Gusev, Asymptotic back strain approach for estimation of effective properties of multiphase materials. *Adv. Eng. Mater.* (accepted)

Title: Glassy state of multiphase and pure polymer materials

Researchers: Stephan A. Baeurli*,**
Atsushi Hotta*
Andrei A. Gusev**

Institute/Group: *Department of Chemical Engineering and Materials, University of California, MRL Building, Santa Barbara, CA 93106, USA
**Institute of Polymers, Department of Materials, ETH Zürich

Description:

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:

S.A. Baeurle, A. Hotta, A.A. Gusev, On the glassy state of multiphase and pure polymer materials. *Polymer* **47** (2006) 6243-6253.

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

Researchers: Stephan A. Baeurli*
Takao Usami**
Andrei A. Gusev***

Institute/Group: *a) Department of Chemistry & Pharmacy, Institute of Physical and Theoretical Chemistry, D-93053 Regensburg, Germany; b) Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA; c) Department of Civil, Environmental & Geomatic Engineering, Institute for Building Materials, ETH, Zurich, Switzerland
** Polymer Design Laboratory, Mitsubishi Chemical Group Science and Technology Research Center, Yokkaichi, Mie 510- 0885, Japan
***Institute of Polymers, Department of Materials, ETH Zürich

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 determinant 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 inter-phases, 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 behaviour of these materials.

References:

S.A. Baeurle, T. Usami, A.A. Gusev, A new multiscale modeling approach to the prediction of mechanical properties of polymer-based nanomaterials. *Polymer* (submitted).

CSE research project

Title: Minimal size of a barchan dune

Researchers: E. J. R. Parteli, [1]
O. Durán, [1]
H. J. Herrmann, [2,3]

Institute/ Group:
[1]. Institut für Computerphysik, ICP, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany.
[2]. Institut für Baustoffe, ETH Hönggerberg, HIF E 12, CH-8093, Zürich, Switzerland.
[3]. Departamento de Física, Universidade Federal do Ceará - 60455-760, Fortaleza, CE, Brazil.

Description:

Barchans are dunes of high mobility which have a crescent shape and propagate under conditions of unidirectional wind. However, sand dunes only appear above a critical size, which scales with the mean length of the grains in saltation trajectories [10, 13, 14]. Indeed, this scaling relation could not explain the proto size of barchan dunes, which often occur in coastal areas of high litoral drift, and the scale of dunes on Mars. In the present work, we show from three dimensional calculations of sand transport that the size and the shape of the minimal barchan dune depend on the wind friction speed and the sand flux on the area between dunes in a field. Our results explain the common appearance of barchans a few tens of centimeter high which are observed along coasts. Furthermore, we find that the rate at which grains enter saltation on Mars is one order of magnitude higher than on Earth, and is relevant to correctly obtain the minimal dune size on Mars.

References: Proceedings for Lunar and Planetary Science

CSE research project

Title: Networks based on collisions among mobile agents

Researchers: Marta C. González, [a]
Pedro G. Lind, [a,b]
Hans J. Herrmann [c,d]

Institute/ Group: [a], Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany
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[c], Departamento de Física, Universidade Federal do Ceará, 60451-970 Fortaleza, Brazil
[d], IfB, HIF E12, ETH Hönggerberg, CH-8093 Zürich, Switzerland

Description:

We investigate in detail a recent model of colliding mobile agents [Phys. Rev. Lett. 96, 088702], used as an alternative approach to construct evolving networks of interactions formed by the collisions governed by suitable dynamical rules. The system of mobile agents evolves towards a quasi-stationary state which is, apart small fluctuations, well characterized by the density of the system and the residence time of the agents. The residence time defines a collision rate and by varying the collision rate, the system percolates at a critical value, with the emergence of a giant cluster whose critical exponents are the ones of two-dimensional percolation. Further, the degree and clustering coefficient distributions and the average path length show that the network associated with such a system presents non-trivial features which, depending on the collision rule, enables one not only to recover the main properties of standard networks, such as exponential, random and scale-free networks, but also to obtain other topological structures. Namely, we show a specific example where the obtained structure has topological features which characterize accurately the structure and evolution of social networks in different contexts, ranging from networks of acquaintances to networks of sexual contacts.

References: to appear in Physica D

CSE research project

Title: Cluster Formation of Clay-like Colloids in Shear Flow

Researchers: Martin Hecht, [1]
Jens Harting, [1]
Hans J. Herrmann, [2,3]

Institute/ Group:
[1.] Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany
[2.] Institut für Baustoffe, Schafmattstr. 6, ETH Zürich, CH-8093 Zürich, Switzerland
[3.] Departamento de Física, Universidade Federal do Ceará Campus do Pici, 60451-970 Fortaleza CE, Brazil

Description:

In Al2O3 suspensions, depending on the experimental conditions very different microstructures can be found, comprising fluid like suspensions, a repulsive structure, and a clustered microstructure. For technical processing in ceramics, the knowledge of the microstructure is of importance, since it essentially determines the stability of a workpiece to be produced. To enlighten this topic, we investigate these suspensions by means of a coupled Stochastic Rotation Dynamics (SRD) and Molecular Dynamics (MD) simulation. In the present paper we utilize the low-k-peak of the structure factor and the nearest neighbor peak of the pair correlation function as analysis tools to observe cluster formation. The first one observes on the length scale of the system size, whereas the latter focuses on short distances to the nearest neighbors. Both observation tools show good agreement among each other. The repulsive microstructure can be identified by means of the mean squared displacement of the particles. The results from different evaluation tools are summarized in a stability diagram.

References: submitted to European Physical Journal E

CSE research project

Title: Damage and Healing in Fatigue Fracture

Researchers: F. Kun, [1]
M. H. A. S. Costa, [2]
R. N. Costa Filho, [2]
J. S. Andrade Jr., [2]
J. B. Soares, [3]
S. Zapperi, [4]
H. J. Herrmann, [5]

Institute/ Group:
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[2]. Departamento de Física, Universidade Federal do Ceará, 60451-970 Fortaleza, Ceará, Brazil
[3]. LMP, DET, Universidade Federal do Ceará, 60451-970 Fortaleza, Ceará, Brazil
[4]. CNR-INFM, Dipartimento di Fisica, Universitá 'La Sapienza', Piazzale Aldo Moro 2, 00185 Roma, Italy
[5]. IfB, HIF, E12, ETH, Hoenggerberg, 8093 Zürich, Switzerland

Description:

We present an experimental and theoretical study of the fatigue failure of asphalt under cyclic compression. Varying the load amplitude, experiments reveal a finite fatigue limit below which the specimen does not break, while approaching the tensile strength of the material a rapid failure occurs. In the intermediate load range, the lifetime decreases with the load as a power law. We introduce two novel theoretical approaches, namely, a fiber bundle model and a fuse model, and show that both capture the major microscopic mechanisms of the fatigue failure of asphalt, providing an excellent agreement with the experimental findings. Model calculations show that the competition of damage accumulation and healing of microcracks gives rise to novel scaling laws for fatigue failure.

References: submitted to Phys. Review Lett

Title: Nodal Auxiliary Space Preconditioning in H(curl) and H(div) spaces

Researchers: Ralf Hiptmair
Jinchao Xu (PennState University)

Institute: Seminar for Applied Mathematics, ETH Zürich

Description:

Variational problem posed on the function spaces $\mathbf{H}(\mathbf{curl},\Omega)$ and $\mathbf{H}(\mathrm{div},\Omega)$, $\Omega\subset\mathbb{R}^3$, play an important role in many mathematical models, in particular in electromagnetism. Their discretization by means of discrete differential forms, edge elements and face elements, respectively, in the lowest order case, leads to large sparse linear systems that can only be solved iteratively.

We developed and analyzed a general approach to preconditioning these linear systems of equations, which exclusively relies on approximate solvers for discrete 2nd-order elliptic problems. We proved mesh-independent effectivity of the preconditioners by appealing to the abstract theory of auxiliary space preconditioning. The main tool are discrete analogues of so-called regular decomposition results in the function spaces $\mathbf{H}(\mathbf{curl},\Omega)$ and $\mathbf{H}(\mathrm{div},\Omega)$.

Numerical experiments in both 2D and 3D confirm the excellent performance of the new auxiliary space preconditioner. The table lists the condition numbers of the preconditioned linear systems arising from an edge element discretization of

$$\mathbf{u}\in\mathbf{H}_0(\mathbf{curl},\Omega):\quad \int_\Omega \mathbf{curl}\,\mathbf{u}\cdot\mathbf{curl}\,\mathbf{v}+\tau\mathbf{u}\cdot\mathbf{v}\,\mathrm{d}x=\int_\Omega \mathbf{f}\cdot\mathbf{v}\,\mathrm{d}x\quad\forall\mathbf{v}\ .$$

In this case we took Ω to be the unit ball and meshes on different levels of refinement were employed.
The new preconditioning strategy allows to harness powerful algebraic multigrid methods available for discrete 2nd-order operators.

		τ		
level	#cells	10^{-4}	1	10^4
1	2197	2.893	2.911	3.021
2	4462	3.334	3.372	3.317
3	8865	3.280	3.288	3.430
4	17260	3.499	3.494	3.329
5	66402	3.955	3.932	3.431
6	95593	4.132	4.102	5.022
7	148554	4.497	4.246	3.513
8	242588	4.340	4.552	3.391

References:

1. R. Hiptmair and J. Xu, *Nodal auxiliary space preconditioning in H(curl) and H(div) spaces*, Report 2006-09, SAM, ETH Zürich, Zürich, Switzerland, 2006.

Title: Solitary Waves in Planar Bragg Gratings

Researchers: Tomas Dohnal

Institute: Seminar for Applied Mathematics
ETH Zürich

Description: We consider Coupled Mode Equations (CME) approximating propagation of quasimonochromatic wavepackets of light in planar Bragg gratings with the Kerr nonlinearity and study bifurcations of localized solitary waves from edges of photonic band gaps. Study of solitary waves in photonic structures is of fundamental importance in nonlinear optics as these conherent structures may find application in optical logic and computing. We consider transverse homogeneous planar gratings which lead to resonance of two counter propagating waves and demonstrate that the occurrence of oscillations in the profiles of bound states [1] for the corresponding CME are due to incompleteness of the band gap in that system. We call these waves "quasi gap solitons (QGS)". Second, it is shown via separation of variables and Floquet theory that the addition of slowly periodic transverse structure on the length scale of the wavepacket envelope opens an infinite number of bandgaps but leaves each incomplete. A rich family of QGS is shown to bifurcate from their edges and continuation curves of these families are numerically computed. For an example see Fig. 1. Finally, in contrast, a Bragg grating in two perpendicular directions leading to resonance of four counterpropagating waves is shown to allow a complete bandgap and to support bifurcations of exponentially localized gap solitons whose asymptotic approximation is given and continuation curves computed. For an example of one of the waves see Fig. 2.

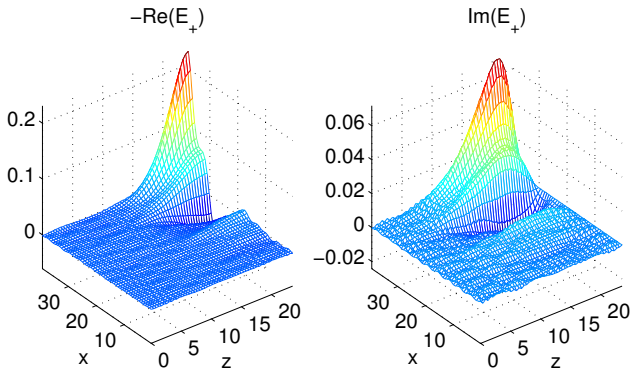


Figure 1: The profile of a solitary wave with speed 0.12 in the slowly transverese periodic Bragg grating (extend by symmmetry).

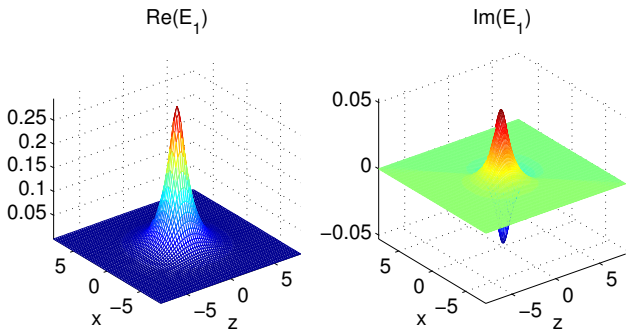


Figure 2: A stationary solitary wave in the Bragg grating with two perpendicular directions.

References:

[1] T. Dohnal and A.B. Aceves, *Optical soliton bullets in (2+1)D nonlinear Bragg resonant periodic geometries*, Studies in Appl. Math., 115:209–232, 2005.

[2] T. Dohnal, "Solitary and Quasi-solitary Waves in Low Contrast Planar Bragg Gratings (title tentative)," in preparation.

Title: Radiative heat transfer for plasma arc simulations

Researchers: Gisela Widmer
Ralf Hiptmair

Institute/ Group: Seminar for Applied Mathematics,
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 radiation equation is stated in five dimensions, with the intensity depending on space and direction, it is a bottleneck of such computations. This project aims at reducing the number of degrees of freedom by applying sparse tensor product and a-posteriori adaptive methods. Sparse tensor product methods have been used to overcome the 'curse of dimension' of multidimensional problems. Applied to the radiation equation, the complexity of the problem is reduced from five to three dimensions up to logarithmic terms.

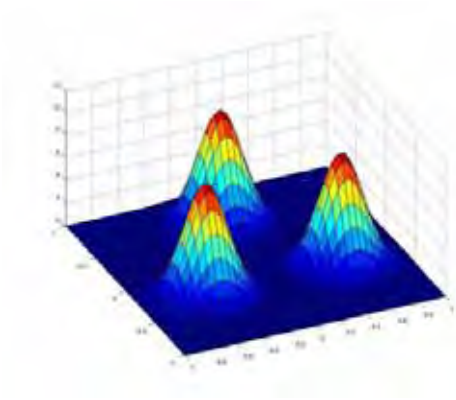


Figure 1: Emission f(x)

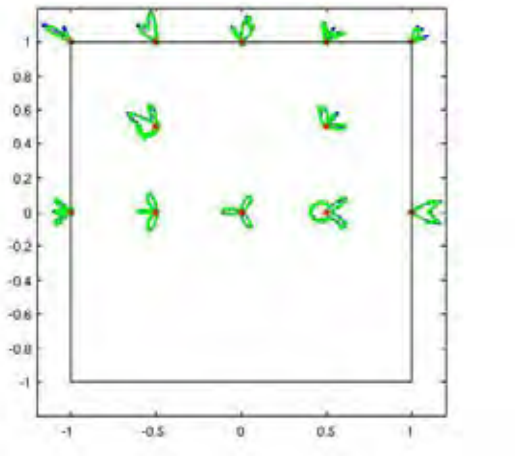


Figure 2: Radiation intensiy in two dimensions. Comparison of sparse grid (green) and full grid (blue) for emission in fig. 1 for absorption $\kappa = 1$.

Title: Virtual modeling of the straightening process with two rolls straighteners

Researchers: Pavel Hora
Longchang Tong
Fabiano Vanini

Institute/ Group: Institute of Virtual Manufacturing

Description:

The virtual modeling of forming processes is difficult in the case of a material behavior, that is not possible to describe with a simple elastic-plastic material model with isotropic hardening and if the process depends on complex and permanently changing boundary conditions, which have to be represented exactly.
Such a complex process for the virtual modeling represents the straightening process of bright steel in a two-roll-straigthening system. The residual stress responsible for the straightness can be predicted only by material models with kinematic hardening. The modeling of the straightening rolling process set high requirements to the contact formulation because of the complex boundary conditions. It can be only modeled with very small increments for adequate accuracy. For the determination of the steady state condition the process has to be modeled over an adequate long period.
In the framework of a CTI-project a special purpose FEM simulation has been developed, which applies enhanced constitutive model of Chaboche and Theodosiu for the exact prediction. Special algorithms modeling the special, quasi-static straightening rolling process have been developed for the reduction of the computing time. The software will be applied for the planning and optimization of the rolling machine as well as for the control of the process robustness after the ending of the 2-1/2 year lasting project.

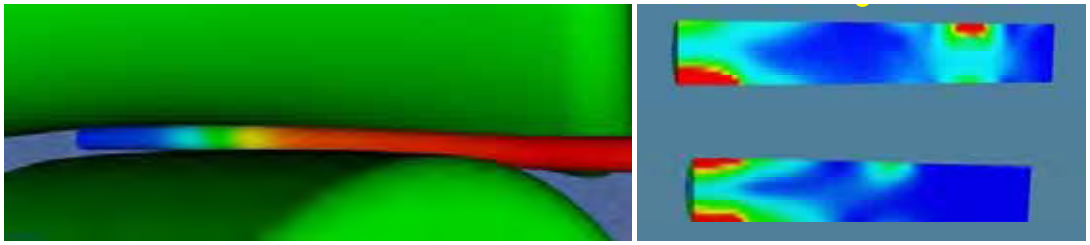


Fig. 1: Plastic strain of the rod during the straightening rolling process

Title: A Constitutive Model for the Simulation of MetaStable Austenitic Stainless Steels

Researchers: Bernd Hochholdinger

Institute/ Group: Institute of Virtual Manufacturing

Description:

A new material model for the simulation of metastable austenitic stainless steels was implemented. This material model uses an approach suggested by Hänsel to include the effect of a deformation based phase transformation from austenite to martensite on the hardening curve. The model consists of two basic equations: the martensite rate equation and a function describing the hardening behavior of the material. The formation of strain induced martensite highly depends on the temperature. Therefore in general a coupled thermo-mechanical analysis with adequate thermal boundary conditions has to be setup. From the test simulations that have been conducted so far, it can be concluded that the material model is capable of modeling the temperature dependent formation of martensite and its effect on the hardening curve.

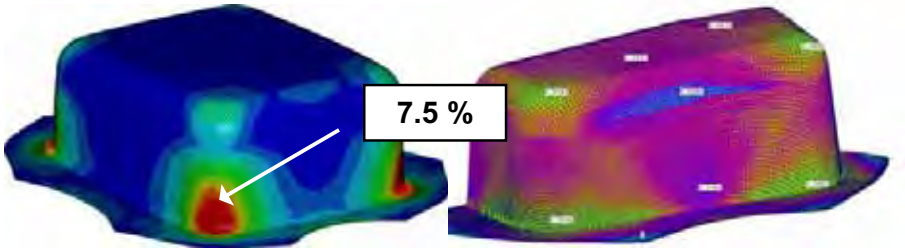


Fig. 1: Martensite volume fraction induced by the forming of a kitchen sink

References:

B. Hochholdinger
A Constitutive Model for the Simulation of MetaStable Austenitic Stainless Steels with LS-DYNA, Proceedings of the FLC06, Zurich, (2006)

Title: Characterization of additives in lubricants for tribological systems with the help of simulations on different length-scales

Researchers: Reto Grueebler
Thomas Bonner

Institute/ Group: Institute of Virtual Manufacturing

Description:

The main goal of the project is the development of simulation techniques towards the understanding of and application towards tribological processes relevant to the industrial manufacturing practice. Here, additives play an important role in the regime of boundary lubrication. Molecular Dynamics simulations help to understand more about the working on the nanoscale in this environment. With the Finite Element Method a bridge to the macroscopic world is built, where the effects from nanotribology are used for the optimization of tribological systems.
With the Molecular Dynamics simulation the anti-wear (AW), in which the molecules are adsorbed on the surface, as well as the extreme pressure (EP), in which EP-layers are formed after chemical reaction, was analyzed. In the AW regime the behavior of the additives of the Irgalube family has been examined. Different types of the Irgalube, i.e. different boundary groups for the AW molecule result in different adsorption and heat capacity properties. For the EP regime the model system aluminum- chloride had been considered, because the chlorine shows a better effectiveness than the other possible EP-elements like sulfur or phosphor. This system is modeled by the Charge Equilibration Method, where the charge of the atoms is considered. To calculate the charges a large system of equations depending on the amount of atoms has to be solved. The calculation of this solution is very time-consuming, whereas it was possible to reduce the calculation time by special algorithms. The results show the lower friction of the tip – substrate system with chloride than without.

Title: Computation of methodology-independent ionic solvation free energies from molecular simulations: II. The hydration free energy of the sodium cation.

Researchers: Mika Kastenholz*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

The raw ionic solvation free energies computed from atomistic (explicit-solvent) simulations are extremely sensitive to the boundary conditions (finite or periodic system, system shape and size) and treatment of electrostatic interactions (Coulombic, lattice-sum or cutoff-based) used during these simulations. In this study, it is shown that correction terms can be derived for the effect of : (A) an incorrect solvent polarization around the ion due to the use of an approximate (not strictly Coulombic) electrostatic scheme; (B) the finite size or artificial periodicity of the simulated system; and (C) improper summation scheme to evaluate the potential at the ion site and the possible presence of a liquid-vacuum interface in the simulated system. Taking the hydration free energy of the sodium cation as a test case, it is shown that the raw solvation free energies obtained using seven different types of boundary conditions and electrostatic schemes commonly used in explicit-solvent simulations (for a total of 72 simulations differing in the corresponding simulation parameters) can be corrected so as to obtain a consistent value for this quantity.

References: Kastenholz, M. & Hünenberger, P.H.
J. Chem. Phys. **124** (2006) 224501/1-224501/20.

Title: Development of a lattice-sum method emulating nonperiodic boundary conditions for the treatment of electrostatic interactions in molecular simulations: A continuum electrostatics study.

Researchers: Mika Kastenholz*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Artifacts induced by the application of periodic boundary conditions and lattice-sum methods in explicit-solvent simulations of (bio-)molecular systems are nowadays a major concern in the computer-simulation community. The present study reports a first step toward the design of a modified lattice-sum algorithm emulating non-periodic boundary conditions, and therefore exempt of such periodicity-induced artifacts. This result is achieved here in the (more simple) context of continuum electrostatics. It is shown that an appropriate modification of the periodic Poisson equation and of its boundary conditions leads to a continuum-electrostatics scheme, which, although applied under periodic boundary conditions, exactly mimics the non-periodic situation. The possible extension of this scheme to explicit-solvent simulations is outlined and its practical implementation will be described in more details in a forthcoming article.

References: Kastenholz, M. & Hünenberger, P.H.
J. Chem. Phys. **124** (2006) 124108/1-124108/12.

Title: Conformational and dynamical properties of disaccharides in water: A molecular dynamics study.

Researchers: Cristina S. Pereira*
David Kony*
Riccardo Baron*
Martin Müller*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Explicit-solvent molecular dynamics simulations (50 ns, 300 K) of the eight reducing glucose disaccharides (kojibiose, sophorose, nigerose, laminarabiose, maltose, cellobiose, isomaltose, and gentiobiose) have been carried out using the GROMOS 45A4 force field (including a recently reoptimized carbohydrate parameter set), to investigate and compare their conformational preferences, intramolecular hydrogen-bonding patterns, torsional dynamics, and configurational entropies. The calculated average values of the glycosidic torsional angles agree well with available experimental data, providing validation for the force field and simulation methodology employed in this study. These simulations show in particular that: (*i*) (1→6)-linked disaccharides are characterized by an increased flexibility, the absence of any persistent intramolecular hydrogen bond and a significantly higher configurational entropy (compared to the other disaccharides); (*ii*) cellobiose presents a highly persistent interresidue hydrogen bond and a significantly lower configurational entropy (compared to the other disaccharides); (*iii*) persistent hydrogen bonds are observed for all disaccharides (except (1→6)-linked) and typically involve a hydrogen donor in the reducing residue and an acceptor in the nonreducing one; (*iv*) the probability distributions associated with the glycosidic dihedral angles ϕ and ψ are essentially unimodal for all disaccharides, and full rotation around these angles occurs at most once or twice for ϕ (never for ψ) on the 50-ns timescale; (*v*) the timescales associated with torsional transitions (except around ϕ and ψ) range from; 30 ps (rotation of hydroxyl groups) to the nanosecond range (rotation of the lactol and hydroxymethyl groups, and around the ω-glycosidic dihedral angle in (1→6)-linked disaccharides).

References: Pereira, C.S., Kony, D., Baron, R., Müller, M., van Gunsteren, W.F. & Hünenberger, P.H.
Biophys. J. **90** (2006) 4337-4344.

Title: Interaction of the sugars trehalose, maltose and glucose with a phospholipid bilayer: A comparative 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 sugars trehalose, maltose, and glucose with a phospholipid bilayer at atomic resolution. Simulations of the bilayer in the absence or in the presence of sugar (2 molal concentration for the disaccharides, 4 molal for the monosaccharide) are carried out at 325 and 475 K. At 325 K, the three sugars are found to interact directly with the lipid headgroups through hydrogen bonds, replacing water at about one-fifth to one-quarter of the hydrogen-bonding sites provided by the membrane. Because of its small size and of the reduced topological constraints imposed on the hydroxyl group locations and orientations, glucose interacts more tightly (at identical effective hydroxyl group concentration) with the lipid headgroups when compared to the disaccharides. At high temperature, the three sugars are able to prevent the thermal disruption of the bilayer. This protective effect is correlated with a significant increase in the number of sugar-headgroups hydrogen bonds. For the disaccharides, this change is predominantly due to an increase in the number of sugar molecules bridging three or more lipid molecules. For glucose, it is primarily due to an increase in the number of sugar molecules bound to one or bridging two lipid molecules.

References: Pereira, C.S. & Hünenberger, P.H.
J. Phys. Chem. B **110** (2006) 15572-15581.

Title: Estimating the configurational entropy from molecular dynamics simulations: Anharmonicity and correlation corrections to the quasi-harmonic approximation.

Researchers: Riccardo Baron*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

During the past decades, the calculation of accurate free-energy differences from molecular simulations has become feasible in practice. In contrast, the reliable estimation of absolute entropies and entropy differences from these simulations is a notoriously difficult problem. This study investigates critically the method to estimate configurational entropies from molecular dynamics simulations based on the quasi-harmonic approximation. The theory, assumptions, and approximations underlying the method are presented, as well as its connection with essential-mode and normal-mode analyses. In particular, the following points are considered: (i) the relationship between quasi-harmonic and essential modes; (ii) the requirement of mass-weighting (or metric-tensor-weighting) in quasi-harmonic analysis; (iii) the effect of anharmonicities in the individual modes on the estimated entropy; (iv) the effect of pairwise (supralinear) correlations among the different modes on the estimated entropy. The analyses are carried out in the context of long (hundreds of nanoseconds) molecular dynamics simulations involving the reversible folding of β-peptides, considering individually the specific properties of the folded and unfolded ensembles. The anharmonicity correction to the quasi-harmonic entropy is small. In contrast, the pairwise (supralinear) correlation correction is large and affects to a larger extent the entropy of the folded state than that of the unfolded state. The proposed procedure to evaluate corrections for anharmonicity and correlation effects allows for an improved calculation of absolute entropies, as well as of entropy differences for molecular systems which undergo conformational transitions.

References: Baron, R., van Gunsteren, W.F. & Hünenberger, P.H.
Trends Phys. Chem. (2006) in press.

Title: Investigation of the transition between the B and Z conformations of DNA by targeted molecular dynamics simulations with explicit solvation.

Researchers: Mika Kastenholz*
Thomas U. Schwartz**
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry
** Department of Biology, Massachusetts Institute of Technology, Cambridge, USA

Description :

The transition between the B and Z conformations of double-helical deoxyribonucleic acid (DNA) belongs to the most complex and elusive conformational changes occurring in biomolecules. Since the accidental discovery of the left-handed Z-DNA form in the late 1970's, research on this DNA morphology has been engaged in resolving questions relative to its stability, occurrence and function in biological processes. While the occurrence of Z-DNA *in vivo* is now widely recognized and the major factors influencing its thermodynamical stability are largely understood, the intricate conformational changes that take place during the B-to-Z transition are still unknown at the atomic level. In the present article, we report simulations of this transition for the 3'-(CGCGCG)-5' hexamer duplex using targeted molecular dynamics with the GROMOS96 force field in explicit water under different ionic-strength conditions. The results suggest that for this oligomer length and sequence, the transition mechanism involves: (*i*) a stretched intermediate conformation, which provides a simple solution to the important sterical constraints involved in this transition; (*ii*) the transient disruption of Watson-Crick hydrogen-bond pairing, partly compensated energetically by an increase in the number of solute-solvent hydrogen bonds; (*iii*) an asynchronous flipping of the bases compatible with a zipper-like progression mechanism.

References: Kastenholz, M.A., Schwartz, T.U. & Hünenberger, P.H. Biophys. J. (2006) in press.

Title: Explicit-solvent molecular dynamics simulations of the polysaccharide schizophyllan in water.

Researchers: David Kony*
Wolfgang Damm**
Serge Stoll***
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry
** Schrödinger Inc., New York, USA
*** Department of Inorganic, Analytical and Applied Chemistry, University of Geneva, Geneva, Switzerland

Description :

Schizophyllan is a $\beta(1\rightarrow3)$-D-glucan polysaccharide with lateral $\beta(1\rightarrow6)$-branched D-glucose that presents a very stiff triple-helical structure under most experimental conditions. In spite of the remarkable stability of this structure (which persists up to 120^oC in water), schizophyllan undergoes a major state transition around 7^oC in water, that has been hypothetized to result from an order-disorder transition in the lateral residues. In the present study explicit-solvent MD simulations of a schizophyllan fragment (complemented by simulations of the tetrasaccharide monomer) are performed at three different temperatures (273K, 350K and 450K) and with two different types of boundary conditions (finite non-periodic or infinite periodic fragment) as an attempt to provide detailed structural and dynamical information about the triple-helical conformation in solution and the mechanism of the low-temperature transition. These simulations suggest that three important driving forces for the high stability of the triple helix are : (*i*) the limited conformational work involved in its formation; (*ii*) the formation of a dense hydrogen-bonding ne t work at its center; (*iii*) the formation of inter-chain hydrogen bonds between main-chain and lateral glucose residues. However, these simulations evidence a moderate and continuous variation of the simulated observables upon increasing the temperature, rather than a sharp transition between the two lowest temperatures that could be associated with the state transition. Although water-mediated hydrogen-bonded association of neighbouring lateral residues is observed, this interaction is not strong enough to promote the formation of an ordered state (correlated motions of the lateral residues) at the lowest temperature considered.

References: Kony, D., Damm, W., Stoll, S., van Gunsteren, W.F. & Hünenberger, P.H.
Biophys. J. (2006) submitted.

Title: Conformation, dynamics, solvation and relative stability of selected β-hexopyranoses in water: A molecular dynamics study.

Researchers: Vincent Kräutler*
Martin Müller*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

The present article reports long time-scale (200 ns) simulations of four β-D-hexopyranoses (β-D-glucose, β-D-mannose, β-D-galactose and β-D-talose) using explicit-solvent (water) molecular dynamics and vacuum stochastic dynamics simulations together with the GROMOS 45A4 force-field. The following observations are made: (*i*) a solvent-induced population shift of the ϕ dihedral angle characterizing the hydroxymethyl group conformation from g+ in vacuum to t in water for compounds where the 4-OH group is axial (β-D-galactose, β-D-talose); (*ii*) the formation of a strong hydrogen-bonded bridge between the 1,3-*syn*-diaxial 2-OH and 4-OH groups in β-D-talose; (*iii*) the formation of a structured solvent environment between the ring and lactol oxygen atoms as well as around the 4-OH group (except for β-D-talose); (*iv*) the rapid and correlated rotational dynamics of the solute exocyclic hydroxyl groups, with the identification of an asynchronous disrotatory pathway for interconverting hydrogen- bonds between vicinal hydroxyl groups; (*v*) a negative correlation between the average number of solute-solvent hydrogen bonds (itself anticorrelated with the number of intra-solute hydrogen bonds) and the apparent solute "hydrophobicity" (reduced solvation free energy). Good agreement is found with available experimental data on the structural, dynamical and thermodynamic properties of these compounds, and the present study therefore provides additional validation for the carbohydrate force field employed.

References: Kräutler, V., Müller, M. & Hünenberger, P.H.
Carbohydrate Res. (2006) submitted.

Title: Simulation of Plasma Arc Behavior in Gas Circuit Breakers (GCB)

Researchers: Dr. Vincent Wheatley
Harish Kumar
Patrick Huguenot
Prof. Dr. R. Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

In this project we investigate issues related to the simulation of plasma arcs in GCB. Such simulations contain a rich variety of physical mechanisms that may include shocks, arc rotation, turbulence, high radiation and arc-root/cathode interaction. Our motivation is that the importance of such mechanisms and what numerical methods are required to capture them is not yet clear.

We postulate that the equations of magnetohydrodynamics govern the flow within the GCB. In order to capture the details of the physics in our target problems, a high resolution numerical method is required. We have chosen to employ a discontinuous Galerkin (DG) method for this reason. This employs high-order polynomial reconstruction on each element, with the fluxes between elements computed using approximate Riemann solvers to account for the presence of discontinuities.

It is known from low-order methods that to accurately resolve flows with discontinuities, advanced Riemann solvers are required. However, DG methods usually employ the simple and highly diffusive Lax-Friedrichs flux. One of our goals is to assess the performance of advanced Riemann solvers in DG methods.

We are investigating different approaches for obtaining boundary conditions for the arc simulations, including a coupled simulation of the current and fields within the cathode. Also, as our numerical methodology advances, we carry out simulations in the full complicated GCB geometry for comparison to experimental and prior numerical results.

References:

[1] T. C. Warburton and G. E. Karniadakis, *A Discontinuous Galerkin Method for the Viscous MHD Equations*, Journal of Computational Physics 152, 608-641 (1999)

[2] M. Wesenberg, *Efficient MHD Riemann Solvers for Simulations on unstructured triangular Grids*, J. Numer. Math., Vol. 10, No 1, pp. 37-71 (2002)

Title: Developing a Divergence-Preserving Finite Volume Method for Maxwell Equations

Researcher: Paolo Corti
Dr. Manuel Torrilhon
Dr. Michael Fey
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The Maxwell equations describe the motion of electric charges and electromagnetic field in a medium. This set of equations can be subdivided in two groups, a first one describing the changes in time of the electromagnetic fields, and a second one - an intrinsic constraint - coupling the fields to the charges.
The time dependence of the charge density is not explicitly given through a partial differential equation alone, as for the field equation. In the continuum we can couple the two sets of equations to derive the rules for the evolution of charge density.
In the continuous case with a physical initial condition, using the evolution of the charge equation automatically satisfies the constraint. We utilize a finite volume formulation of Torrilhon and Fey [1] - which fulfills the constraint inherently - to avoid non-physical solutions.

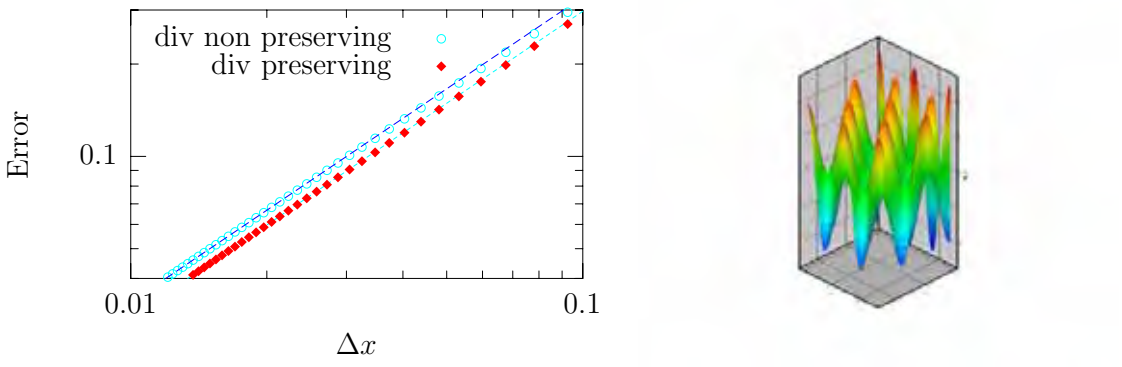


Figure 1: Two 2D simulations for TE wave are illustrated. On the left an l_2 error comparison between a standard 1st order FV method and a divergence-preserving version of the same method. Both are of 1st order convergence, but the divergence-preserving one is slightly better. The initial data for B_z is on the right.

References:

[1] M. Torrilhon and M. Fey, *Constraint-preserving Upwind Methods for Multidimensional Advection Equations*, SIAM J. Num. Anal. 42/4, (2004), pp.1694-1728

Title: The Stability of Numerical Simulations of Complex Stochastic Differential Equations

Researchers: Christian Perret
Dr. Wesley P. Petersen
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zurich

Description:

When dealing with some simulations of SDEs, a loss of accuracy almost independent of the time-step refinement and number of paths can occur after a relatively short time for many methods. An example of a hard-necked SDE is the one given in [1], which numerical solution behaves badly after $t \approx 0.3$. Splitting of drift methods as introduced in [2] have been tried on this process and seem to improve the stability of the results, but not to the desired extent. The goal of this dissertation is thus to develop some new techniques to deal with the unstable behavior of certain SDEs. In particular, the objectives are:

1. to find regularization and splitting techniques which allow numerical solutions of SDEs to remain stable for long time integrations.

2. to study stochastic gauges and their relationships to integrability conditions. Apparently, choices of gauges which preserve positivity of the weights are not as arbitrary as in [1]. It is likely these gauges must be considered to be Lagrange multipliers which must be chosen according to integrability conditions [3,4] of the resulting SDE system with constraints.

3. to study the behavior of oscillating SDEs and to find appropriate integration methods as in [5]. The problem from [1] is not highly oscillating but the long time oscillating behavior is not well behaved.

References:

[1] P. Deuar and P.D. Drummond, *Stochastic gauges in quantum dynamics for many-body simulations*, Comput. Phys. Commun., 142 (2001) pp. 442-445.

[2] W. P. Petersen, *A General Implicit Splitting for Stabilizing Numerical Simulations of Itô Stochastic Differential Equations*, SIAM J. Numer. Anal., 35 (1998), pp. 1439-1451.

[3] W. Römisch and R. Winkler, *Stochastic Differential Algebraic Equations in Circuit Simulations*, Modeling,Simulation, and Optimization of Integrated Circuits, K. Antreich, R. Bulirsch, et al editors, Birkhäuser, Basel (2003) pp. 303-318.

[4] U. M. Ascher and L. R. Petzold, *Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations*, SIAM Books (1998).

[5] L. R. PETZOLD, *An Efficient Numerical Method for Highly Oscillatory Ordinary Differential Equations*, Univ. of Illinois, Urbana-Champaign, pre-print UIUCDCS-R-79.

Title: Compact Third Order Logarithmic Limiting for Non-Linear Hyperbolic Conservation Laws

Researcher: Miroslav Čada
Dr. 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 five-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. These functions were optimized for simplicity and efficiency. The resulting methods handle discontinuities as well as local extrema within the standard semi-discrete MUSCL algorithm using only a single limiter function.

In order to match the spatial discretization we adjust the time integration scheme to be third-order accurate as well. A stability analysis of third-order Runge-Kutta schemes applied to the new spatial operator shows an improved CFL condition such that simulations with CFL < 1.5 are stable.

We will illustrate the performance of this scheme with several numerical experiments, including gas dynamic, MHD flows and Grad's 13–moment equations.

Title: The Dynamics of Debris Flows

Researchers: Julia Kowalski
Dr. Perry Bartelt (Swiss Federal Research Institute WSL)
Dr. Jim McElwain (University of Cambridge)
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Debris flows constitute a major hazard in mountainous areas during summer time. They consist of mobilized sediments spanning a wide range of grain sizes and the flows are fully or partly saturated with water. Well established physical models describe them as depth-averaged one-phase flows with a non-Newtonian rheology. The set of hyperbolic PDEs is closely related to the shallow water equations. A numerical approximation is realized by applying a standard second order Godunov solver and operator splitting is used to incorporate the source terms. Although that works quite well, still a difficulty is, that one can hardly account for different flow regimes. Those can arise due to a variable degree of saturation. With this work we try to overcome that problem by analysing a different model approach. Starting with the mixture theory equations, the fluid and the solid phase are considered separately. Coupling is realized by viscous drag and Terzaghis effective earth pressure theory. Again the homogeneous system has hyperbolic character and currently a numerical solver is developed. A detailed study of similarities and differences between both approaches will follow as well as a comparison to large field scale data from our debris flow observation site in the Illgraben, Kanton Wallis. This project is part of the research activities of the Swiss Federal Institute for Forest, Snow and Landscape Research in the field of rapid mass movements.

References:

[1] B. McArdell, P. Bartelt and J. Kowalski, *Field observations of basal forces and fluid pressures in a debris flow*, Geophysical Research Letters, (submitted 10/2006)

Title: Turbulent reactive flow

Researchers: Dr. Benjamin Rembold
Daniel W. Meyer
Michael Hegetschweiler
Gaurav Anand
Michael Wild
Mathias Hack
Prof. 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. This also is the main reason why they are not more widely used in industry. Motivated by this deficiency, we developed a new hybrid particle/finite-volume PDF solver, which proved to be much faster than previous solution algorithms. Since one of our objectives is to apply PDF methods in industry on a more regular basis, we recently generalized this hybrid algorithm for problems with complex 3D geometries (implemented in C++). Moreover, to make large, complex studies feasible, the code was parallelized using a domain decomposition approach and MPI. The object oriented design will facilitate the integration of all the models we are currently developing.

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. The projects related to the last two topics were initiated recently and therefore no results can be presented yet.

References:

P. Jenny and B. Rembold. Modeling Interaction of Turbulence with Premixed Combustion Using a Joint PDF Approach. Conference on Turbulence and Interactions TI2006, Porquerolles, France, May 29-June 2, 2006

D. W. Meyer and P. Jenny. A Mixing Model for Turbulent Flows Based on Parameterized Scalar Profiles. Physics of Fluids, 18(3), 2006

D. W. Meyer and P. Jenny. Consistent Inflow and Outflow Boundary Conditions for Transported Probability Density Function Methods. Journal of Computational Physics, submitted

D. W. Meyer and P. Jenny. Parameterized Scalar Profile Mixing Model for Turbulent Combustion Simulations. 77th Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik, Berlin, Germany, March 27-31, 2006

M. Hegetschweiler and P. Jenny. Model of Partially Premixed Turbulent Combustion with PDF Methods. 77th Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik, Berlin, Germany, March 27-31, 2006

B. Rembold and P. Jenny. A Lagrangian Joint PDF Approach for Turbulent Premixed Combustion. 77th Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik, Berlin, Germany, March 27-31, 2006

B. Rembold, M. Grass and P. Jenny. Parallel Hybrid Particle/Finite Volume Algorithm for Transported PDF Methods Employing Sub-Time Stepping. Journal of Computational Physics, submitted

B. Rembold and P. Jenny. A multiblock joint PDF finite-volume hybrid algorithm for the computation of turbulent flows in complex geometries. Journal of Computational Physics, in press, available online since 22 June 2006

Title: Multi-phase flow in porous media

Researchers: Dr. Ivan Lunati
Manav Tyagi
Prof. 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, the MSFV method was extended by gravity, capillary pressure and compressibility effects. We also investigated the potential of the MSFV method for other applications, i.e. to solve the incompressible Navier-Stokes equations and to study blood flow regulation in a human brain. Of particular algorithmic interest is that the MSFV algorithm is based on solving many small independent tasks and therefore it is an ideal target for massive parallel computing.

Uncertainty assessment: Another problem, which is intrinsic to flow and transport in porous media, is the uncertainty assessment of the solution as a result of uncertain input data (e.g. permeability). In collaboration with Professor Hamdi Tchelepi from the Petroleum Engineering Department at Stanford University, we addressed this issue using a PDF approach. Therefore, first a transport equation for the joint velocity-concentration (e.g. of a contaminant) PDF was developed. Then, a particle solution algorithm was devised, implemented and tested. Conceptually, this new approach has a number of crucial advantages compared with established methods and we intend to generalize it for multi-phase flow.

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 stochastic particle method (SPM), in which individual (infinitesimal) fluid volumes are modeled. 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, a proof of concept study was completed and currently, the method is extended in order to demonstrate its capability to deal with memory effects. It was also shown how consistent macroscopic equations can be derived and that they contain unclosed terms, which require no modeling in the SPM. An ultimate goal of this work is to devise closure models for these terms, such that the macroscopic equations can be solved by efficient finite-volume simulators.

References:

P. Jenny, S. H. Lee and H. Tchelepi. Fully implicit adaptive multi-scale finite-volume algorithm for multi-phase flow in porous media. Journal of Computational Physics, 2006

P. Jenny, H. A. Tchelepi and D. A. Meyer. Probability density function (PDF) modeling for uncertainty assessment of transport in porous media. Journal of Computational Physics, submitted

P. Jenny, H. Tchelepi and D. W. Meyer. Uncertainty Assessment of Transport in Porous Media Based on a Probability Density Function Method. ECMOR X – 10th European Conference on the Mathematics of Oil Recovery, Amsterdam, The Netherlands, 4 Sep 2006

P. Jenny and I. Lunati, Multi-scale finite-volume method for stiff elliptic problems. 77th Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik, Berlin, Germany, March 27-31, 2006

I. Lunati and P. Jenny. Multiscale Finite-Volume Method for Compressible Multiphase Flow in Porous Media. Journal of Computational Physics, 216, 616-636, 2006

I. Lunati and P. Jenny. Multi-Scale Finite-Volume Method for Density-Driven Multiphase Flow in Porous Media. Journal of Computational Geosciences, submitted

I. Lunati and I Lunati. Treating Highly Anisotropic Subsurface Flow with the Multi-Scale Finite-Volume Method. SIAM Journal of Multiscale Modeling and Simulation, submitted

I. Lunati and P. Jenny. A multiscale finite-volume method for three-phase flow influenced by gravity. CMWR XVI - Computational Methods in Water Resources, Copenhagen, Denmark, June 19-22, 2006

I. Lunati and P. Jenny. The Multiscale Finite Volume Method: A flexible tool to model physically complex flow in porous media. ECMOR X – 10th European Conference on the Mathematics of Oil Recovery, Amsterdam, The Netherlands, 4 Sep 2006

M. Tyagi, P. Jenny, I. Lunati, and H.A. Tchelepi. Multi-scale approach for multiphase transport in porous media using stochastic particles. CMWR XVI – Computational Methods in Water Resources, Copenhagen, Denmark, June 19-22, 2006

M. Tyagi, P. Jenny, I. Lunati, and H. A. Tchelepi. Stochastic particle method for non-linear hyperbolic problems. 77th Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik, Berlin, Germany, March 27-31, 2006

Title: Radiation and light scattering in turbid media

Researchers: Prof. 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. In the future, more physics will be incorporated, e.g. capabilities to deal with optical surface effects, anisotropic media, spatially varying scattering characteristics, re-emission and wavelength dependence. Moreover, the model may be applied to compute energy distribution within combustion devices due to radiation.

References:

P. Jenny, M. Vöge, S. Mourad and T. Stamm. Modeling Light Scattering in Paper for Halftone Print. CGIV – Third European Conference on Color in Graphics, Imaging and Vision, University of Leeds, UK, June 19-22, 2006

P. Jenny, S. Mourad, T. Stamm, M. Vöge and K. Simon. Computing Light Statistics in Heterogeneous Media Based on a Mass Weighted Probability Density Function (PDF) Method. JOSA, submitted

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 finite volume method is employed 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. It is investigated how these 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. In addition, the validity of the description of blood as a Newtonian fluid is tested for various conditions.

Title: Incompressible Navier-Stokes flow

Researchers: Dr. Giuseppe Bonfigli
Prof. 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 recently extended and modified to solve the Poisson equation for pressure arising in incompressible Navier-Stokes simulations. Preliminary results indicate that the MSFV results are virtually identical with the corresponding fine-scale solutions. Since the computational cost of MSFV calculations scales linearly with the problem size and is ideally suited for massive parallel computing, we plan to apply the method for huge DNS and LES studies. First, however, this MSFV method requires further validation.

References:

G. Bonfigli and M. Kloker. Secondary instability of crossflow vortices: validation of the stability theory by DNS. J. Fluid Mech, submitted

G. Bonfigli. Numerical simulation of transition and early turbulence in a 3-d boundary layer perturbed by superposed stationary and traveling crossflow vortices. PhD Thesis, University of Stuttgart, 2006

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

Researchers: Giuseppe Bonfigli, Rolf Henniger, Andreas Jocksch, Leonhard Kleiser, Jörg Ziefle

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

Description:

Most engineering and geophysical flows occur at high Reynolds numbers and are thus turbulent. Due to their wide range of length and time scales such flows are not amenable to Direct Numerical Simulations (DNS) in which all relevant scales need to be resolved. In Large-Eddy Simulations (LES) one only resolves the large scales, while their interaction with the non-resolved subgrid scales is modeled. In the Approximate Deconvolution Model (ADM) for LES, the unclosed correlations are computed directly from the approximately unfiltered flow field and the interaction between resolved and non-resolved scales is taken into account by a relaxation term. This approach has been tested and found to give excellent results for a range of flows, all at a fraction (order one percent) of the cost that would be needed for a DNS of the same flows. Similar results have been obtained with our newly developed high-pass filtered eddy-viscosity models.
In one of our projects, simulations of turbulent spots in compressible boundary layers have been carried out in order to compile a set of data quantifying turbulent spot growth within transitional compressible boundary layers. This data can be applied for modeling of transition in RANS flow solvers handling complex flow cases. The investigation of turbulent spot growth may be a significant step towards establishing LES for an industrial application specifically with transitional flow.
Furthermore, the ADM approach was implemented in an industrial-type finite volume code (NSMB), including an extension to flexible multiblock geometries. After the successful validation using the canonical periodic-hill channel configuration, we shifted focus to a flow case of more industrial relevance. Our current research focuses on a turbulent jet issuing into an oncoming boundary layer. This so-called "jet in crossflow" (JICF) configuration is a problem occurring in a wide variety of applications such as film cooling of turbomachinery blades, fuel injection in combustors, plumes of smoke stacks or vertical/short take-off and landing (V/STOL) aircraft. To assess the validity of our simulation approach, a generic JICF configuration consisting of a turbulent round jet issuing perpendicularly into a laminar boundary layer was investigated at two different jet-to-crossflow velocity ratios. The mean-flow results agree well with experimental and numerical reference data, and sophisticated visualisations of the mean and instantaneous flow fields reveal the known relevant flow structure and dynamics, especially the complex vortex systems in the near field of the mixing region.

References: See separate list.

Title: Large-Eddy Simulation and Stability Investigation of Free Shear Flows

Researchers: Felix Keiderling, Leonhard Kleiser, Sebastian Müller

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

Description:
Swirling flows occur in many engineering applications and industries. Curvature effects from the azimuthal component of velocity impose a radial pressure gradient and influence the development of the shear layer. Typical features of swirling jets include the development of recirculation zones, two or more states occurring at the same values of control parameters (bistability), and jump transition between flow states. These effects are of both fundamental and practical interest and are observed e. g. in tornadoes, over delta wings of aircraft and in vortex devices. Accurate prediction of such flows by LES is a challenging task requiring accurate numerics as well as appropriate subgrid-scale models. To obtain accurate time dependent solutions, high order approximations with spectral resolution properties have been employed for spatial discretization. The implementation of the cylindrical coordinate Navier-Stokes solver has been supplemented by extensive validation studies.
Recent investigations focused on swirling mixing layers. Here, corresponding base flows have been computed numerically by solving the compressible boundary layer equations in cylindrical coordinates for axisymmetric swirling mixing layers. A subsequent linear spatial stability analysis revealed a multitude of viscous instability waves which are spatially amplifying. These instabilities waves, modeled as individual wave-like solutions, are superposed with the laminar base flow to specify an inflow condition for large-eddy simulation as well as direct numerical simulation. These investigations provide a better understanding of the early nonlinear evolution and interaction of these instabilities. A high-resolution simulation is being performed in order to obtain high-fidelity reference data of a flow problem with highly increased physical complexity and to analyze the detailed flow structure as well as swirl-enhanced mixing mechanisms.
Furthermore, we performed LES of a compressible turbulent swirling jet with strong swirl including vortex breakdown using the aforementioned instability-mode forcing. The goal is to assess the predictive capability of Large-Eddy Simulation with the Approximate Deconvolution Model for a swirling jet flow configuration which has been previously investigated in experiments. Swirling jet flows present a severe challenge for turbulence modeling since the energy transfer is usually different from the isotropic turbulence case. Therefore, the traditional eddy-viscosity approaches are not expected to be a suitable means for the computation of such flows.

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:

Jet noise reduction has found increasing interest in recent years due to increasingly strict noise immission regulations. However, it has remained largely empirical. Aeroacoustic noise prediction tools are still to be developed, and they are inherently tied to turbulent flow simulations. With the continued increase of computer power, simulations for relevant Reynolds numbers come into reach of time-dependent large-eddy simulations (LES). It is believed that the noise generating mechanisms can be further understood and thus steps toward noise control can be taken.
Our work within 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 that allow to predict the emitted far-field noise accurately and efficiently. As a subgrid-scale model we employ the Approximate Deconvolution Model (ADM) for LES. 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. Presently we investigate a round jet flow (and its associated noise) for a moderate Reynolds number and a high subsonic Mach number. To this end, a DNS/LES code developed for cylindrical geometries is applied for simulations of circular jet flows with direct computation of noise radiation into the near field.
The emitted jet noise in the acoustic far-field can be determined most efficiently with a hybrid method. Hybrid methods extrapolate the information of an underlying DNS/LES to the far-field and thereby couple the fluid flow with an acoustic field. By exploiting analogies between the governing equations of fluid flow and the acoustic wave propagation the aerodynamically generated noise can be determined. To this end, two acoustic far-field solvers were developed. Both directly interface with the previously described DNS/LES solver. One far-field solver is based on a surface integral formulation (method 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 (e.g. data from the LES).

References: See separate list.

Title: Simulation of Particle-laden Flows

Researchers: Rolf Henniger, Leonhard Kleiser, Anna Kubik

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

Description:

This project is concerned with the direct numerical simulation of disperse two–phase flows, in which a large number of small particles are suspended in a carrier fluid. We consider dilute suspensions, i. e. flows with small particle concentrations where the particle–fluid interaction is the predominant process while direct particle–particle interactions may be neglected (two–way coupling). The particles are assumed to be much smaller than the smallest relevant scales of the fluid motion. This allows us to model the particles as point–forces without resolving their finite size. Each particle is tracked along its trajectory (Lagrangian tracking), while the fluid equations are solved in an Eulerian framework.
One of the studied fundamental phenomena was the settling of an initially random particle suspension in homogeneous turbulence. The mean particle settling velocity is increased by the preferential sweeping effect. Additionally, enhancement of the settling velocity is caused by the particles exerting a collective downward drag force on the fluid in regions of increased particle concentration. A new large eddy simulation (LES) study was conducted enabling us to perform direct comparisons with experiments at microscale Reynolds numbers of a few hundred.
Furthermore, turbulent, wall-bounded particle-laden attached and separated flows were investigated using the setup of a plane channel and backward-facing step (BFS). To account for the wall–particle interaction, models of this process were extended and refined. Two-way coupling for the particulate flow was implemented allowing for studies of turbulence modification. It is confirmed for the plane channel flow that particle feedback causes the turbulence intensities to become more non-isotropic as the particle loading is increased (for the ranges studied). The particles tend to increase the characteristic length scales of the fluctuations in the streamwise velocity, which reduces the transfer of energy between the streamwise and the transverse velocity components. The particle concentration exhibits a maximum close to the wall and a slight increase in the middle of the channel. Fully developed particle-laden channel flow was found to be the most favorable inflow condition for the BFS flow. Significant levels of local enhancement and attenuation of the streamwise component of the fluid turbulence is observed in the channel extension region of the BFS. No modification of the turbulence is found in the separated shear layer or in the re-development region behind the reattachment, although there were significant particle loadings in these regions.

References: See separate list.

Title: Particulate flow in the human inner ear: an analytic model for BPPV

Researchers: Dominik Obrist, Stefan Hegemann*

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser
* Dept. of Otorhinolaryngology, University Hospital Zurich, CH-8092 Zurich

Description:

Particulate flow in the semicircular canals of the human inner ear is suspected to be the most common cause for vertigo. This pathologic condition is known as benign paroxysmal positional vertigo (BPPV) and affects almost 10% of the older people. BPPV may be caused by calcite particles that float freely in the semicircular canals (canalithiasis).
In a first step, we studied the fluid dynamics of the semicircular canals without any particles, i.e., the healthy organ. An analytic solution for an idealized flow configuration was found. An analysis of the eigenmodes revealed the dynamic structure of the flow. Furthermore, we derived explicit expressions that relate the flow field directly to the angular velocity of the head.
In order to study canalithiasis we added an analytic model for the particle dynamics to the governing equations. We studied these coupled equations for the particulate flow in the semicircular canals by numerical and analytical methods.
The numerical study was based on a compact finite difference scheme for the spatial discretization and an implicit time integration scheme to cope with the stiffness of the governing equations. This study revealed the mechanisms of canalithiasis from a phenomenological point of view. It also yielded extensive data on the characteristic features of the vertigo (its onset, strength and duration) as a function of the particle size and the number of particles.
The analytical study suggested an approriate definition of a Stokes number St for this flow configuration. We found that there are two different flow regimes that exhibit different phenomena: the small particle regime ($St > 1$) and the large particle regime ($St < 1$). The critical particle size ($St = 1$) was shown to lie within the physiological range of particle sizes. Based on an analysis of the eigensolutions of the linearized equations we developed a reduced-order model. From this we were able to derive explicit expressions that connect the particle and canal properties (including the Stokes number) directly to the onset, strength and duration of the vertigo.
Finally, it was demonstrated how the analytical and numerical results can be used to interpret data gained from clinical experiments with BPPV patients.

References: See separate list.

Title: Information from coarse-grained models subjected to nonequilibrium situations. Brownian and molecular dynamics, theory and applications.

Researchers: PD Dr. Martin Kröger [1]
Dr. Patrick Ilg [1]
Prof. Vlasis G. Mavrantzas [2]
Prof. Brian J. Edwards [3]

Institute: [1] Polymer Physics, Department of Materials, ETH Zürich
[2] University of Patras, Greece
[3] The University of Tennessee, U.S.A.

Description:

We are concerned with the nonequilibrium dynamics and structure of complex fluids based on simple micro- and mesoscopic physical models [1,2] which are not rigorously solvable by analytic methods. Special emphasis is placed on the finitely extendable nonlinear elastic (FENE) chain models which account for molecular stretch, bending, and topology. More coarse-grained descriptions such as primitive path models, and elongated particle models are developed as well. We focus on their inherently anisotropic material - in particular rheological - properties via deterministic and stochastic approaches. Models are implemented in order to enable the analysis of the microscopic origins of the nonlinear viscoelastic behavior of polymeric and magnetic materials [1,3]. In this project we cover the range from flexible to semiflexible polymers in melts, structural suspensions including ferrofluids in field-induced anisotropic phases. For polymer melts, we are currently investigating the statics and dynamics of entanglement networks (shortest multiple disconnected path) based on an efficient geometric algorithm which became recently available [4,5].

References:

[1] M. Kröger, *Simple models for complex nonequilibrium fluids*, Phys. Rep. **390** (2004) 453.

[2] M. Kröger, *Models for polymeric and anisotropic liquids* (Springer, Berlin, 2005)

[3] P. Ilg, M. Kröger, *Anisotropic self-diffusion in ferrofluids studied via Brownian dynamics simulation*, Phys. Rev. E **72** (2005) 031504.

[4] M. Kröger, *Shortest multiple disconnected path for the analysis of entanglements in two- and three-dimensional polymeric systems*, Comput. Phys. Commun. **168** (2005) 209.

[5] K. Foteinopoulou, N.C. Karayiannis, V.G. Mavrantzas, M. Kröger, *Primitive path identification and entanglement statistics in polymer melts*, Macromolecules **39** (2006) 4207.

1. Title: "Measuring" electron delocalization in π-conjugated systems

2. Researchers: Maurizio Bruschi[2]
Maria Grazia Giuffreda[1]
Hans Peter Lüthi[1]

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

4. Description:

For the design of donor/acceptor functionalized π-conjugated compounds, electron delocalization is a widely used concept to make structure-property predictions. In this work we present a method based on the Natural Bond Orbital (NBO) analysis, which allows studying conjugation these compounds on the basis of individual conjugation paths. The method maps rather complex information obtained from quantum chemical calculations onto simple concepts used by the general chemist, and has been proven useful in a number of applications. Based on this method it was possible, for example, to quantitatively address the issues of efficiency of cross (*geminal*) versus through (*cis/trans*) conjugation, or to explain the effect of the insertion of a triple bond in a chain of double bonds.

5. References:

[1] M.G. Giuffreda, M. Bruschi, and H.P. Lüthi, *Chemistry Eur. J.*, 2004, *10*, 5671-5680.
[2] M. Bruschi, M.G. Giuffreda, and H.P. Lüthi, *Chimia* 2005, *59,* 1-6.
[3] M. Bruschi, PhD Thesis, ETH Zürich (No. 16343), 2005.

1. Title: *Through* versus *cross* conjugation in polytriacetylene oligomers: a computational analysis

2. Researchers: Maurizio Bruschi[2]
Maria Grazia Giuffreda[1]
Hans Peter Lüthi[1]

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

4. Description:

In this project we perform a systematic investigation of the molecular and electronic properties of unsubstituted polytriacetylene (PTA) and *iso*-polytriacetylene (*iso*-PTA) oligomers, which are characterized by through (*cis, trans*) and cross (*geminal*) π-conjugation pathways, respectively. The goal of the study is to compare the efficiency of through and cross conjugation on the basis of the computed molecular geometries, electron affinities, ionization potentials, excitation energies, and non-linear optical properties for oligomers of increasing chain length. The computations show that for the cross conjugated oligomers, these properties show very short effective conjugation lengths, indicating that electron delocalization past the cross-linked carbon atoms is very limited. This may be different in the molecular anions and cations, however [1].

We also find that the incorporation of triple bonds in a polyacetylene (PA) chain, to give poly-diacetylene (PDA) or polytriacetylene (PTA), increases the total amount of π-delocalization, but, on the other hand, reduces the efficiency with which π-delocalization extends along the chain. This observation can be explained by means of the orbital interaction patterns along the polymer chain. Whereas the interactions between like orbitals (double with double, triple with triple bonds) leads to smooth energy profiles, the interaction between unlike orbitals is usually smaller. This creates a rugged interaction energy profile along the chain; the relatively weaker interaction between double and triple bonds also results in a more limited flow of charge, i.e. a lesser delocalization energy [2].

5. References:

[1] M. Bruschi, M.G. Giuffreda, H.P. Lüthi, *ChemPhysChem* 2005, *6*, 511-519.
[2] M. Bruschi, M.G. Giuffreda, H.P. Lüthi, manuscript in preparation.

1. Title: Electron delocalization in cyanoethynylethenes and their donor-substituted derivatives

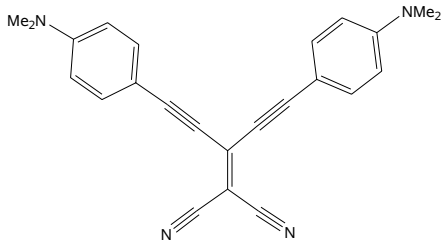
2. Researchers: Maria Grazia Giuffreda[1]
Peter Limacher[1]
Nicolle Moonen[2]
Hans Peter Lüthi[1]
François Diederich[2]

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

4. Description:

Cyanoethynylethenens and their donor-substituted derivates are new class of compounds showing potential for application as NLO materials. The goal of this study is the analysis of mixed donor/acceptor substitution patterns and of differences between the various conjugation paths (*geminal*, *trans*, and *cis)* within the same molecule or among different constitutional isomers. We further relate the efficiency of conjugation with the overall stability and other properties.

The analysis of the conjugation pathways shows some unexpected features. The *geminal* cyano-cyano conjugation paths are very efficient, and strongly respond to the environment: donor presence "boosts" the delocalization energy of the *geminal* CN-CN path, making it to a strong discriminator between isomers. The donor-acceptor paths, on the other hand, prefer *cis/trans* conjugation. Given these "rules" it is not surprising that the constitutional isomer shown in the figure below is the most stable in its class (i.e. the class of bis-cyano-bis-dimethylanilino ethenes).



5. References:

[1] M.G. Giuffreda, N. Moonen, H.P. Lüthi, F. Diederich, *Chemistry Eur. J.*, to be submitted

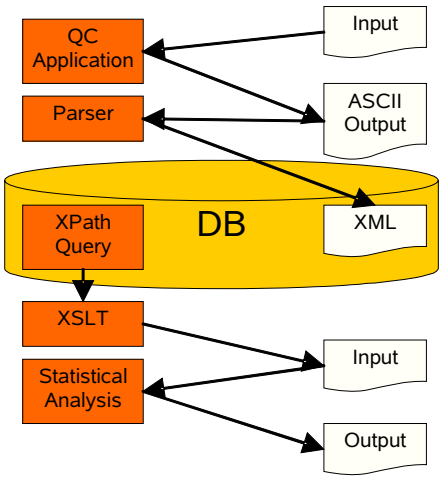
1. Title: Statistical Analysis of Quantum Chemical Data Using Generalized XML/CML Archives for the Derivation of Molecular Design Rules

2. Researchers:
Andreas Elsener[1]
Martin Brändle[2]
Peter Bühlmann[3]
Claire Samson[1]
Hans Peter Lüthi[1]

3. Institute/Group:
[1]Laboratory of Physical Chemistry, ETH Zurich
[2]Chemistry Biology Pharmacy Information Center, ETH Zurich
[3]Seminar for Statistics, ETH Zurich

4. Description:

The rational design of novel compounds with tailored properties requires rules ("knowledge") describing the relationship between the molecular and electronic structure and the properties. Today, structure and property information can be generated by means of computations at very high throughput. The main challenge remaining is the transformation of this information to knowledge.



In this work we describe a highly automated procedure ("workflow"; see Figure) for the analysis of data obtained from quantum chemical computations on a training set of over 1'500 donor / acceptor functionalized ethynylethenes. The data generated as part of this workflow are archived in an XML/CML database and processed by means of statistical analysis methods. This production and analysis "machinery" is applied towards the interference of dependencies between the electron delocalization energy and the properties of the training set. The study shows that the electron delocalization energy is a valid descriptor for functionalized π-conjugated compounds. XML/CML turn out to be very useful for program interoperability and data analysis.

5. References:

[1] A. Elsener, M. Brändle, P. Bühlmann, C. Samson, H.P. Lüthi,
Chimia (invited contribution), manuscript in preparation

Title: Probabilistic Methods for High Dimensional PDEs Using the Feynman Kac Representation.

Researchers: F. M. Buchmann
W. P. Petersen

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Monte-Carlo methods for high dimensional systems are very attractive because the statistical errors are independent of the dimensionality. The statistical errors are $O(N^{-1/2})$, where N is the sample size, and the proportionality is independent of the domain dimension d. The basic idea of MC methods for partial differential equations (PDE) is to simulate independent sample paths of a stochastic differential equation (SDE), whose drift and diffusion coefficients are taken from the PDE. The solution of the PDE is given by expectations (averages) of functions of these sample paths. Non-linear and problems with complicated boundary conditions are variants on this basic idea.

Two procedures for boundary finding have been explored: (1) a bounded increment approach, wherein the step-size is chosen so that paths are never allowed to leave the domain but stop within a *stopping layer*; and (2) an estimated excursion method, where the Brownian increments are Gaussian, and statistical estimates of the exit time are done by Brownian bridges. Potential and Poisson-like problems up to $d = 128$ have been studied. All of our tests were run on the ETH Beowulf clusters *Asgard*, *Hraidar*, and *Gonzales*.

References:

[1] F. M. Buchmann and W. P. Petersen, An Exit Probability Approach to Solve High Dimensional Dirichlet Problems, SIAM J. on Sci. and Stat. Comp., vol. 28, no. 3, pp. 1153-1166, (2006).

Title: Asset pricing for idiosyncratically incomplete markets

Researchers: Semyon Malamud
Eugene Trubowitz
Wesley Petersen

Institute(s): Seminar for Applied Mathematics
and Department of Mathematics
ETH Zürich

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:

[1] S. Malamud and E. Trubowitz, Asset pricing for idiosyncratically incomplete markets, preprint, ETHZ (2006).

[2] S. Malamud, W. Petersen and E. Trubowitz, Asset Pricing in Strongly Heterogeneous Economies, ETHZ (2006), in preparation.

[3] J. Campbell, and J. Cochrane, J. of Political Economy, 107 (2), p. 205–251 (1999).

[4] G. M. Constantinides and D. Duffie, J. of Political Economy, 104 (2), p.219–240 (1996).

Title: Similarity measures for NMR (1D and 2D) and IR spectra

Researchers: Lóránt Bódis
Ernö Pretsch

Institute/ Group: Laboratory of Organic Chemistry
Group of Prof. E. Pretsch
In cooperation with
Dr. A. Ross, F. Hoffmann-La Roche Ltd.
Dr. P. Portmann, Upstream Solutions, Zürich

Description:

A new method has been developed for calculating the similarity degree of two spectra. Its performance has been optimized using computer-generated ^{1}H NMR spectra. The method is compared with a recently proposed local cross-correlation method. Using a test set, its discriminative power between related and unrelated spectra is found to be better than with other methods described previously. Better results are also obtained when comparing measured spectra from a database with the corresponding estimated ones or with estimated spectra of randomly assigned structures. More recently, the method has been adapted for 2D NMR and infrared spectra.

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

Researchers: M. Quack*
J. Stohner**

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

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 (2006)
[2] J. Stohner and M. Quack in "Trends and Perspectives in Modern Computational Science" 1, pages 000 – 000, Brill Academic Publishers, Leiden 2006, (in press).

Title: Electroweak Quantum Chemistry and the Dynamics of Parity Violation in Chiral Molecules

Researchers: M. Quack

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

Description:

The theoretical, computational and experimental status of the field is reviewed.

References:

[1] Martin Quack in "Modelling Molecular Structure and Reactivity in Biological Systems", Proc. 7th WATOC Congress , Capetown 2005, pages 3 – 38, (K. Naidoo, J. Brady, M. Field, J. Gao and M. Hann, eds.), Royal Society of Chemistry, Cambridge 2006, (ISBN 0854046682).

Title: Stereomutation Tunneling Switching Dynamics and Parity Violation in Chlorineperoxide Cl–O–O–Cl

Researchers: M. Quack
M. Willeke

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

Description:

In a search for efficient spectroscopic avenues toward experiments on molecular parity violation, we investigate the stereomutation tunneling processes in the axially chiral chlorine isotopomers of Cl_2O_2 by the quasiadiabatic channel reaction path Hamiltonian (RPH) approach and the corresponding parity violating potentials by means of quantum chemical calculations including our recently developed Multiconfiguration linear response (MC-LR) approach to electroweak quantum chemistry. The calculated ground-state torsional tunneling splittings for all isotopomers of Cl_2O_2 are much smaller than the parity violating energy differences $\Delta_{pv}E$ between the enantiomers of these molecules and therefore parity violation is predicted to dominate the quantum dynamics of stereomutation at low energies. We also compare these with torsional ground-state tunneling splittings and parity violating energy differences of the whole series of axially chiral $HXYH^{(+)}$ isotopomers (with X, Y = $Cl^{(+)}$, O, S, Se, Te). A comparison with our previous results for the homologous molecule Cl_2S_2 shows that for Cl_2O_2 a spectroscopic high-resolution analysis should be easier and the energy region of large tunneling splittings should be more easily accessible by IR excitation. We thus propose a scheme using "tunneling switching" with vibrational excitation in order to carry out the measurement of time-dependent parity violation in superposition states of initially well-defined parity. We discuss the advantages and drawbacks of such an experiment that can be carried out entirely in the IR spectral range (for Cl_2O_2 or related molecules).

References:

[1] M. Quack and M. Willeke, J. Phys. Chem. A **110,** 3338 – 3348 (2006)
[2] M. Quack and M. Willeke, in "Proceedings 15th Symposium on Atomic and Surface Physics and Related Topics", SASP 2006 Obergurgl, 4. - 9. Febr. 2006, pages 233 – 236, (V. Grill and T. D. Märk, eds.), Innsbruck University Press (IUP), Innsbruck, 2006 (ISBN 3-901249-82-6).

Title: The NH and ND stretching fundamentals of $^{14}NH_2D$

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

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

Description:

High resolution (0.004 cm^{-1} instrumental bandwidth) interferometric Fourier transform infrared spectra of mixtures of ammonia-HD isotopomers were measured on a BOMEM DA002 spectrometer under essentially Doppler limited conditions. We report the analysis of the ND and NH stretching fundamentals of $^{14}NH_2D$ with term values $T_\upsilon(s)$ = 2506.5087(9) cm^{-1} and $T_\upsilon(a)$ = 2505.8952(10) cm^{-1} for the ν_1 fundamental, $T_\upsilon(s)$ = 3365.2435(9) cm^{-1} and T_υ (a) = 3367.5892(10) cm^{-1} for the ν_{3a} fundamental and T_υ (s) = 3438.8633(12) cm^{-1} and T_υ (a) = 3439.0315(14) cm^{-1} for the ν_{3b} fundamental. This notation for the fundamentals is chosen for simplicity and for analogy with the case of NH_3 and ND_3. The degenerate modes of NH_3 and ND_3, whose degeneracy is lifted in NH_2D are distinguished by the subscripts *a* and *b*, being symmetric, respectively antisymmetric with respect to the ND-plane of symmetry. About 20 molecular parameters of the effective S-reduced Hamiltonian could be determined accurately for each fundamental. Assignments were established with certainty by means of ground state combination differences. The results are important for and are discussed in relation to the mode selective inhibition of inversion at the nitrogen atom by exciting ND and NH stretching vibrations, for treatments of isotope effects on inversion of ammonia through effective hamiltonians as well as true molecular hamiltonians on high dimensional potential hypersurfaces.

References:

[1] M. Snels, H. Hollenstein and M. Quack, J. Molec. Spectrosc. **237**, 143 – 148 (2006).

Title: Intramolecular Primary Processes: Recent Results and New Questions

Researchers: M. Quack

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

Description:

We outline the Zürich approach to derive intramolecular primary processes from high resolution spectroscopy. We then review recent results on intramolecular vibrational redistribution (IVR) and on tunneling processes. Time scales for fast intramolecular energy redistribution range from less than 100 femtoseconds (fs) to many nanoseconds (ns). Tunneling processes for hydrogen bond dynamics in hydrogen bonded clusters such as $(HF)_2$ fall in the picosecond (ps) to nanosecond ranges, where both rearrangement and predissociation of the hydrogen bonds occur. Fast stereomutation tunneling processes in chiral molecules such as H_2O_2 can be observed in the picosecond to nanosecond time ranges. All these processes are highly nonstatistical showing extreme "non-RRKM" behaviour. Certain slow tunneling processes for stereomutation cover times exceeding many times the age of the Universe. However, well before this limit is reached, tunneling between enantiomers is suppressed by asymmetry arising from the parity violating weak nuclear force. Measurements of the processes of time dependent parity violation on the time scale of milliseconds to seconds could indirectly provide information on properties of the standard model of high energy physics including lifetimes and masses of the short lived heavy particles such as the Z-Boson with a sub-yoctosecond (ys) lifetime and the still hypothetical Higgs-particle. In a speculative final part of the paper we present possible consequences of a hypothetical CPT violation on the one hand and of a molecular theory of thought and decision making on the other hand.

References:

[1] M. Quack in "Proceedings, 15th Symposium on Atomic and Surface Physics and Related Topics", SASP 2006 Obergurgl, 4. - 9. Febr. 2006, pages 81 – 85, (V. Grill and T. D. Märk, eds.), Innsbruck University Press (IUP), Innsbruck, 2006 (ISBN 3-901249-82-6).

Title: Recent results on Parity Violation in Chiral Molecules: Camphor and the Influence of Molecular Parity Violation

Researchers: J. Stohner*
M. Quack**

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:

We report fully anharmonic vibrational frequencies for some selected fundamentals of totally 75 for camphor. The pure vibrational anharmonic frequencies have been obtained with a quartic force-field calculated by *ab initio* or density functional (DFT) methods. A cut through the parity violating potential energy hyper-surface has also been determined as a function of reduced dimensionless normal coordinates $\vec{q}$ and fitted to a multi-dimensional polynomial expansion. This polynomial has been used to calculate parity-violation induced relative frequency shifts as expectation values using anharmonic vibrational wavefunctions for some of the fundamentals, which fall into the CO_2-laser emission range. Anharmonicity strongly influences the relative frequency shift as will be shown by comparison with calculations neglecting anharmonic couplings in camphor and some other molecules.

References:

[1] J. Stohner and M. Quack in "Proceedings, 15th Symposium on Atomic and Surface Physics and Related Topics", SASP 2006 Obergurgl, 4. - 9. Febr. 2006, pages 196 – 199, (V. Grill and T. D. Märk, eds.), Innsbruck University Press (IUP), Innsbruck, 2006 (ISBN 3-901249-82-6).

Title: High Resolution Spectroscopy of Aromatic Compounds

Researchers: S. Albert
M. Quack

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

Description:

The infrared spectra of pyridine, C_6H_5N, and chlorobenzene, C_6H_5Cl were measured with the Bruker IFS125 HR Zürich Prototype (ZP) 2001 Fourier transform spectrometer at room temperature in a 3 m glass cell and in a White-type cell with effective optical path lengths between 9.3 and 19.6 m. The spectra were recorded with a resolution of 0.0008-0.0015 cm^{-1} in the range 600-1300 cm^{-1}. The pyridine spectra were analysed in the ν_{18a} and ν_{15} regions using an effective Hamiltonian. A Coriolis resonance between the ν_{18a} and ν_{18b} states as well as between the ν_{15} state and a dark state attributed to $\nu_4 + \nu_{16b}$ were detected and analysed. The spectrum of chlorobenzene was assigned in the ν_{10b} region. *C*-type transitions were identified. Extensive numerical simulations of the spectra are carried out.

References:

[1] S. Albert and M. Quack in "Proceedings, 15th Symposium on Atomic and Surface Physics and Related Topics", SASP 2006 Obergurgl, 4. - 9. Febr. 2006, pages 213 – 216, (V. Grill and T. D. Märk, eds.), Innsbruck University Press (IUP), Innsbruck, 2006 (ISBN 3-901249-82-6).

Title: Ultrafast Redistribution of Vibrational Energy After Overtone Excitation of CH_3I - Three Different Time Scales

Researchers: V. Krylov
E. Miloglyadov
M. Quack
G. Seyfang

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

Description:

The redistribution of vibrational energy after overtone excitation was investigated for CH_3I in femtosecond pump-probe experiments by time delayed UV-absorption spectroscopy. Dependent on the near-IR excitation frequency three different relaxation times have been measured reaching from τ_1^{IVR} = 200 – 400 fs, τ_2^{IVR} = 4 - 6 ps to τ_3^{IVR} = 250 – 400 ps. This wide range of relaxation times is explained by different intramolecular coupling schemes for the initially excited vibrational levels. Numerical calculations are used in the analysis of the experiments.

References:

[1] V. Krylov, E. Miloglyadov, M. Quack, and G. Seyfang in "Proceedings, 15th Symposium on Atomic and Surface Physics and Related Topics", SASP 2006 Obergurgl, 4. - 9. Febr. 2006, pages 229 – 232, (V. Grill and T. D. Märk, eds.), Innsbruck University Press (IUP), Innsbruck, 2006 (ISBN 3-901249-82-6).

Title: Rovibrational Analysis of the ν_4, $2\nu_6$ Fermi Resonance Band of $CH^{35}ClF_2$ by Means of a Polyad Hamiltonian Involving the Vibrational Levels ν_4, $2\nu_6$, $\nu_6 + \nu_9$ and $2\nu_9$ and Comparison with *ab initio* Calculations

Researchers: S. Albert
H. Hollenstein
M. Quack
M. Willeke

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

Description:

High resolution FTIR spectra of the $\nu_4/2\nu_6$ band system in the region 750–850 cm^{-1} were measured with our Bruker IFS 125 HR Zürich prototype (ZP2001) spectrometer using an instrumental resolution of better than 0.001 cm^{-1} (FWHM, unapodized or 1/MOPD = 0.001 cm^{-1} with the maximum optical path difference MOPD). The spectra were analysed by means of a polyad Hamiltonian built up from the $\nu_4/2\nu_6$ Fermi dyad and the $2\nu_6$, $\nu_6 + \nu_9$, $2\nu_9$ Coriolis triad which share the level $2\nu_6$.The levels $\nu_6 + \nu_9$ and $2\nu_9$ are not directly observed but are included as dark states. Spectroscopic parameters for $\nu_6 + \nu_9$ and $2\nu_9$ as well as the Coriolis coupling constants for the Coriolis triad were transferred from the Coriolis dyad ν_6, ν_9 using previously reported values. The analysis included both isotopomers $CH^{35}ClF_2$, and $CH^{37}ClF_2$. The deperturbed band centres of ν_4 and $2\nu_6$ obtained from the fit are $\tilde{\nu}_4^0 = 812.9300$ cm^{-1} and $2\tilde{\nu}_6^0 = 825.4091$ cm^{-1} for $CH^{35}ClF_2$, and $\tilde{\nu}_4^0 = 809.8311$ cm^{-1} and $2\tilde{\nu}_6^0 = 815.5846$ cm^{-1} for $CH^{37}ClF_2$. The Fermi resonance coupling matrix element obtained for $CH^{35}ClF_2$ is $F = -7.6839$ cm^{-1}. We also report *ab initio* calculations on the MP2 level of theory with aug-cc-pVDZ and aug-cc-pVTZ basis sets pertaining to (q_4), (q_6) and (q_4, q_6) subspaces. These results agree well with the empirical findings and allow us to assign a sign to certain coupling constants which cannot be obtained from the analysis of the experimental spectra.

References:

[1] S. Albert, H. Hollenstein, M. Quack and M. Willeke, Mol. Phys. **104**, 2719 – 2735 (2006)
[2] S. Albert, H. Hollenstein, M. Quack and M. Willeke in "Proceedings 19th Coll. on High Resolution Molecular Spectroscopy", Salamanca 11 – 16 Sept. 2005, pages 123 – 124, (D. Bermejo, J. L. Domenech, M. A. Moreno eds), Sociedad Española de Óptica, Salamanca, 2005 (ISBN 84-609-6737-9).

Title: Modeling Weather and Climate on European and Alpine scales

Researchers: Bodo Ahrens, Peter Brockhaus, Andreas Dobler, Erich Fischer, Joachim Gurtz, Martin Hirschi, Cathy Hohenegger, Simon Jaun, Eric Jäger, Michael Litschi, Daniel Lüthi, Christoph Schär, Reinhard Schiemann, Jürg Schmidli, Sonia Seneviratne, Reto Stöckli, Mark Verbunt

Institute/Group: Institute for Atmospheric and Climate Science, ETH Zürich
Group of Prof. 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. Previous results of our group have indicated that climate change might be associated not only with a mean warming, but also with pronounced increases in interannual (year-to-year) variability. These results have been confirmed by a recent analysis of climate-change simulations from the IPCC fourth assessment report. We have also addressed the underlying physical mechanisms, and find that land-surface processes play a prominent role. This is due to the partitioning of the surface net radiation balance into evapotranspiration and heating, which is strongly affected by the availability of soil moisture. Our research in this area is funded by the Swiss National Science Foundation (NCCR Climate) and the European Commission (projects ENSEMBLES and CECILIA).

Research on weather aspects is motivated by the emergence of high-resolution cloud-resolving models. Such models offer promising prospects in numerical weather prediction as well as quantitative precipitation and flood forecasting. During the last year, we have devoted much effort towards understanding intrinsic predictability limitations that derive from moist convection. Results show that at high spatial resolution, the chaotic dynamical nature of the atmosphere becomes even more pronounced than at the resolutions currently used in numerical weather prediction systems. This implies that weather and flood forecasting should strongly rely on probabilistic systems using ensemble (Monte Carlo) methods. Recent work on probabilistic precipitation forecasting is currently being extended towards probabilistic flood forecasting system. A special case study is underway for the devastating August 2005 flood, which affected large parts of Switzerland. Some of this work is funded by a COST initiative and relies on international collaboration within MAP D-PHASE.

References: A series of papers has been published in the peer-reviewed scientific literature, among them one in *Nature* (see references for further details).

Title: Sparse Galerkin FEM of elliptic problems with stochastic data

Researchers: Marcel Bieri
Christoph Schwab

Institute: Seminar for applied mathematics (SAM)

Description:

We solve elliptic partial differential equations where the coefficients are given as random fields. A Monte-Carlo simulation is a possible but very slow convergent approch for solving this kind of problem. Therefore we use a different method, the so-called Stochastic Finite Element Method (SFEM,[1]), based on the discretization of the random fields in terms of polynomials of random variables. This discretization, however, turns out to lead to a very high-dimensional but deterministic problem to be solved. The main goal of the project is to overcome this high complexity by using

- sparse approximation techniques, such as sparse tensor product spaces and sparse polynomial chaos expansions [2].
- computer parallelism to efficiently overcome potential bottlenecks in our proposed algorithm.

Implementation, parallelization and testing of the SFEM algorithm 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

[1] R.G. Ghanem and P.D. Spanos. Stochastic Finite Elements, a spectral approach. Dover edition. Dover Publications, Inc., Mineola, New York.

[2] R.-A. Todor and C. Schwab. Convergence Rates for Sparse Chaos Approximations of Elliptic Problems with Stochastic Coefficients. Tech. Report 2006-05, Seminar for applied mathematics, ETH Zürich.

Title: Sparse Second Moment Analysis of Elliptic PDEs in Stochastic Domains

Researchers: H. Harbrecht (Univ. Bonn)
R. Schneider (CAU Kiel)
Ch. Schwab (SAM, ETH)

Institute: Seminar for Applied Mathematics
ETH Zürich

Description: We consider the numerical solution of Dirichlet problems in domains with random boundary perturbations. Assuming normal perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution for the Dirichlet problem in the stochastic domain.

Using a variational boundary integral equation formulation on the unperturbed, reference boundary and a wavelet discretization, we present and analyze an algorithm to approximate the random solution's two-point correlation function at essentially optimal order in essentially $\mathcal{O}(N)$ work and memory, where N denotes the number of unknowns required for consistent discretization of the boundary of the domain.

Numerical experiments with Gaussian Boundary Perturbations in R^3 show that the sparse tensor discretization allows to reduce the number N of degrees of freedom on the reference boundary from $N = O(10^16)$ that would be required for the full tensor product discretization of the Covariance function to $O(10^9)$ for our sparse tensor product discretization without loss in accuracy.

References:

[1] H. Harbrecht, R. Schneider and Ch. Schwab, *Sparse Second Moment Analysis for Elliptic Problems in Stochastic Domains*, submitted.

[2] Ch. Schwab and R.A. Todor, *Sparse wavelet methods for operator equations with stochastic data*, pplications of Mathematics **51**(2) 145-180 (2006).

Title: Pricing algorithms for financial derivatives on multivariate jump processes

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

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Lévy copulas are used to construct d-dimensional Lévy models. Option prices are solutions of partial integrodifferential equations. These are solved by sparse tensor product finite element spaces. Since the multidimensional Lévy densities have singularities at the origin and possibly on the axes, variable order, composite quadrature formulas are needed for the computation of the integral part. We give numerical examples for different payoff functions.

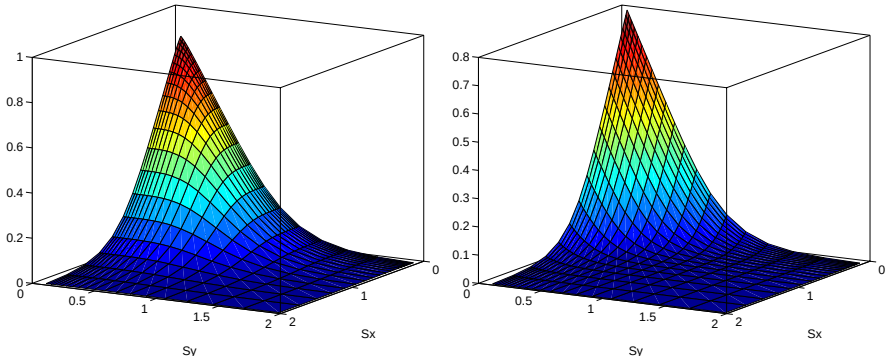


Figure 1: Maximum put option (left) and basket option (right)

References:

[1] J. Kallsen and P. Tankov, *Characterization of dependence of multidimensional Lévy processes using Lévy copulas*, Journal of Multivariate Analysis. 97 (2006)

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

Title: Anisotropic Stable Lévy Copula Processes – Analytical and Numerical Aspects

Researcher: PD Dr. Walter Farkas*
Nils Reich**
Prof. Christoph Schwab**

Institute: * Swiss Banking Institute, University of Zurich,
** 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 of tempered stable type.
The dependence among the marginals' jump structure is parametrized by a Lévy copula. 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 Kolmogoroff 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, and C. Schwab, *Anisotropic stable* L*évy copula processes - analytical and numerical aspects*, Research Report No. 2006-08, Seminar for Applied Mathematics, ETH Zürich

Title: Numerical analysis for anisotropic multivariate Lévy processes

Researcher: Nils Reich

Institute: Seminar for Applied Mathematics, ETH Zürich.

Description:

In this work arbitrage-free prices u of financial derivatives on $d \geq 2$ assets are considered where the underlyings are modeled by Markov processes of Lévy type. They satisfy a high dimensional parabolic partial integrodifferential equation (PIDE) $\partial_t u + \mathcal{A}u = 0$ on $[0,1]^d$. Numerical pricing of these contracts by sparse Finite Element Methods requires the efficient discretization of the infinitesimal generator $\mathcal{A}$ of X.
For a wide class of operators we obtain a new sparse grid based wavelet compression scheme for *anisotropic* tensor product wavelets that (asymptotically) reduces the matrix complexity from originally $\mathcal{O}(h^{-2d})$ to $\mathcal{O}(h^{-1})$.

References:

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

[2] W. Farkas, N. Reich, and C. Schwab, *Anisotropic stable* L*évy copula processes - analytical and numerical aspects*, Research Report No. 2006-08, Seminar for Applied Mathematics, ETH Zürich

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: Hysteretic memory effects in disordered magnets

Researchers: H. G. Katzgraber[*]
G. T. Zimanyi[**]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**] University of California Davis

Description:

We study the return point as well as the complementary point memory effect numerically with paradigmatic models for random magnets and show that already simple systems with Ising spin symmetry can reproduce the experimental results of Pierce et al. where both memory effects become more pronounced for increasing disorder and return point memory is always better than complementary point memory.

References:

H. G. Katzgraber and G. T. Zimanyi, Phys. Rev. B 74, 020405(R) (2006)

Title: Universality in three-dimensional spin glasses

Researchers: H. G. Katzgraber [*]
M. Körner *
A. P. Young **

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California Santa Cruz

Description:

We study universality in three-dimensional Ising spin glasses by large-scale Monte Carlo simulations of the Edwards-Anderson Ising spin glass for several choices of bond distributions, with particular emphasis on Gaussian and bimodal interactions. A finite-size scaling analysis suggests that three-dimensional Ising spin glasses obey universality.

References:

H. G. Katzgraber, M. Körner, and A. P. Young, Phys. Rev. B 73, 224432 (2006)

Title: Simulations of ultracold bosonic atoms in optical lattices with anharmonic traps

Researchers: O. Gygi, H. G. Katzgraber, M. Troyer [*]
Stefan Wessel [**]
G. G. Batrouni [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Universität Stuttgart, Germany
[***] Universite de Nice-Sophia Antipolis, France

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:

O. Gygi, H. G. Katzgraber, M. Troyer, Stefan Wessel, and G. G. Batrouni, Phys. Rev. A 73, 063606 (2006)

Title: Feedback-optimized parallel tempering Monte Carlo

Researchers: H. G. Katzgraber [*]
S. Trebst [**]
D. Huse[***]
M. Troyer *

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Microsoft Research and KITP UC Santa Barbara
[***] Princeton University

Description:

We introduce an algorithm to systematically improve the efficiency of parallel tempering Monte Carlo simulations by optimizing the simulated temperature set. Our approach is closely related to a recently introduced adaptive algorithm that optimizes the simulated statistical ensemble in generalized broad-histogram Monte Carlo simulations. Conventionally, a temperature set is chosen in such a way that the acceptance rates for replica swaps between adjacent temperatures are independent of the temperature and large enough to ensure frequent swaps. In this paper, we show that by choosing the temperatures with a modified version of the optimized ensemble feedback method we can minimize the round-trip times between the lowest and highest temperatures which effectively increases the efficiency of the parallel tempering algorithm. In particular, the density of temperatures in the optimized temperature set increases at the bottlenecks of the simulation, such as phase transitions. In turn, the acceptance rates are now temperature dependent in the optimized temperature ensemble. We illustrate the feedback-optimized parallel tempering algorithm by studying the two-dimensional Ising ferromagnet and the two-dimensional fully-frustrated Ising model, and briefly discuss possible feedback schemes for systems that require configurational averages, such as spin glasses.

References:

H. G. Katzgraber, S. Trebst, D. Huse, and M. Troyer, J. Stat. Mech P03018 (2006)

Title: Probing tails of energy distributions using importance sampling in the disorder with a guiding function

Researchers: M. Körner, H. G. Katzgraber [*]
A. K. Hartmann [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Theoretische Physik, Universität Göttingen

Description:

We propose a simple and general procedure based on a recently introduced approach that uses an importance-sampling Monte Carlo algorithm in the disorder to probe to high precision the tails of ground-state energy distributions of disordered systems. Our approach requires an estimate of the ground-state energy distribution as a guiding function which can be obtained from simple-sampling simulations. In order to illustrate the algorithm, we compute the ground-state energy distribution of the Sherrington-Kirkpatrick mean-field Ising spin glass to eighteen orders of magnitude. We find that if the ground-state energy distribution in the thermodynamic limit is described by a modified Gumbel distribution as previously predicted, then the value of the slope parameter m is clearly larger than 6 and of the order 11.

References:

M. Körner, H. G. Katzgraber, and A. K. Hartmann, J. Stat. Mech P04005 (2006)

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

Researchers: H. G. Katzgraber[*]
A.P. Young[**]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**]University of California, Santa Cruz

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:

H. G. Katzgraber and A.P. Young, Phys. Rev. B accepted

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

Researchers: H. G. Katzgraber [*]
F. Krzakala[**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] ESPCI, Paris

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:
H. G. Katzgraber, F. Krzakla, Phys. Rev. Lett. submitted (cond-mat/0606180)

Title: Precise finite-sample quantiles of the Jarque-Bera adjusted Lagrange multiplier test

Researchers: D. Würtz*
H.G. Katzgraber**

Institute/Group: * Theoretische Physik, ETH Zürich
** Theoretische Physik, ETH Zürich

Description:
It is well known that the finite-sample null distribution of the Jarque-Bera Lagrange Multiplier (LM) test for normality and its adjusted version (ALM) introduced by Urzua differ considerably from their asymptotic chi^2(2) limit. Here, we present results from Monte Carlo simulations using 10^7 replications which yield very precise numbers for the LM and ALM statistic over a wide range of critical values and sample sizes. This enables a precise implementation of the Jarque-Bera LM and ALM test for finite samples.

References:

Econ.Lett. Submitted (math.ST/0509423)

Title: Spin, charge and orbital fluctuations in a multi-orbital Mott-insulator

Researchers: A. Koga [*]
N. Kawakami [**]
T.M. Rice[***]
M. Sigrist[****]

Institute/Group: [*] Department of Applied Physics, Osaka University
[**]Department of Applied Physics, Osaka University
[***] Theoretische Physik, ETH Zürich
[****]Theoretische Physik, ETH Zürich

Description:
The two-orbital degenerate Hubbard model with distinct hopping integrals is studied by combining dynamical mean-field theory with quantum Monte Carlo simulations. The role of orbital fluctuations for the nature of the Mott transition is elucidated by examining the temperature dependence of spin, charge, and orbital susceptibilities as well as the one-particle spectral function. We also consider the effect of the hybridization between the two orbitals, which is important particularly close to the Mott transition points. The introduction of the hybridization induces orbital fluctuations, resulting in the formation of a Kondo-like heavy-fermion behavior, similarly to *f*-electron systems, but involving electrons in bands of comparable width.

References:

Phys. Rev. B72, 045128 (2005).

Title: Critical properties of doped coupled spin-Peierls chains

Researchers: N. Laflorencie[*]
D. Poilblanc[**]
M. Sigrist[***]

Institute/Group: [*] Laboratoire de Physique Théorique, Université Paul Sabatier
[**] Laboratoire de Physique Théorique, Université Paul Sabatier
[***]Theoretische Physik, ETH Zürich

Description:

Using numerical Real Space Renormalisation Group methods as well as Stochastic Series Expansions Quantum Monte Carlo simulations a generic model of diluted spin-1/2 impurities interacting at long distances is investigated. Such a model gives a generic description of coupled dimerized spin-Peierls chains doped with non-magnetic impurities at temperatures lower than the spin gap. A scaling regime with temperature power-law behaviors in several quantities like the uniform or staggered susceptibilities is identified and interpreted in terms of large clusters of correlated spins.

References:

Phys. Rev. B71, 104427 (2005)

Title: Quantum fluctuations and excitations in antiferromagnetic quasicrystals

Researchers: S. Wessel[*] and I. Milat[*]

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

Description:

We study the effects of quantum fluctuations and the excitation spectrum for the antiferromagnetic Heisenberg model on a two-dimensional quasicrystal, by numerically solving linear spin-wave theory on finite approximants of the octagonal tiling. Previous quantum Monte Carlo results for the distribution of local staggered magnetic moments and the static spin structure factor are reproduced well within this approximate scheme. Furthermore, the magnetic excitation spectrum consists of magnonlike low-energy modes, as well as dispersionless high-energy states of multifractal nature. The dynamical spin structure factor, accessible to inelastic neutron scattering, exhibits linear-soft modes at low energies, self-similar structures with bifurcations emerging at intermediate energies, and flat bands in high-energy regions. We find that the distribution of local staggered moments stemming from the inhomogeneity of the quasiperiodic structure leads to a characteristic energy spread in the local dynamical spin susceptibility, implying distinct nuclear magnetic resonance spectra, specific for different local environments.

References:

Phys. Rev. B71, 104427 (2005)

Title: Slave-boson theory of the Mott transition in the two-band Hubbard model

Researchers: A. Rüegg, M. Indergand, S. Pilgram and M. Sigrist

Institute/Group: *Theoretische Physik, ETH Zürich

Description:
We apply the slave-boson approach of Kotliar and Ruckenstein to the two-band Hubbard model with an Ising like Hund's rule coupling and bands of different widths. On the mean-field level of this approach we investigate the Mott transition and observe both separate and joint transitions of the two bands depending on the choice of the inter- and intra-orbital Coulomb interaction parameters. The mean-field calculations allow for a simple physical interpretation and can confirm several aspects of previous work. Beside the case of two individually half-filled bands we also examine what happens if the original metallic bands possess fractional filling either due to finite doping or due to a crystal field which relatively shifts the atomic energy levels of the two orbitals. For appropriate values of the interaction and of the crystal field we can observe a band insulating state and a ferromagnetic metal.

References:
European Physical Journal B48, 55 (2005)

Title: Enhanced coherence of antinodal quasi-particles in dirty *d*-wave superconductor

Researchers: K. Wakabayashi, T.M. Rice, M. Sigrist

Institute/Group: Theoretische Physik, ETH Zürich

Description:
Recent ARPES experiments show a narrow quasiparticle peak at the gap edge along the antinodal [1,0]-direction for the overdoped cuprate superconductors. We show that within weak coupling BCS theory for a d-wave superconductor the s-wave single-impurity scattering cross section vanishes for energies of the gap edge. This coherence effect occurs through multiple scattering off the impurity. For small impurity concentrations the spectral function has a pronounced increase of the (scattering) lifetime for antinodal quasiparticles but shows a very broad peak in the nodal direction, in qualitative agreement with experiment and in strong contrast to the behavior observed in underdoped cuprates.

References:
Phys. Rev. B72, 214517 (2005)

Title: Quasiparticle Dynamics in the Kondo Lattice Model at Half Filling

Researchers: S. Trebst[*], M. Sigrist[*]
H. Monien[**]
A. Grzesik[***]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**]Computational Laboratory, ETH Zürich
[***]Physikalisches Institut, Universität Bonn

Description:
We study spectral properties of quasiparticles in the Kondo lattice model in one and two dimensions including the coherent quasiparticle dispersions, their spectral weights and the full two-quasiparticle spectrum using a cluster expansion scheme. We investigate the evolution of the quasiparticle band as antiferromagnetic correlations are enhanced towards the RKKY limit of the model. In both the 1D and the 2D model we find that a repulsive interaction between quasiparticles results in a distinct antibound state above the two-quasiparticle continuum. The repulsive interaction is correlated with the emerging antiferromagnetic correlations and can therefore be associated with spin fluctuations. On the square lattice, the antibound state has an extended s-wave symmetry.

References:
Phys. Rev. B73, 165101 (2005)

Title: Frustrated three-leg spin tubes: from spin ½ with chirality to spin 3/2

Researchers: J.-B. Fouet[*]
A. Läuchli, S. Pilgram[**]
R.M. Noack[***]
F. Mila[****]

Institute/Group: [*]IRRMA, Lausanne
[**]Theoretische Physik, ETH Zürich
[***]Fachbereich Physik, Philipps Universität Magdeburg
[****]Ecole Polytechnique FéDérale de Lausanne

Description:
Motivated by the recent discovery of the spin tube [(CuCl$_2$tachH)$_3$Cl]Cl$_2$, we investigate the properties of a frustrated three-leg spin tube with antiferromagnetic intra-ring and inter-ring couplings. We pay special attention to the evolution of the properties from weak to strong inter-ring coupling and show on the basis of extensive density matrix renormalization group and exact diagonalization calculations that the system undergoes a first-order phase transition between a dimerized gapped phase at weak coupling that can be described by the usual spin-chirality model and a gapless critical phase at strong coupling that can be described by an effective spin-3/2 model. We also show that there is a magnetization plateau at 1/3 in the gapped phase and slightly beyond. The implications for [(CuCl$_2$tachH)$_3$Cl]Cl$_2$ are discussed, with the conclusion that this system behaves essentially as a spin-3/2 chain.

References:
Phys. Rev. B73, 014409 (2006)

Title: A band structure analysis of the coexistence of superconductivity and magnetism in (Ho,Dy)Ni_2B_2C

Researchers: A.O. Shorikov, V.I. Anisimov[*]
M. Sigrist[**]

Institute/Group: [*]Institute of Metal Physis, Ekaterinburg
[**]Theoretische Physik, ETH Zürich

Description:
The phenomenological theory of complex interplay of superconductivity and magnetism in Ho1-*x*Dy*x*Ni2B2C by Doh *et al* (1999 *Phys. Rev. Lett.* **83** 5350) is based on the multi-band picture with at least one band which is strongly dominated by Ni 3d-electron orbitals. These orbitals are insensitive to the antiferromagnetic order of the (Ho, Dy) 4f-electrons, found in these alloys. In the present study we show by detailed analysis of the band structure that indeed such a band can be identified. This provides a microscopic justification of the basic idea underlying the phenomenological discussion.

References:
J. Phys.: Condens. Matter *18*, 5973 (2006)

Title: Optimized ensemble Monte Carlo simulations of dense Lennard-Jones fluids

Researchers: Simon Trebst, Emanuel Gull, Matthias Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:
We apply the recently developed adaptive ensemble optimization technique to simulate dense Lennard-Jones fluids and a particle-solvent model by broad-histogram Monte Carlo techniques. Equilibration of the simulated fluid is improved by sampling an optimized histogram in radial coordinates that shifts statistical weight towards the entropic barriers between the shells of the liquid. Interstitial states in the vicinity of these barriers are identified with unprecedented accuracy by sharp signatures in the quickly converging histogram and measurements of the local diffusivity. The radial distribution function and potential of mean force are calculated to high precision.

References:
J. Chem. Phys. **123**, 204501 (2005)

Title: Simulation results for an interacting pair of resistively shunted Josephson junctions

Researchers: Philipp Werner[*]
Matthias Troyer[**]
Gil Refeael[***]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**]Department of Physics, California Institute of Technology
[***]Kavli Institute of Theoretical Physics, UCSB

Description:
Using a new cluster Monte Carlo algorithm, we study the phase diagram and critical properties of an interacting pair of resistively shunted Josephson junctions. This system models tunnelling between two electrodes through a small superconducting grain, and is described by a double sine-Gordon model. In accordance with theoretical predictions, we observe three different phases and crossover effects arising from an intermediate coupling fixed point. On the superconductor-to-metal phase boundary, the observed critical behaviour is within error-bars the same as in a single junction, with identical values of the critical resistance and a correlation function exponent which depends only on the strength of the Josephson coupling. We explain these critical properties on the basis of a renormalization group (RG) calculation. In addition, we propose an alternative new mean-field theory for this transition, which correctly predicts the location of the phase boundary at intermediate Josephson coupling strength.

References:
J. Stat. Mech P12003 (2005)

Title: Symmetry projection schemes for Gaussian Monte Carlo methods

Researchers: Fakher F. Assaad[*]
Phillip Werner, Phillipe Corboz, Emanuel Gull, Matthias Troyer[**]

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

Description:
A novel sign-free Monte Carlo method for the Hubbard model has recently been proposed by Corney and Drummond. High precision measurements on small clusters show that ground state correlation functions are not correctly reproduced. We argue that the origin of this mismatch lies in the fact that the low temperature density matrix does not have the symmetries of the Hamiltonian. Here we show that supplementing the algorithm with symmetry projection schemes provides reliable and accurate estimates of ground state properties.

References:
Phys. Rev. B**72**, 224518 (2005)

Title: Cluster Monte Carlo Algorithms for Dissipative Quantum Systems

Researchers: Phillip Werner, Matthias Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:
We review efficient Monte Carlo methods for simulating quantum systems which couple to a dissipative environment. A brief introduction of the Caldeira-Leggett model and the Monte Carlo method will be followed by a detailed discussion of cluster algorithms and the treatment of long-range interactions. Dissipative quantum spins and resistively shunted Josephson junctions will be considered.

References:
Prog. Theor. Phys. Suppl. **160**, 395 (2005)

Title: A Massively Parallel Particle-in-Cell Code for the Simulation of Field-Emitter Based Electron Sources

Researchers: Arno Candel, Matthias Troyer[*]
Micha Dehler[**]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**]Paul Scherrer Institut, Villigen

Description:
For the realistic of sources using arrays, the sub-micron resolution required for the emitters leads to models not suitable for current serial codes. Thus, a parallel high-performance 3D Particle-In-Cell code, called *Capone*, has been implemented in C++ using the POOMA II framework on the Linux platform. Sophisticated C++ expression template techniques deliver Fortran performance combined with high-level programming and development comfort. For the computation of external fields, matching parallel field solvers are in development with the electrostatic one being completed.
The Maxwell field solver is on the Finite Integration Algorithm on a non-uniform rectilinear grid. Anisotropic and m constants and perfect electric/magnetic materials stored in triangulated grid cells are supported as well as open, electric and magnetic boundary conditions. Self-consistent macro-particle pushing is accomplished by integrating the classical relativistic equations of motion in combination with charge-conserving current scattering onto the computational grid. Parallelization is performed by partitioning the calculation domain into patches associated to individual processors. Fields are statically distributed while Particles are concurrently distributed to processors according to their position to allow fast local interpolation.

References:
Nuclear Instruments and Methods in Physics Research A **558**, 154 (2006)

Title: Critical Temperature and Thermodynamics of Attractive Fermions at Unitarity

Researchers: Evgeni Burovski[*]
Nikolay Prokof'ev[*], [**], [***]
Boris Svistunov[*], [**]
Matthias Troyer[****]

Institute/Group: [*]Department of Physics, University of Massachusetts
[**] Russian Research Center "Kurchakov Institute, Moscow
[***]Dipartimento di Fisica, Universita di Trento and BEC-INFM, Povo
[***] Theoretische Physik, ETH Zürich

Description:
The unitarity regime of the BCS-BEC crossover can be realized by diluting a system of two-component lattice fermions with an on-site attractive interaction. We perform a systematic-error-free finite-temperature simulations of this system by diagrammatic determinant Monte Carlo. The critical temperature in units of Fermi energy is found to be T_c / E_F = 0.152(7). We also report the behavior of the thermodynamic functions, and discuss the issues of thermometry of ultracold Fermi gases.

References:
Phys. Rev. Lett. **96**, 160402 (2006)

Title: Optimized parallel tempering simulations of proteins

Researchers: Simon Trebst[*]
Matthias Troyer[**]
U.H. E. Hansmann[***]

Institute/Group: Computational Laboratory, ETH Zürich[*]
Theoretische Physik, ETH Zürich[**]
Department of Physics, Michigan Technological University[***]

Description:
We apply a recently developed adaptive algorithm that systematically improves the efficiency of parallel tempering or replica exchange methods in the numerical simulation of small proteins. Feedback iterations allow us to identify an optimal set of temperatures/replicas which are found to concentrate at the bottlenecks of the simulations. A measure of convergence for the equilibration of the parallel tempering algorithm is discussed. We test our algorithm by simulating the 36-residue villin headpiece subdomain HP-36 where we find a lowest-energy configuration with a root-mean-square deviation of less than 4 Å to the experimentally determined structure.

References:
J. Chem., Phys. **124**, 174903 (2006)

Title: Phase diagram of Bose-Fermi mixtures in one-dimensional optical lattices

Researchers: Lode Pollet, Matthias Troyer[*]
K. van Houcke, S.N.A. Rombouts[**]

Institute/Group: Theoretische Physik, ETH Zürich[*]
Subatomaire en Stralingsfysica, Universiteit Gent[**]

Description:
The ground state phase diagram of the one-dimensional Bose-Fermi Hubbard model is studied in the canonical ensemble using a quantum Monte Carlo method. We focus on the case where both species have half filling in order to maximize the pairing correlations between the bosons and the fermions. In case of equal hopping we distinguish among phase separation, a Luttinger liquid phase, and a phase characterized by strong singlet pairing between the species. True long-range density waves exist with unequal hopping amplitudes.

References:
Phys. Rev. Lett. **96**, 250402 (2006)

Title: D-wave resonating valence bond states of ultracold fermionic atoms in optical lattices

Researchers: Simon Trebst, Matthias Troyer[*]
Ulrich Schollwöck[**]
Peter Zoller[***]

Institute/Group: Theoretische Physik, ETH Zürich[*]
Theoretische Physik, RWTH Aachen[**]
Theoretische Physik, Universität Innsbruck[***]

Description:
In view of the apparently exponential complexity of fermionic simulations in two and more dimensions, we consider a controlled quantum simulation to probe the ground state properties of the two-dimensional Hubbard model. We present a controlled experimental setup to adiabatically construct superfluid d-wave resonating valence bond (RVB) states of fermionic atoms confined in a 2D optical lattice. The key idea is to start from a pure initial state which is adiabatically transformed to d-wave RVB states at ultralow temperatures of a few percent of the Fermi temperature. We discuss hole doping techniques and describe a simple experimental measurement to study d-wave pairing.The proposed experiment can be used to effectively probe ground state properties of the repulsive Hubbard model on (coupled) plaquettes, ladders and the 2D square lattice. The proposal is within the capabilities of current technology, and shows how an adiabatic quantum simulator could answer a question that cannot currently be reliably answered by classical computational methods.

References:
Phys. Rev. Lett. **96**, 250402 (2006)

Title: A continuous-time solver for quantum impurity models

Researchers: Philipp Werner, Armin Comanac, A.J. Millis[*]
Luca De Medici[*], [**]
Matthias Troyer[***]

Institute/Group: Department of Physics, Columbia University[*]
Centre de Physique Théorique, Ecole Polytechnique, Palaiseau[**]
Theoretische Physik, ETH Zürich[***]

Description:
We present a new continuous time solver for quantum impurity models such as those relevant to dynamical mean field theory. It is based on a stochastic sampling of a perturbation expansion in the impurity-bath hybridization parameter. Comparisons to quantum Monte Carlo and exact diagonalization calculations confirm the accuracy of the new approach, which allows very efficient simulations even at low temperatures and for strong interactions. As examples of the power of the method we present results for the temperature dependence of the kinetic energy and the free energy, enabling an accurate location of the temperature-driven metal-insulator transition.

References:
Phys. Rev. Lett. **97**, 076405 (2006)

Title: The fate of vacancy-induced 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, Cornell University, [****]
Department of Physics, CUNY, Staten Island[*****]
Theoretische Physik, ETH Zürich[******]

Description:
We study different solid phases of Helium-four, by means of Path Integral Monte Carlo simulations based on a recently developed "worm" algorithm. Our study includes simulations that start off from a high-T gas phase, which is then "quenched" down to T=0.2 K. The low-T properties of the system crucially depend on the initial state. While an ideal hcp crystal is a clear-cut insulator, the disordered system freezes into a "superglass", i.e., a metastable amorphous solid featuring off-diagonal long-range order and superfluidity.

References:
Phys. Rev. Lett. **97**, 080401 (2006)

Title: The Fermi-Hubbard model at Unitarity

Researchers: Evgeni Burovski[*]
Boris Svistunov[*, **]
Nikolay Prokof'ev[***]
Matthias Troyer[****]

Institute/Group: Department of Physics, University of Massachusetts[*]
Kurchatov Institute, Moscow[**]
BEC-INFM, Universita di Trento[***]
Theoretische Physik, ETH Zürich[****]

Description:
We simulate the dilute attractive Fermi-Hubbard model in the unitarity regime using a diagrammatic determinant Monte Carlo algorithm with worm-type updates. We obtain the dependence of the critical temperature on the filling factor and, by extrapolating to 0, determine the universal critical temperature of the continuum unitary Fermi gas in units of Fermi energy: Tc/ F=0.152(7). We also determine the thermodynamic functions and show how the Monte Carlo results can be used for accurate thermometry of a trapped unitary gas.

References:
New J. Phys. **8**, 153 (2006)

Title: Ramping fermions in optical lattices across a Feshbach resonance

Researchers: Helmut G. Katzgraber, Matthias Troyer" Aniello Esposito*

Institute/Group: Theoretische Physik, ETH Zürich*

Description:
We study the properties of ultracold Fermi gases in a three-dimensional optical lattice when crossing a Feshbach resonance. By using a zero-temperature formalism, we show that three-body processes are enhanced in a lattice system in comparison to the continuum case. This poses one possible explanation for the short molecule lifetimes found when decreasing the magnetic field across a Feshbach resonance. Effects of finite temperatures on the molecule formation rates are also discussed by computing the fraction of double-occupied sites. Our results show that current experiments are performed at temperatures considerably higher than expected: lower temperatures are required for fermionic systems to be used as quantum simulators. In addition, by relating the double occupancy of the lattice to the temperature, we provide a means for thermometry in fermionic lattice systems, previously not accessible experimentally. The effects of ramping a filled lowest band across a Feshbach resonance when increasing the magnetic field are also discussed: fermions are lifted into higher bands due to entanglement of Bloch states. Our results are in good agreement with recent experiments.

References:
Phys. Rev. A, 0510194 (2006)

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 N\'eel 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:
Preprint, submitted to Phys. Rev. Lett.

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

Researchers: Christophe Fumeaux
Dirk Baumann
Krishnaswamy Sankaran
Rüdiger Vahldieck

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

Description:

This project considers the development a general-purpose 3D solver for the accurate numerical simulations of electromagnetic (EM) fields. The solver is based on the Finite-Volume Time-Domain (FVTD) method. The FVTD algorithm presents the advantage of being applied in fully unstructured meshes (e.g. made of tetrahedrons). This represents a significant advantage for the discretization of complex geometries, i.e. for the modeling of curved or slanted surfaces, for the resolution of small details within larger structures and in connection with different materials showing a large dielectric contrast.
The development of the FVTD method is pursued along two complementary paths. First, theoretical developments aim at improving the FVTD algorithm for better accuracy and computational efficiency. In-house developments include a novel definition of ports for S-parameter extraction [2] and the finite-volume implementation of accurate absorbing boundary conditions (ABC) based on perfectly matched layers (PML) [4] [5]. In the second line of investigation, the FVTD algorithm is applied to the solution of challenging real-world problems. Among the applications, spiral antennas in conformal configurations and dielectric resonator antennas have been investigated [1] [3] [6].

References:

[1] C. Fumeaux, D. Baumann, R. Vahldieck, "FVTD characterization of substrate effects for Archimedean spiral antennas in planar and conformal configurations", ACES Journal, vol. **20**(3),186-197 (November 2005)
[2] D. Baumann, C. Fumeaux, R. Vahldieck, "Field-based scattering-matrix extraction scheme for the FVTD method exploiting a flux-splitting algorithm", IEEE Transactions on Microwave Theory and Techniques **MTT-53**(11), 3595-3605 (November 2005)
[3] C. Fumeaux, D. Baumann, R. Vahldieck, "Finite-Volume Time-Domain analysis of a cavity-backed Archimedean spiral antenna"; IEEE Transactions on Antennas and Propagation **AP-54**(3), 844-851 (March 2006)
[4] K. Sankaran, C. Fumeaux, R. Vahldieck, "Cell-centered finite-volume based perfectly matched layer for time domain Maxwell system", IEEE Transactions on Microwave Theory and Techniques **MTT-54**(3), 1269-1276 (March 2006)
[5] K. Sankaran, C. Fumeaux, R. Vahldieck, "Uniaxial and radial anisotropy models for finite-volume Maxwellian absorber", IEEE Transactions on Microwave Theory and Techniques, in press (2006)
[6] G. Almpanis, C. Fumeaux, R. Vahldieck, "Novel Broadband Dielectric Resonator Antennas Fed Through Double-Bowtie-Slot Excitation Scheme", Accepted for publication in ACES Journal (2006)

Title: Simulation and Optimization of Metamaterials

Reseachers: Christian Hafner
Kakhaber Tavzarashvili
Nicolas Guérin
Cui Xudong
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 and optimization of metamaterials for microwave and optical applications 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 above are combined with various numerical optimizers for parameter optimization (gradient methods, downhill simplex, evolutionary strategies, genetic algorithms, particle swarm optimization, and genetic programming algorithms were implemented and applied) 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. were developed, implemented and applied).

References:

In 2005 and 2006 four book chapters in three book and seven papers in reviewed journals were published.

Title: Design and analysis of evanescently coupled unitraveling-carrier photodetectors for sub-THz applications

Researchers: Damir Pasalic
Rüdiger Vahldieck

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

Description:

Photodetectors with broad bandwidth and high efficiency are key components of modern optical and wireless communication systems, high-frequency measurement systems, and photonic local oscillators for generation of high power microwave and millimeter wave signals by optical heterodyning. To satisfy the current and future system requirements, new and innovative designs are required to improve photodetector performance. Two main requirements place on high-end photodetectors are broad bandwidth and high output power. Recently proposed unitraveling-carrier (UTC) photodetectors (PDs) utilize only electrons as active carriers. Therefore, they can achieve very broad bandwidths and high output powers. However, the proposed UTC PD is a side-illuminated device with a low coupling efficiency between the feeding optical fiber and the PD due to the very thin absorbing layer. To mitigate the coupling problem, the UTC PD evanescently coupled with a multimode optical waveguide has been proposed. The modes in the optical waveguide are similar to those in the optical fiber; thus a very good coupling can be achieved. The optical power is then evanescently couple with the photodetector. External efficiencies of over 60% can be achieved. However, one of the main challenges in the design of evanescently coupled UTC photodetectors is their modeling. The geometry of the devices is highly complex, as well as the physical processes taking place in them. In this project, we have focused on modeling and design of high speed evanescently coupled UTC PDs. For this purpose, we use the hybrid drift-diffusion—TLM method developed in our last project for analysis of traveling-wave photodetectors (TWPDs). The method combines a semiconductor simulation based on the 2-D drift-diffusion method and a full-wave electromagnetic simulation based on the TLM method. It was used for analysis of different types of TWPDs and excellent agreement with experimental results was obtained. One of the main advantages of this method is its generality. Therefore, it was easily modified to allow simulation of the evanescently coupled UTC photodetectors.

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, and vehicle-mounted vertical monopoles and free-standing horizontal dipoles in the 20 100 MHz 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:
A full report will be filed to ArmaSuisse (Bern, Switzerland) in October 2006.

Title: Force field evaluation for biomolecular simulation: free enthalpies of solvation of polar and apolar compounds in various solvents

Researchers: Daan P. Geerke
Wilfred F. van Gunsteren

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

Description:

Recently, the GROMOS biomolecular force field parameter set 53A6 - which has been parameterized to reproduce experimentally determined free enthalpies of hydration and solvation in cyclohexane of amino acid side-chain analogs - was presented. To investigate the transferability of the new parameter set, we calculated free enthalpies of solvation of a range of polar and apolar compounds in different solvents (methanol, dimethyl sulfoxide (DMSO), acetonitrile, and acetone) from molecular dynamics simulations using the GROMOS 53A6 force field. For methanol and DMSO, parameters were used that are available in the 53A6 parameter set. For acetonitrile, a recently developed model was taken and for acetone, two models available in literature were used. We found that trends in and values for the solvation free enthalpies are in satisfactory agreement with experiment, except for the solvation in acetone for which deviations from experiment can be explained in terms of the properties of the models used.

References: ChemPhysChem **7** (2006) 671-678

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

Researchers: Riccardo Baron[1]
Alex H. de Vries[1,2]
Philippe H. Hünenberger[1]
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:

Molecular liquids can be modeled at different levels of spatial resolution. In atomic-level (AL) models, all (heavy) atoms can be explicitly simulated. In coarse-grained (CG) models, particles (beads) that represent groups of covalently bound atoms are used as elementary units. Ideally, a CG model should reproduce the thermodynamic and structural properties of the corresponding AL model after mapping to the lower-resolution scale. In the present work, two such models are investigated: (i) the classical GROMOS atomic-level model; (ii) a CG model recently proposed by Marrink et al., which maps approximately four non-hydrogen atoms to one bead [*J. Phys. Chem. B* **2004**, *108*, 750]. The study is restricted to *n*-alkanes whose aliphatic fragments are abundantly found in lipids of biological interest. Additionally, *cis*-9-octadecene is included, as a template chain of the lipid dioleoylphosphatidylcholine (DOPC). The two representations of molecules in the liquid phase are compared in terms of average molecular structures, extent of configurational space sampled, and single-molecule entropies. An approximate method is used to estimate the rotational contributions to the absolute configurational entropy. Good correspondence between the AL and CG representations is found. The loss in configurational entropy due to the reduction in degrees of freedom upon coarse-graining of the model is estimated.

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

Title: Biomolecular modeling: goals, problems, perspectives

Researchers: Wilfred F. van Gunsteren[1]
Dirk Bakowies[1]
Riccardo Baron[1]
Indira Chandrasekhar[1]
Markus Christen[1]
Xavier Daura[2]
Peter Gee[1]
Daan P. Geerke[1]
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Chris Oostenbrink[3]
Merijn Schenk[1]
Daniel Trzesniak[1]
Nico F. A. van der Vegt[4]
Haibo B. Yu[5]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zurich, Switzerland,
[2]Universitat Autonoma de Barcelona, Bellaterra, Spain
[3]Vrije Universiteit, Amsterdam, The Netherlands
[4]Max-Planck-Institute for Polymer Research, Mainz, Germany
[5]Department of Chemistry, University of Wisconsin, USA

Description:

Computation based on molecular models is playing an increasingly important role in biology, biological chemistry, and biophysics. Since only a very limited number of properties of biomolecular systems is actually accessible to measurement by experimental means, computer simulation can complement experiment by providing not only averages, but also distributions and time series of any definable quantity, for example, conformational distributions or interactions between parts of systems. Present day biomolecular modeling is limited in its application by four main problems: 1) the force-field problem, 2) the search (sampling) problem, 3) the ensemble (sampling) problem, and 4) the experimental problem. These four problems are discussed and illustrated by practical examples. Perspectives are also outlined for pushing forward the limitations of biomolecular modeling.

References: Angew. Chem. Int. Ed. **45** (2006) 4064-4092
Angew. Chem **118** (2006) 4168-4198

Title: Configurational entropy change of netropsin and distamycin upon DNA minor-groove binding

Researchers: Jožica Dolenc[1,2]
Riccardo Baron[2]
Chris Oostenbrink[3]
Jože Koller[1]
Wilfred F. van Gunsteren[2]

Institute/ Group: [1]Faculty of Chem and Chem. Techn., University of Ljubljana, Slovenia
[2]Laboratory of Physical Chemistry, ETH Zurich, Switzerland;
[3]Vrije Universiteit, Amsterdam, The Netherlands

Description:

Binding of a small molecule to a macromolecular target reduces its conformational freedom, resulting in a negative entropy change that opposes the binding. The goal of this study is to estimate the configurational entropy change of two minor-groove-binding ligands, netropsin and distamycin, upon binding to the DNA duplex d(CGCGAAAAACGCG)· d(CGCGTTTTTCGCG). Configurational entropy upper bounds based on 10-ns molecular dynamics simulations of netropsin and distamycin in solution and in complex with DNA in solution were estimated using the covariance matrix of atom-positional fluctuations. The results suggest that netropsin and distamycin lose a significant amount of configurational entropy upon binding to the DNA minor groove. The estimated changes in configurational entropy for netropsin and distamycin are -127 JK^{-1} mol^{-1} and -104 JK^{-1} mol^{-1}, respectively. Estimates of the configurational entropy contributions of parts of the ligands are presented, showing that the loss of configurational entropy is comparatively more pronounced for the flexible tails than for the relatively rigid central body.

References: Biophysical Journal **91** (2006) 1460-1470

Title: Configurational entropies of lipids in pure and mixed bilayers from atomic-level and coarse-grained molecular dynamics simulations

Researchers: Riccardo Baron[1]
Alex H. de Vries[2]
Philippe H. Hünenberger[1]
Wilfred F. van Gunsteren[1]

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

Description:

Single-chain and single-fragment configurational entropies of lipid tails in hydrated lipid bilayers are evaluated from molecular dynamics simulations using the quasi-harmonic approximation. The entropy distribution along individual acyl tails is obtained and compared to that of corresponding hydrocarbon chains in the liquid phase. We consider pure dipalmitoylphosphatidylcholine and mixed dioleoylphosphatidylcholine/dioleoylphosphatidylethanolamine bilayers. The systems are modeled at different levels of spatial resolution: In an atomic-level (AL) model all (heavy) atoms are explicitly simulated; in a coarse-grained (CG) model particles (beads) representing groups of covalently bound atoms are used, which map approximately four non-hydrogen atoms to one interaction site. Single-chain and single-fragment entropies and correlations between the motions of (single) acyl chains are compared. A good correspondence is found between the flexibility of the AL and CG models. The loss in configurational entropy due to the reduction in the number of degrees of freedom upon coarse-graining of the model is estimated. The CG model shows about 4 times faster convergence of the chain entropies than the more detailed AL model. Corrections to the quasi-harmonic entropy estimates were found to be small for the CG model. For the AL model, the correction due to mode anharmonicities is small, but the correction due to pairwise (supralinear) mode correlations is sizable.

References: J. Phys. Chem. B **110** (2006) 15602-15614 with suppl. mat.

Title: Molecular dynamics simulations of liquid methanol and methanol-water mixtures with polarizable models

Researchers: Haibo Yu[1]
Daan P. Geerke[2]
Haiyan Liu[3]
Wilfred F. van Gunsteren[2]

Institute/ Group: [1]Department of Chemistry, University of Wisconsin, USA
[2]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[3]University of Science and Technology of China, Hefei, China

Description:

A polarizable model for simulation of liquid methanol, compatible with the COS/G2 water model, has been developed using the Charge-on-Spring (COS) technique. The model consists of three point charges, with one polarizable center on the oxygen atom. The Lennard-Jones parameters on the oxygen atom together with the molecular polarizability were varied to reproduce the experimental heat of vaporization and density of liquid methanol at ambient conditions. We examined the energies of various methanol dimers in the gas phase and compared them with values obtained from ab initio calculations. The model was then used to study the thermodynamic, dynamic, structural, and dielectric properties of liquid methanol as well as of a methanol-water mixture. A microscopic picture of the structure of pure liquid methanol and of the methanol-water mixture is provided. Good agreement was found between the results from our model simulations and available experimental and ab initio calculation data. In particular, the experimental dielectric permittivity of 32 could be reproduced, which had been shown to be difficult when using nonpolarizable models.

References: J. Comput. Chem. **27** (2006) 1494-1504

Title: A protein under pressure: molecular dynamics simulation of the Arc repressor

Researchers: Daniel. Trzesniak[1]
Roberto D. Lins[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]EPFL Lausanne, Switzerland

Description:

Experimental NMR results for the Arc Repressor have shown that this dimeric protein dissociates into a molten globule at high pressure. This structural change is accompanied by a modification of the hydrogen–bonding pattern of the intermolecular β–sheet: it changes its character from intermolecular to intra–molecular with respect to the two monomers. Molecular dynamics (MD) simulations of the Arc Repressor, as a monomer and a dimer, at elevated pressure have been carried out with the aim to study this hypothesis and to identify the major structural and dynamical changes of the protein under such conditions. The monomer appears less stable than the dimer. However, the complete dissociation has not been seen due to the long timescale needed to observe this phenomenon. In fact, the protein structure altered very little when raising the pressure. It became slightly compressed and the dynamics of the side chains and the unfolding process slowed down. Raising both, temperature and pressure, a tendency of conversion of intermolecular into intra–molecular hydrogen bonds in the β–sheet region has been detected, supporting the mentioned hypothesis. Also the onset of denaturation of the separated chains was observed.

References: Proteins **65** (2006) 136-144

Title: Sampling of rare events using hidden restraints

Researchers: Markus Christen
Anna-Pitschna E. Kunz
Wilfred F. van Gunsteren

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

Description:

A method to enhance sampling of rare events is presented. It makes use of distance or dihedral-angle restraints to overcome an energy barrier separating two metastable states or to stabilize a transition state between the two metastable states. In order not to perturb these metastable end states themselves, a prefactor is introduced into the restraining energy function, which smoothly increases the weight of this function from zero to one at the transition state or on top of the separating energy barrier and then decreases the weight again to zero at the final state. The method is combined with multi-configurational thermodynamic integration and applied to two biomolecular systems, which were difficult to treat using standard thermodynamic integration. As first example the free energy difference of a cyclic α-aminoxy-hexapeptide-ion complex upon changing the ion from Cl^- to Na^+ was calculated. A large conformational rearrangement of the peptide was necessary to accommodate this change. Stabilizing the transition state by (hidden) restraints facilitates that. As a second example, the free energy difference between the $^4C_1$ and the $^1C_4$ conformation of β-*D*-glucopyranoside was calculated. In unrestrained simulations the change from the $^4C_1$ into the $^1C_4$ conformation was never observed because of the high energy barrier separating the two states. Using (hidden) restraints, the transition from the $^4C_1$ into the $^1C_4$ state and back could be enforced without perturbing the end states. As comparison, for the same transitions the potential of mean force as obtained by using dihedral-angle constraints is provided.

References: J. Phys. Chem. B **110** (2006) 8488-8498

Title: Multigraining: an algorithm for simultaneous fine-grained and coarse-grained simulation of molecular systems

Researchers: Markus Christen
Wilfred F. van Gunsteren

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

Description:

A method to combine fine-grained and coarse-grained simulations is presented. The coarse-grained particles are described as virtual particles defined by the underlying fine-grained particles. The contribution of the two grain levels to the interaction between particles is specified by a grain-level parameter λ. Setting $\lambda = 0$ results in a completely fine-grained simulation, whereas $\lambda = 1$ yields a simulation governed by the coarse-grained potential energy surface with small contributions to keep the fine-grained covalently bound particles together. Simulations at different λ-values may be coupled using the replica-exchange molecular dynamics method (REMD) to achieve enhanced sampling at the fine-grained level.

References: J. Chem. Phys. **124** (2006) on-line DOI: 10.1063/1.2187488

Title: Pathway dependence of the efficiency of calculating free energy and entropy of solute-solute association in water

Researchers: Daniel Trzesniak
Wilfred F. van Gunsteren

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

Description:

In this study we investigate two alternative pathways to compute the free energy and the entropy of small molecule association (ΔF_{assoc} and ΔS_{assoc}) in water. The first route (direct pathway) uses thermodynamic integration as function of the distance *R* between the solutes. The mean force and the mean covariance of the force with the energy in solution are calculated from molecular dynamics (MD) simulation followed by integration of these quantities with respect to the reaction coordinate *R*. The alternative approach examined (solvation pathway) would first remove the solutes from the solution using thermodynamic integration as function of a solvation coupling parameter λ, change the solute-solute distance in vacuo and then solvate back the solute pair at the new separation distance. The system studied was a pair of CH_4 molecules in water. We investigate the influence of the CH_4-water interaction strength on the obtained ΔF_{assoc} and ΔS_{assoc} values by changing van der Waals and Coulomb interaction and evaluated the accuracy and efficiency for the two pathways. We find that the direct route seems more suitable for the calculation of free energies of hydrophobic solutes while the solvation pathway performs better when calculating entropy changes for solutes that have a stronger interaction with the solvent.

References: Chem. Phys. (2006) on-line Doi:10.1016/j.chemphys.2006.09.012

Title: Simulation of an all-beta(3)-icosapeptide containing the twenty proteinogenic side chains: effect of temperature, pH, counterions, solvent and force field on helix stability

Researchers: Daniel Trzesniak[1]
Bernhard Jaun[2]
Raveendra I. Mathad[2]
Wilfred F. van Gunsteren[1]

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

Description:

Simulations of various β-peptides have in the last years clarified several issues concerning peptide folding equilibria and interpretation of experimental data, especially from NMR and CD spectroscopy. These simulations involved different temperatures, pH-values, ionic strengths, solvents, and force-field parameters, but a variation of these factors for one β-peptide has not yet been done. To investigate the influence of varying these factors, we analyze the helix stability of an all-β^3-icosapeptide bearing all twenty proteinogenic amino acid side chains, which is experimentally observed to fold into a 3_{14}-helix in methanol but not in water. Structural aspects, such as hydrogen-bonded rings and salt bridges are discussed and a comparison with NMR primary (NOE distance bounds and ^{3}J-values) and secondary (NMR derived model structures) data is made. We further investigate the reasons for the 3_{14}-helix stability/instability in methanol/water. Of all factors studied, the presence of counter-ions seems to be the one inducing most significant effects in the simulations.

References: Biopolymers (2006) on-line DOI: 10.1002/bip.20601 with supporting mat.

Title: On searching in, sampling of, and dynamically moving through conformational space of biomolecular systems: a review

Researchers: Markus Christen
Wilfred F. van Gunsteren

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

Description:

Methods to search for low-energy conformations, to generate a Boltzmann-weighted ensemble of configurations, or to generate classical-dynamical trajectories for molecular systems in the condensed liquid phase are briefly reviewed with an eye to application to biomolecular systems. After having chosen the degrees of freedom and method to generate molecular configurations, the efficiency of the search or sampling can be enhanced in various ways: (i) efficient calculation of the energy function and forces, (ii) application of a plethora of search enhancement techniques, (iii) use of a biasing potential energy term, and (iv) guiding the sampling using a reaction or transition pathway. The overview of the available methods should help the reader to choose the combination that is most suitable for the biomolecular system, degrees of freedom, interaction function, and molecular or thermodynamic properties of interest.

References: J. Comput. Chem. (2006) in press

Title: Catalytic mechanism of Cyclophilin as observed in molecular dynamics simulations: pathway prediction and reconciliation of X-ray crystallographic and NMR solution data

Researchers: Daniel Trzesniak
Wilfred F. van Gunsteren

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

Description:

Cyclophilins are proteins which catalyze X-proline cis-trans inter-conversion, where X represents any amino acid. Its mechanism of action has been investigated over the past years but still generates discussion, especially because until recently structures of the ligand in the cis and trans conformations for the same system were lacking. X-ray crystallographic structures for the complex Cyclophilin A and HIV-1 capsid mutants with ligands in the cis and trans conformations suggest a mechanism where the N-terminal portion of the ligand rotates during the cis-trans isomerization. However, a few years before, a C-terminal rotating ligand was proposed to explain NMR solution data. In the present study we use molecular dynamics (MD) simulations to generate a trans structure starting from the cis one. From simulations starting from the cis and trans structures obtained through the rotational pathways, the seeming contradiction between the two sets of experimental data could be resolved. The simulated N-terminal rotated trans structure shows good agreement with the equivalent crystal structure and, moreover, is consistent with the NMR data. These results illustrate the use of MD simulation at atomic resolution to model structural transitions and to interpret experimental data.

References: Prot. Sci. (2006) in press

Title: Biomolecular structure refinement based on adaptive restraints using local-elevation simulation

Researchers: Markus Christen
Bettina. Keller
Wilfred F. van Gunsteren

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

Description:

Introducing experimental values as restraints into molecular dynamics (MD) simulation to bias the values of particular molecular properties, such as nuclear Overhauser effect intensities or distances, dipolar couplings, ^{3}J-coupling constants, chemical shifts or crystallographic structure factors, towards experimental values is a widely used structure refinement method. Because multiple torsion angle values φ correspond to the same ^{3}J-coupling constant and high-energy barriers are separating those, restraining ^{3}J-coupling constants remains difficult. A method to adaptively enforce restraints using a local elevation (LE) potential energy function is presented and applied to ^{3}J-coupling constant restraining in an MD simulation of hen egg-white lysozyme (HEWL). The method succesfully enhances sampling of the restrained torsion angles until the 37 experimental ^{3}J-coupling constant values are reached, thereby also improving the agreement with the 1630 experimental NOE atom-atom distance upper bounds. Afterwards the torsional angles φ are kept restrained by the built-up local-elevation potential energies.

References: PNAS (2006) submitted with suppl. mat.

Title: Configurational entropy elucidates the role of salt-bridge networks in protein thermostability

Researchers: John H. Missimer[1]
Michel O. Steinmetz[1]
Riccardo Baron[2]
Fritz K. Winkler[1]
Richard A. Kammerer[3]
Xavier Daura[2,4]
Wilfred F. van Gunsteren[2]

Institute/ Group: [1]Paul Scherrer Institute, Villigen, Switzerland
[2]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[3]Faculty of Life Sciences, University of Manchester, Manchester, UK
[4]Universitat Autonoma de Barcelona, Bellaterra, Spain

Description:

Detailed knowledge of how networks of surface salt bridges contribute to protein thermal stability is essential not only to understand protein structure and function but also to design thermostable proteins for industrial applications. Experimental limitations, however, hinder examination of salt bridge networks and assessment of their energetic contribution to protein stability. Using explicit-solvent molecular dynamics simulations, we investigate here the stability of a short polypeptide designed to fold into a stable trimeric coiled coil with a well-packed hydrophobic core and an optimal number of intra- and interhelical surface salt bridges. We find that the increase of configurational entropy of the backbone and side-chain atoms and decreased pair correlations with increased temperature are consistent with nearly constant atom–positional root-mean-square fluctuations, increased salt-bridge occupancies and stronger electrostatic interactions in the coiled coil. Thus, our study of the coiled coil suggests a mechanism in which well-designed salt-bridge networks could accommodate stochastically the disorder of increased thermal motion to produce thermostability.

References: J. Mol. Biol. (2006) submitted with supporting material

Title: Molecular dynamics simulations of the native and partially-folded states of ubiquitin: influence of methanol cosolvent, pH, and temperature on the protein structure and dynamics

Researchers: David B. Kony
Philippe H. Hünenberger
Wilfred F. van Gunsteren

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

Description:

A series of explicit-solvent molecular dynamics simulations of the protein ubiquitin are reported, that investigate the effect of environmental factors (presence of methanol cosolvent in the aqueous solution, neutral or low pH value, room or elevated temperature) on the structure, stability and dynamics of the protein. The simulations are initiated either from the native structure of the protein or from a model of a partially folded state (A-state) that is known to exist at low pH in methanol-water mixtures. The main results of the simulations are: (i) the ubiquitin native structure is remarkably stable at neutral pH in water; (ii) the addition of the methanol cosolvent enhances the stability of the secondary-structure but weakens tertiary interactions within the protein; (iii) this influence of methanol on the protein structure is enhanced at low pH, while the effect of lowering the pH in pure water is limited; (iv) the Astate of ubiquitin can be described as set of relatively rigid secondary structure elements (a native-like β-sheet and α-helix plus two non-native α-helices) connected by flexible linkers.

References: Proteins (2006) submitted

Title: On using oscillating time-dependent restraints in MD simulation

Researchers: Bettina Keller[1]
Markus Christen[1]
Chris Oostenbrink[2]
Wilfred F. van Gunsteren[1]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Switzerland
[2]Vrije Universiteit, Amsterdam, The Netherlands

Description:

The use of time-dependent restraints in molecular simulation in order to generate a conformational ensemble for molecules that is in accordance with measured ensemble averages for particular observable quantities is investigated. Using a model system consisting of liquid butane and the cyclic peptide antamanide the reproduction of particular average ^{3}J-coupling constant values in a molecular dynamics simulation is analysed. It is shown that the multiple-valuedness and the sizeable gradients of the Karplus curve relating ^{3}J-coupling constants measured in NMR experiments to the corresponding torsional-angle values cause severe problems when trying to restrain a ^{3}J-coupling constant to a value close to the extrema of the Karplus curve. The introduction of a factor oscillating with time into the restraining penalty function alleviates this problem and enhances the restrained conformational sampling.

References: J. Biomol. NMR (2006) submitted

Title: Simulation of Global Climate and Climate Change with General Circulation Models

Researchers: Martin Wild
Andreas Roesch
Peter Tschuck
Martin Schraner
Atsumu Ohmura

Institute/ Group: Institute for Atmospheric and Climate Sciences ETH
Global Climate Modeling Group

Description:

The most powerful tools to investigate the sensitivity of the Earth's climate to anthropogenic perturbations are three dimensional numerical models of the climate system (GCMs). In the framework of National Competence Centre for Climate Research (NCCR Climate), we are maintaining and running a global climate model (ECHAM5) at the Swiss Centre for Scientific Computing (CSCS). Results of these simulation are currently entering the 4th assessment report of the UN-Intergovernmental Panel on Climate Change (IPCC AR4).
Currently we are in the process of porting the ECHAM5 to the Cray XT3 in Manno. Specifically, we use a research version of the ECHAM5, which includes a sophisticated aerosol scheme (HAM, Hamburg Aerosol Model). This modelling system allows an unprecedented assessment of the impact of changes in anthropogenic aerosol and greenhouse gas emissions on global climate. The ECHAM5-HAM simulations with detailed aerosol and cloud microphysics processes have the potential to reproduce various recently discovered variations in climate variables which have not been captured so far in GCMs. Amongst them are the reduction of sunlight received at the surface up to the mid 1980s ("global dimming") as well as its' recent recovery ("global brightening") (Wild et al. 2005), the related reversal in the surface radiative forcing of the global hydrological cycle from being negative between 1960 and 1990 to becoming positive thereafter, the associated decrease in land precipitation in the 1970s and 1980s with an increase thereafter, or, more regionally, the increase in Sahelian droughts in the 1970s and 1980s and a recovery thereafter. The successful simulation of these aspects of the climate system is a prerequisite for reliable projections of the related changes in scenario simulations over the coming decades. With the ECHAM5-HAM model, we intend to carry out simulations over the period 1950-2050. The aim is to first reproduce the main aspects of the variations of the components of global climate system over the past 50 years under observed forcings of aerosol and greenhouse gases, and then process to scenario simulations of the coming decades.

References: See separate list

Title: Simulation and Analysis of Blue Lasers

Researchers: Bernd Witzigmann
Valerio Laino
Mathieu Luisier
Dölf Aemmer

Institute/ Group: Integrated Systems Laboratory/
Computational Optoelectronics Group

Description:

We are analyzing novel generation blue lasers with the aid of microscopic multi-physics simulations. Blue semiconductor light emitters at around 400nm are fabricated in the Gallium-Nitride material system. The optical and electronic properties of this material are not yet fully understood. We are developing theoretical models and computer aided design tools in order to analyze measured characteristics and gain understanding about the structural aspects and material parameters. In particular, the electroluminescence has been investigated using a quantum-kinetic many-particle program that has been developed in our group. This rigorous theory allows extracting information about the material quality and composition by comparison to measurement. Moreover, the sources of losses in the optical waveguide are another subject of investigation. Here, an in-house finite-element software to solve the vectorial Maxwell equations with open boundary conditions is employed and customized.

References:

In 2005 and 2006 seven papers in reviewed journals were published on the topic of blue lasers.

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:
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.

Pérez, D.R. and Wüthrich, K.
NMR assignment of the Xenopus laevis prion protein fragment xlPrP(98-226)
J. Biomol. NMR **31** (2005), 260

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: 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

At the 2005 Annual Workshop on November 24, C4 completed its first year under the new Steering Committee consisting of Dr. Wanda Andreoni (IBM Zürich Research Laboratory), Prof. Jürg Hutter (University of Zürich), Prof Wilfred F. van Gunsteren and PD Dr. Hans P. Lüthi (both ETH Zürich).

The Workshop was held in a new format which caters to more scientific excitement as well as to a greater exchange between the ever increasing C4 community. For that matter, the Computer Aided Drug Design Group of the Novartis Corporation was invited as a guest. Among other, the Novartis researchers, lead by Dr. Richard Lewis and Prof. Manuel Peitsch, formed the jury that visited the nearly thirty posters presented by the C4 community, granting awards to the best presentations and the best presenters. The guest of the 2006 Workshop will be the Kenneth Pitzer Center for Theoretical Chemistry of the UC Berkeley (January 4 and 5, 2007).

In the past year, C4, for the first time, offered tutorials on advanced topics of molecular modeling and simulation. In October 2005, Jürg Hutter and Marcella Iannuzzi presented a one-week tutorial on Car-Parrinello Molecular Dynamics. In October 2006, the second C4 tutorial was on the topic of dynamical electron correlation, presented by Dr. David Tew and Prof Wim M. Klopper of the University of Karlsruhe. Both tutorials were presented by leaders in the respective fields, giving the participants, close to 30 in number, insight into the state-of-the-art and the future perspectives 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 14 lectures, presented by researchers from academia (12) and from industry (2). The seminars, that take place every second Thursday during the semester, enjoy a remarkable popularity: thirty to fifty attendants is the “normal crowd”.

In April 2006, C4 inaugurated its new compute-resource, a 32 node Opteron cluster consisting of two dual-core CPUs from IBM. Four of the nodes are “fat nodes” with 16 GBytes of memory and 600 GBytes of local disk storage; the other nodes have 8 and 128 GBytes of memory and external storage, respectively. Obélix and the boars (i.e. the server and the compute nodes) are operated by the ETH Zürich Informatikdienste. This resource allows running computations or production campaigns difficult to execute on other resources.

The goals of C4, namely to seek new frontiers and opportunities in molecular modeling and simulation, to cater to the flow of know-how, to be a major contributor towards computational science for the participating institutions, and to serve as a platform for the interaction with external partners resulted in a “return on investment” of nearly scientific 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 C4 and CS&E community.

Hans P. Lüthi
October 31, 2006

6.2 CSCS – Swiss National Supercomputing Centre

Swiss National Supercomputing Centre
Galleria 2 – Via Cantonale
CH-6928 Manno (Switzerland)

High Performance Computing in Switzerland

CSCS is the Swiss National Supercomputing Centre, providing, developing and promoting technical and scientific services for the Swiss research community in the fields of high-performance and high-throughput computing.

The Steering Board of CSCS, that oversees the activities of the centre and guides it in accordance with the performance agreement set out in 2004, was initially elected for 2 years. ETH-Board confirmed all members of the Steering Board for the next 2-year period in December 2005. At the same time Prof. Ulrich Suter stepped down as Vice President of Research to be replaced by Prof. Dimos Poulikakos. We look forward to working with the new Vice President over the coming years.

The newly formed Scientific Review Committee met in Zurich in October for the scientific evaluation of the 44 submitted projects. During 2005 the CSCS resources served 38 large projects from most academic institutions of Switzerland. The acquisition of the Horizon system allowed us to form a working partnership with the Paul Scherrer Institute (PSI) leading to an enriching and challenging exchange between the two institutions. Other existing partnerships with CERN's LCG project and the Swiss Bio Grid have continued to unfold throughout the year. We were also able to sign a new contract with MeteoSwiss for the continued support of their compute needs by CSCS. CSCS has continually been involved with educational activities, workshops and conference activities throughout 2005 – confirming the trend set out in the previous year. 2006 will see these activities progress further.

In order to maintain the level of compute power equivalent to the worldwide ranking of ETH and the quality science performed in Switzerland CSCS put out a request for purchase (RFP) under the code name of "Terrane", published with agreement of the Steering Board in September, that would complement the existing architectures available at CSCS and replace the outgoing technology. Terrane system will go into production in 2nd half of 2006.

Mid 2006 CSCS lauched the call for proposals for a new application scheme called ALPS (Advanced Large Projects in Supercomputing) to enable scientific breakthroughs by offering large amounts of CPU and collaborative support. 8 projects were proposed, 3-4 may be considered for this new scheme.

Figure 1: CSCS' Infrastructure

HPC technology development

The main activities of the Technical and Operational Services Section have been
- the operation and maintenance of our HPC servers, data management and storage systems, networks, and dedicated pre- and post-processing systems
- the commissioning and testing of the new Cray XT-3 HPC and the new IBM SP5 server
- improvements to the capability, accessibility, and availability of CSCS' infrastructure.

All our HPC servers are now accessible through a new front-end computer. Besides providing increased compute power and storage, the new CSCS front-end provides world-wide accessibility through a secure SSH connection to our computing resources as well as to all related documentation and real-time information on the status of all resources.

In addition to the existing communication line to Zurich, SWITCH, the operator of the Swiss education and research network, has installed a new line connecting Manno to Lausanne. The new line improves the availability and reliability of our connection to our users. Preliminary tests on operating these connections at a speed of 10GB/s have been made in preparation for increased future requirements.

The CSCS-internal network has been adapted to meet new requirements of the grid community. New security requirements stem from the fact that – contrary to the users of our HPC servers – not all members of a grid community are known and registered with CSCS.

The throughput and stability of our archive system have been improved through the addition and reconfiguration of high speed/high capacity tape drives. The performance for small files and for multiple file access in a directory has been significantly improved through the installation of a SamFS/QFS disk archive.

We have installed group videoconferencing equipment allowing us to strengthen communication with some of our user communities. In order to streamline this communication, we have also reorganized all user data and consolidated it in a single database.

Finally, fast computers consume plenty of power and produce plenty of heat. In order to meet the gross power and cooling requirements of the Cray XT-3 installed in 2005 and of the IBM SP5 server in 2006, we have increased the power supply of CSCS from 750kVA to 1200kVA. The capacity of the backup battery system has been increased accordingly.

Development of the high-performance computing infrastructure

2005 was a milestone in the development of the computing infrastructure at CSCS. The procurement project Horizon started in autumn of 2004 and ended with the delivery of a Cray XT3. This massively-parallel computer, the first installation of its kind in Europe and the fourth in the world, consists of 1'100 AMD Opteron processors, which are interconnected by a custom very high-bandwidth, low-latency network with a 3D-torus topology. The new computer is able to deliver 5.8 Tflops or 5.8 trillion floating point calculations per second. It offers a total memory of 2.2 TBytes and a global shared parallel file system of 28 TBytes. It operates a special software stack, including a micro-kernel on the compute part of the system, which yields very high efficiency for computational experiments involving hundreds or thousands of processors in parallel. Horizon went through a period of intense testing and verifications by CSCS and a large number of pilot users in late 2005, and it finally went into general production in January 2006.

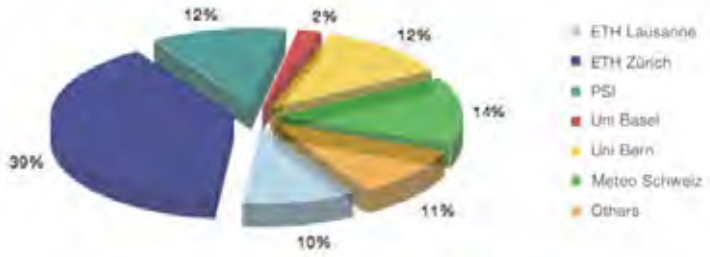
With Horizon, CSCS has entered a new level of parallel computing, going from tens of processors on the previous NEC and IBM computers, to up to 1'000 processors per single experiment. This new level of parallelism enables CSCS' researchers to carry out scientific research they were not able to do before. Already during the pre-production period in 2005, two research groups working with CSCS reported that they have run computational experiments they could not run before. New users, coming from new institutions, have applied to work on Horizon and we expect exciting scientific results from this machine in the near future.

As Horizon significantly extended the capabilities of CSCS computing infrastructure, the next development step was designed to increase the capacities of the systems of the centre. CSCS identified the importance of offering our users compute facilities for a lower level of parallelism, with some shared memory capacity, and with a high level of compatibility to other systems. Thus, CSCS stays flexible and open in terms of technology and application portfolio and it has economic solutions for all kinds of computational needs. The strategy also takes into account the fact that every computational research project, even if targeted at running big, massively parallel experiments, requires heavy computational resources on a lower level of parallelism for preparing, validating, and complementing the large-scale experiments. If a proposed research project is evaluated by the CSCS Scientific Review Committee as scientifically sound and to be supported, CSCS must offer the full spectrum of services for fulfilling all computational requirements of the project. Of course, resources of lower-level parallelism are also available at other institutions in Switzerland. CSCS will therefore not cover the full national need for these kinds of facilities but share this offer with compute services at the universities and research sites.

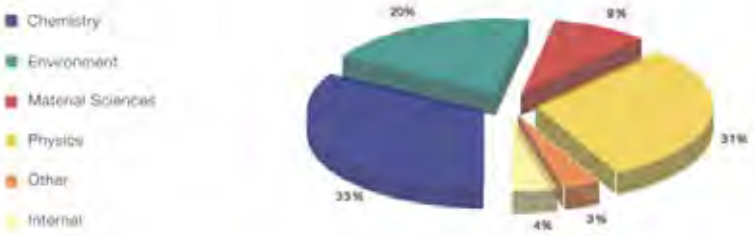
Consequently, CSCS launched the Terrane procurement with a public call for tender in late 2005. In addition to the requirements concerning the level of parallelism, we targeted a system that has some shared memory capacity, offers a sound performance per node, i.e. strong single processors, and is easy to use and to migrate to. Therefore, we followed our strategy already published in the Annual Report 2004, which envisaged a system of current HPC market standards to be inserted into CSCS' HPC portfolio in 2006. The Terrane project was awarded to a 768 processor IBM Power-5-system. It arrived at CSCS in the summer of 2006 and will be open to our users for early access, porting, and testing from October to December 2006.

Facts & Figures 2005

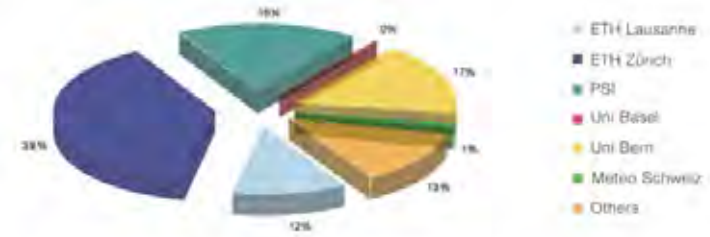
Cost of machines per institution based on direct costs during reporting period



Cost of machines per discipline based on direct costs during reporting period

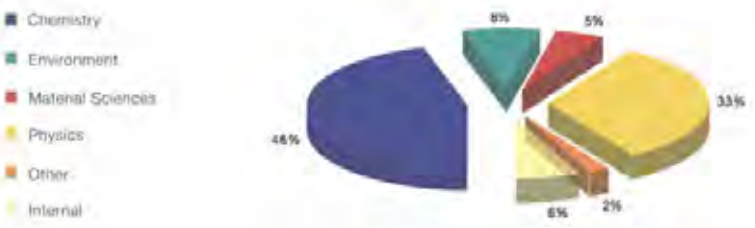


Share of cooperate resources based on produced CPU hours per institution during the reporting period



the field «others» includes broaching, testing and benchmarking of XT3

Share of cooperate resources based on produced CPU hours per discipline during the reporting period



List of Large User Projects 2005

Name	Organiszation	Project Title
Arbenz P.	ETH Zürich	Large scale eigenvalue problems in opto-electronic semiconductor lasers and accelerator cavities
Baiker A.	ETH Zürich	Hydrogenation reactions in heterogeneous enatioselective catalysis and homogeneous catalysis in supercritical CO_2
Bakowies D.	ETH Zürich	Atomizations energies from ab-inition calculations without empirical corrections
Beniston M.	Uni Fribourg	Global and regional climate modelling
Besson O.	Uni Neuchâtel	Numerical solution of Navier Stokes equation in shallow domains
Bey I.	EPF Lausanne	Coupling tropospheric chemistry and aerosols in the general circulation model ECHAM
Bürgi Th.	Uni Neuchâtel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper W.A.	EPF Lausanne	Computation of stellarator coils, equilibrium and stability
Deubel D.	ETH Zürich	Quantum chemical studies on the interaction of anticancer drugs with biological targets
Fäh D.	ETH Zürich	Numerical modelling of seismic local effect estimation on complex sites
Fichtner W.	ETH Zürich	Computational science and engineering in microelectronics and optoelectronics
Folini D.	EMPA	Inverse modeling to monitor source regions of air pollutants in Europe
Hasenfratz P.	Uni Bern	Chiral symmetric dirac oparator in lattice QCD
Hauser A.	Uni Genève	Photophysics and photochemistry of transition metal compounds: Theoretical Approaches
Helm L.	EPF Lausanne	Iperfine interaction anysotropy on first and second coordination sphere water molecules, in paramagnetic metal ion solutions
Hutter J.	Uni Zürich	Development and application of ab-initio molecular dynamics methods
Jakob A.	PSI	Molecular modelling of radionuclide mobility and retardation in clay minerals
Joos F.	Uni Bern	Carboclime: modelling carbon cycle climate feedbacks
Keller J.	PSI	Air quality modeling in Switzerland
Kleiser L.	ETH Zürich	Numerical simulation of transitional, turbulent and multiphase flows

Name	Organization	Project Title
Koumoutsakos P.	ETH Zürich	Simulations using particle methods optimization of real world problems using evolutionary algorithms multiscale modelling, simulations and optimization of complex systems
Leriche E.	EPF Lausanne	Direct numerical simulation ot the buoyancy-driven turbulence in a cavity: the DNSBDTC project
Leutwyler S.	Uni Bern	Proton and hydrogen atom transfer in solvent clusters and nucleic acid base pairs: theory and dynamics
Leyland P.	EPF Lausanne	Large scale simulation for aerospace applications
Lohmann U.	ETH Zürich	Effect of aerosols on clouds and climate
Lüthi H.P.	ETH Zürich	Computational quantum chemistry of large molecules
Meuwly M.	Uni Basel	Electronic structure calculations for molecular dynamics simulations of iron-containing, reactive centers of biomolecules. Theoretical investigations of iridium-catalyzed reactions.
Oganov A.	ETH Zürich	Computational mineral physics and cristallography
Ohmura A.	ETH Zürich	Global climate change: modelling climate variability on decadel time scales
Parlange M.B.	EPF Lausanne	Large eddy simulation of atmospheric boundary layer flow over complex terrain
Parinello M.	ETH Zürich	Simulating chemical reactions with Car-Parrinello metadynamics
Pasquarello A.	EPF Lausanne	Disordered network-forming materials
Posternak M.	EPF Lausanne	Computational physic in condesed matter
Poulikakos D.	ETH Zürich	Biothermofluidics for Cerebrospinal fluid diagnostic and control-development of a knowledge base Explosive vaporization phenomena in microenclosures
Röthlisberger U.	EPF Lausanne	Mixed quantum mechanics / molecular mechanics study of systems of biological interest
Samland M.	Uni Basel	The Milky way and its satellite warf galaxies
Schär Ch.	ETH Zürich	Modelling weather and climate on european and alpine scales
Sennhauser U.	EMPA	Nanoxid
Stocker Th.	Uni Bern	Monalisa: modelling and reconstruction of north Atlantic climate system variability

Name	Organization	Project Title
Van Lenthe H.	ETH Zürich	Identifying genetic determinats of bone strengh - a high troughput phenomics approach in mice
Van Swygenhoven H.	PSI	Molecular dynamics computer simulation of nanostructured materials
Vogel P.	EPF Lausanne	New organic chemistry with sulfur dioxide. Electron releasing homoconjugated carbonyl group

Papers published by CSCS in 2005

Favre J., Foggia Th., Garcin H., Parkinson E. % Braune A.; Simulation of a full Pelton turbine, Return on experience & Handling of large data sets, 23rd CADFEM Users' Meeting 2005

Marmo R., Valle M.; Visualizzazione scientifica: un aiuto per capire, Mondo Digitale, AICA, n. **4**, December 2005, p. 45–58

Valle M.; STM3: a chemistry visualization platform, Zeitschrift für Kristallographie Vol. **220** (2005) Issue 5-6 Pages, 585-588

Valle M., Favre J., Parkinson E., Perrig A. & Farhat M.; Scientific Data Management for Visualization Implementation Experience, Simulation and Visualization 2005 Magdeburg, March 3 – 4, 2005

The Swiss ATLAS Computing Prototype. By S. Gadomski, C. Haeberli, F. Orellana, G.L.Volpato. May 2005. 18pp. ATLAS Note: ATL-SOFT-PUB- 2005-003; CERN-ATL-COM-SOFT-2005-007.

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6.3 Information Technology Services

The following resources are available:

- Hewlett Packard Superdome Cluster consisting of
    - 1 HP Superdome (Stardust): 64 Itanium2 CPUs (1500 MHz), 128 GB Memory, 400 GB local Disk, 2 TB SAN Disk, HP/UX Operating System
    - 1 HP Superdome (Pegasus): 32 Itanium2 CPUs (1500 MHz), 64 GB Memory, 400 GB local Disk, 2 TB SAN Disk, 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 two Beowulf Clusters co-owned with the Departments Biology, Environmental Sciences, Physics, Mathematics, Material Sciences and Computer Science. One cluster (“Hreidar”) consists of 188 dual processor AMD Opteron 244 systems with 4 GB memory and Ethernet network, the other (“Gonzales”) consists of 288 dual processor AMD Opteron 250 systems with 8 GB memory and Quadrics High Bandwidth/Low Latency network. During the course of

2007 the Gonzales cluster will be extended by approximately 600 CPUs and the Hreidar cluster by 150 CPUs. 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 cluster is 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 we see already the second group of students entering the Master program in CSE. As procedures for accepting students from outside ETH had not been in place in the period of this report we did not advertise the Master program. However, we have set up a body to handle the admission of students from outside ETH. Hence we shall advertise our CSE Master program in the next year and we expect to receive a larger international student body next fall. As the curriculum becomes more international the course material will have to be more and more in English and of course the lectures as well. The tailoring of courses to the needs of students in CSE will continue.

We are planning for a small, more workshop like, conference with our first group of Master students and scientists involved in CSE and its teaching in summer of 2007 to assess the Bachelor and the Master program. This will give us the necessary feedback to optimize our programs.

Together with colleagues of the University of Zürich we are organizing the International Congress on Industrial and Applied Mathematics, ICIAM 2007, which will be held in Zürich, July 16 -20. A considerable part of this congress will cover also the CSE domain. You find more of the program already now on the web, http://www.iciam07.ch/. This web page is constantly updated, so visit it frequently. In particular there will be industrial days where researchers from industry will present their problems and researchers from academia will present solution tools, case studies and so on. There will also be a minisymposium on CSE where many leaders in these curricula, especially from Europe will report on what is done elsewhere. In addition, there will be students reporting on their experience. To celebrate Euler's 300 anniversary there will be an Euler lecture.

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 19, 2006
Rolf Jeltsch

8

Publications* in 2005/2006

*only CSE-related articles
in refereed journals

Group of G. Blatter

H. G. Katzgraber and G. T. Zimanyi
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Phys. Rev. B **74**, 020405(R) (2006)

H. G. Katzgraber, S. Trebst, D. Huse, and M. Troyer
Feedback-optimized parallel tempering Monte Carlo
J. Stat. Mech P03018 (2006)

H. G. Katzgraber, M. Körner, and A. P. Young
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Phys. Rev. B **73**, 224432 (2006)

M. Körner, H. G. Katzgraber, and A. K. Hartmann
Probing tails of energy distributions using importance sampling in the disorder with a guiding function
J. Stat. Mech P04005 (2006)

O. Gygi, H. G. Katzgraber, M. Troyer, Stefan Wessel, and G. G. Batrouni
Simulations of ultracold bosonic atoms in optical lattices with anharmonic traps
Phys. Rev. A **73**, 063606 (2006)

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Ramping fermions in optical lattices across a Feshbach resonance
Phys. Rev. A, accepted (cond-mat/0510194).

L. W. Lee, H. G. Katzgraber, and A. P. Young
Critical behavior of the three- and ten-state Potts glass
Phys. Rev. B, accepted (cond-mat/0605010)

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Temperature and Disorder Chaos in three-dimensional Ising Spin Glasses
Phys. Rev. Lett., submitted (cond-mat/0606180)

D. Würtz and H. G. Katzgraber
Precise finite-sample quantiles of the Jarque-Bera adjusted Lagrange multiplier test
Econ. Lett. Submitted (math.ST/0509423).

Group of S. Bonhoeffer

Brandin, E, Thorstensson, R, Bonhoeffer, S, Albert, J
Rapid viral decay in simian immunodeficiency virus-infected macaques receiving quadruple antiretroviral therapy
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High epitope expression levels increase competition between T cells
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Novak, M, Pfeiffer, T, Lenski, RE, Sauer, U, Bonhoeffer, S
Experimental tests for an evolutionary trade-off between growth rate and yield in E-coli
AMERICAN NATURALIST (2006) 168:242-251

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Mutation accumulation in space and the maintenance of sexual reproduction
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Regoes, RR, Bowen, EF, Cope, AV, Gor, D, Hassan-Walker, AF, Prentice, HG, Johnson, MA, Sweny, P, Burroughs, AK, Griffiths, PD, Bonhoeffer, S, Emery, VC
Modelling cytomegalovirus replication patterns in the human host: factors important for pathogenesis
PROCEEDINGS OF THE ROYAL SOCIETY B-BIOLOGICAL SCIENCES (2006) 273:1961-1967

Kouyos, RD, Otto, SP, Bonhoeffer, S
Effect of varying epistasis on the evolution of recombination
GENETICS (2006) 173:589-597

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Emergence of drug-resistant influenza virus: Population dynamical considerations
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Stable virulence levels in the HIV epidemic of Switzerland over two decades
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Salathe, M, Scherer, A, Bonhoeffer, S
Neutral drift and polymorphism in gene-for-gene systems
ECOLOGY LETTERS (2005) 8:925-932

Brandin, E, Brostrom, C, Gille, E, Bonhoeffer, S, Albert, J
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AIDS RESEARCH AND HUMAN RETROVIRUSES (2005) 21:608-610

Pfeiffer, T, Soyer, OS, Bonhoeffer, S
The evolution of connectivity in metabolic networks
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Evolution of cooperation by generalized reciprocity
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TRENDS IN MICROBIOLOGY (2005) 13:269-277

Muller, V, Bonhoeffer, S
Guanine-adenine bias: a general property of retroid viruses that is unrelated to host-induced hypermutation
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The evolution of groups of cooperating bacteria and the growth rate versus yield trade-off
MICROBIOLOGY-SGM (2005) 151:637-641 Request reprint

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Epitope down-modulation as a mechanism for the coexistence of competing T-cells
JOURNAL OF THEORETICAL BIOLOGY (2005) 233:379-390

Funk, GA, Jansen, VAA, Bonhoeffer, S, Killingback, T
Spatial models of virus-immune dynamics
JOURNAL OF THEORETICAL BIOLOGY (2005) 233:221-236

Group of K. Boulouchos publications

C.E. Frouzakis, A.G. Tomboulides, P.F. Fischer, P. Papas, R.M. Rais, P.A. Monkewitz, K. Boulouchos, Three-dimensional numerical simulations of cellular jet diffusion flames, *Proc. Combust. Inst.*, **30**, 185–192, (2005).

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Thermodynamic theory of incompressible hydrodynamics,
Phys. Rev. Lett. **94 (8)**, 80602 (2005).

S. Ansumali, I. V. Karlin, C. E. Frouzakis and K. B. Boulouchos,
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Physica A **359**, 289305 (2006).

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