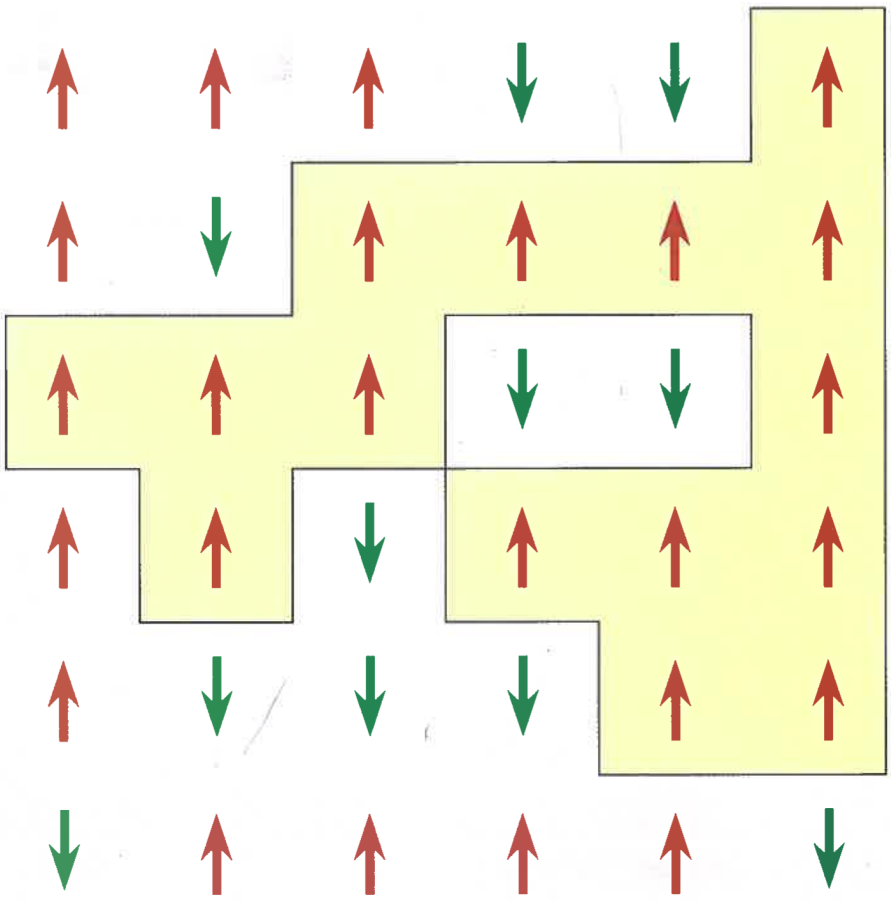
CSE

Computational Science and Engineering

Annual Report
2001/2002



Eidgenössische Technische Hochschule Zürich

CSE

Computational Science and Engineering

Annual Report 2001 / 2002

July 2001 to July 2002

Impressum:

Editors:

Rolf Jeltsch, Kaspar Nipp, Wilfred van Gunsteren
ETH Zürich

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Cover:

Snapshot of a spin configuration of the two-dimensional Ising model close to the phase transition to an ordered magnetic phase. Standard local updates, flipping one spin at a time are very inefficient in changing the structure of large aligned domains. Cluster updates, flipping large clusters - such as the one marked in yellow - are more efficient by many orders of magnitude and allow accurate simulations of phase transitions in magnetic systems.
(By Matthias Troyer, Institute of Theoretical Physics, ETH Zürich.)

Printing:

Fröhlich Druck AG, www.froehlich.ch

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Introduction

This is the second Annual Report of Computational Science and Engineering, CSE, at the ETH. The first one has been a success and it was rather useful to show all persons interested in research and education in CSE, students and colleagues, visitors and people form other universities, 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.

The ETH went ahead with the implementation of the "Strategische Erfolgs-Position", SEP, in Computational Science and Engineering by founding the Computational Laboratory (CoLab) in June 2002. Its director is Professor Petros Koumoutsakos and as Scientific Coordinator Dr. Sabine Attinger has been hired. A program for Postdoctoral Students has been started and the first participants took up their research this fall. For more information see the web page http://www.colab.ethz.ch.

The other major event was the decision by the rector, Prof. K. Osterwalder, to ask for a redesign of the current curriculum in CSE ("Rechnergestützte Wissenschaften") into a Bachelor and a Master program in CSE. At first glance, the major ingredient of the planned change is that students enter the Bachelor program after one year of basic studies and achieve a Bachelor of Science in CSE after an additional four semesters. The Master program builds upon this education and comprises two semesters of studies and a Master thesis of four months. Hence, the overall time covered by the CSE program remains the same, although significant changes have been made. Due to the support by the rector it will be possible to create a number of new courses which are more taylored towards the CSE students. It is planned that in the fall of 2003 the first students will enroll in the new Bachelor program.

At this point we thank the Schulleitung for supporting CSE in research and education. In particular, we thank the rector, Professor K. Osterwalder, and the Vicepresident Research, Professor U.W. Suter, for their financial support to produce this report. Moreover, we thank all those at the ETH who have contributed to this report.

Zürich, October 20, 2002
Rolf Jeltsch, Fachberater und Mitglied des Ausschusses Rechnergestützte Wissenschaften

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Education

For the winter semester 2002/2003 it was planned to establish a Bachelor/Master program in CSE. Unfortunately, this program may not be started this fall. The Rektor of the ETH only admitted a few Bachelor/Master pilot programs all starting with the first year. The major objection was that the general ETH regulations concerning Bachelor/Master programs had not been worked out until late this summer.

Instead of adopting a CSE Bachelor/Master program a minor reform of the CSE curriculum has been implemented. A new course 'Computational Statistics' has been added to the CSE core courses and a new application area 'Astrophysics' has been established. It is run by the Institute of Astrophysics of the University of Zurich under Professor Ben Moore. Moreover, the number of 'gap exams' to be taken by each student has been reduced from three to two.

The Bachelor/Master program in CSE is planned to be implemented in the winter semester 2003/2004 beginning with students in their second year having done their first year studies in one of the following fields: mechanical or electrical engineering, computer science, chemistry, mathematics, physics. The Bachelor studies will take two more years and will result in a Bachelor of Science ETH in CSE. The Master studies building upon a Bachelor in CSE will take one and a half years including the 4 months of the Master thesis and will lead to a Master of Science ETH in CSE. The courses in the Master program are planned to be given in English and it is hoped to attract excellent students from abroad to this program.

In the academic year 2001/2002 15 new students have resumed their CSE studies at ETH; 13 of those students had taken their basic studies at ETH, 1 at the Fachhochschule Burgdorf and 1 at the Fachhochschule Rapperswil in the following fields: Mathematics 1 student, Physics 5, Computer Science 3, Mechanical Engineering 3, Electrical Engineering 1, Environmental Sciences 2. The presentation of the CSE curriculum for ETH students of the 4-th semester of May 28 attracted around 50 persons. It is hoped that a fair number of them will start with the CSE studies this fall.

In the past academic year 3 students have successfully finished their CSE studies and have received a CSE diploma, one of them with distinction. They chose the following fields of specialization: Robotics, Software Engineering and Theoretical Physics. In the following list we give the name of the students, the title of the diploma thesis and the name and the institute of the adviser.

Diploma Theses

S. Benkler	Numerical Solutions of the Nonlinear Hartree Equation (M. Troyer and J. Fröhlich, Theoretical Physics)
K. Meyer	Optimale Impulssteuerung eines unteraktuierten Roboters (C. Glocker, Mechanical Systems)
F. Scheurer	Mehragentenplanen mit Hilfe von Model-Checking-Methoden (A. Biere and T. Gross, Computer Systems)

The total number of CSE students enrolled in the past academic year was 26. Listed below are the term papers written by the CSE students in the past two semesters.

Term Papers

A. Adensamer	Molecular dynamic simulation in carbon nanotubes (P. Koumoutsakos, Computer Science)
A. Adensamer	Simulation von Wasserstoff auf Palladiumoberflächen (M. Troyer, Theoretical Physics)
M. Bergdorf	Polarization around ions in a dielectric continuum (W. van Gunsteren, Computational Chemistry)
M. Bergdorf	Application of self-organizing feature maps to turbulent flow simulations (P. Koumoutsakos, Computer Science)
A. Burri	Dynamik von Kreuzungen in Verkehrssimulationen (K. Nagel, Scientific Computing)
A. Jost	Semantische Kategorisierung von Bildern (B. Schiele, Scientific Computing)
U. Kalatchoff	3D and 2D tracking of a motion point with fixed cameras (P. Verschure, Neuroinformatics)
M. Köpfli	Krylow-Methoden für Systeme mit mehreren rechten Seiten (M. Gutknecht, Applied Mathematics)
R. Lauper	gFEM for periodic lattice materials (C. Schwab, Applied Mathematics)
R. Lauper	Editierbare Kamera-Animation für AVS und Anwendung auf CFD-Daten einer Benzinpumpe (M. Gross, Scientific Computing)
S. Müller	Analyse von Marktpreisen für Elektrizitätsoptionen mit Hilfe von Neuronalen Netzwerken (J. Benasconi, ABB)
M. Rütti	Design und Implementation einer Matlab-Toolbox für orthogonale Polynome und Gauss-Quadraturformeln (W. Gander, Scientific Computing)
G. Stark	Maximum entropy data analysis (M. Troyer, Theoretical Physics)
G. Widmer	Optimales inverses Design (R. Jeltsch, Applied Mathematics)

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 19, 2002
Kaspar Nipp, Mitglied des Ausschusses Rechnergestützte Wissenschaften

For detailed information on the Diploma Studies in CSE at the ETH Zürich see:
http://www.cse.ethz.ch

3
CSE Case Studies Seminar

The CSE Case Studies Seminar takes place each semester on Thursdays, 15 - 17 hours. Speakers from ETH, from other universities as well as from industry are invited to give a 2x45 minutes talk on an applied topic. The idea is to show the students a case study of an application problem containing the problem setting, the modelling, the mathematical approach and the simulation on a computer. In addition, such a case study should show what is going on in the field of CSE and what are the job perspectives for a CSE engineer. The seminars of the past academic year are given in the two following lists.

Case Studies Seminar WS01/02

1. 11. 01	E. Kissling, Geophysik Seismic Tomography
8. 11. 01	Xavier Daura, Informatikgestützte Chemie Computer Simulation in Biochemistry
15. 11. 01	L. Scapozza, Pharmazeutische Biochemie Computational Science within Life Sciences
22. 11. 01	F. Kappel, Universität Graz Modellierung des Herz-Kreislaufsystems
6. 12. 01	W. Benz, Physikalisches Institut der Uni Bern Formation and Evolution of Planetary Systems
10. 1. 02	A. Troxler, Seminar für Angewandte Mathematik Aerodynamisches Design von Gasturbinenkomponenten
17. 1. 02	W. Flury, Esoc / ESA, Darmstadt Optimierung von interplanetaren Bahnen mit solar-elektrischem Antrieb und Gravity Assists
24. 1. 02	Jochen Maurer, Time-steps, Affoltern am Albis Pricing and Risk Analysis of Energy Portfolios

Case Studies Seminar SS02

11. 4. 02	J. Häuser, CLE Gmbh., Salzgitter, Deutschland Computer Simulation for Rocket Design and Launching
18. 4. 02	A. Gusev, Polymere Computer-aided Design of Advanced Structures from Short Fiber and Platelet Reinforced Materials
25. 4. 02	A. Prohl, Seminar für Angewandte Mathematik Mikromagnetismus – Modellierung und Numerik
2. 5. 02	P. Flohr, Alstom Ltd., Baden Dättwil CFD Analysis for Industrial Gas Turbine Combustors
16. 5. 02	P. Hasenfratz, Theoretische Physik, Uni Bern Quarks, Gluons and Hadrons on the Lattice
13. 6. 02	A. Biland, Teilchenphysik Simulation, Rekonstruktion und Analyse grosser Experimente
20. 6. 02	S. Stolz, Fluiddynamik Large Eddy Simulation Based on Approximate Deconvolution

4
Computational Highlight

Computational highlight
Simulations of classical and quantum phase transitions

by M. Troyer, Theoretische Physik, ETH Zürich

Introduction

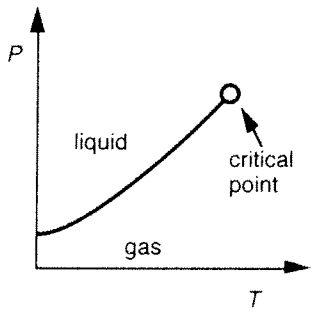
The simulation of phase transitions is one of the big challenges for numerical simulations, for two reasons: when going across the phase transition we need to change the nature of the system throughout our simulation volume – which is hard by itself – while at the same time the relevant length scales diverge and huge systems need to be studied. These challenges are worth tackling however for a unique reason that makes these simulations very rewarding: the properties at second order phase transitions are universal, meaning they do not depend on the microscopic details of the model or material. Simulations of a simplified toy model will, as long as the symmetries are correct, give results that are directly and accurately applicable to a large class of materials, without worrying about material details!

The simulation of classical phase transition has a history of half a century, dating back to the seminal paper of Metropolis and coworkers[1] in 1953. Algorithmic breakthroughs in classical system in the past twenty years, and for quantum systems in the last decade now allow highly precise simulations and provide a stringent checks on analytical.

Here I want to present an overview of the history of this field, the challenges that were overcome and those that remain. I will not go into deep technical details and the article should be understandable to all computational scientists and engineers.

Statistical mechanics and phase transitions

Statistical mechanics is a branch of physics going back to the late 19th century as a microscopic foundation for thermodynamics. It explains that the macroscopic behavior of systems, such as gases, solids and liquids (which are phenomenologically well described by thermodynamics) can be explained microscopically if only we could exactly calculate the movement of all particles. For ideal or weakly interacting gases it is indeed possible to analytically derive the laws of thermodynamics based on such microscopic models. Attention has then shifted to explaining the nature of *phase transitions* between these different states of matter. In many cases the phase transitions are of "*first order*". Let us consider a gas-liquid system starting in the liquid phase. When changing a control parameter, such as increasing the temperature or decreasing the pressure, the free energy of the gas drops with respect to that of the liquids. Once the free energy of the gas becomes lower than that of the liquid, the liquid evaporates to a gaseous state in a phase transition. This discontinuous phase transition is characterized by a coexistence of both phases (gas and liquid or liquid and solid) at the phase transition. While the free energy is continuous at the transition, its derivatives are not, hence the name "first order" transition since the first derivatives of the free energy are discontinuous.

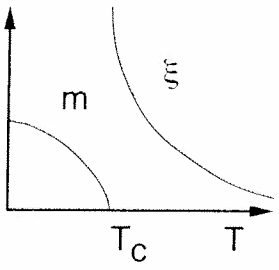


Let us next follow this first order phase transition by raising the temperature and tuning the pressure such as to always stay on the phase transition line. The difference between liquid and gas will become harder to observe and finally the phase transition line ends

[1] N.Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H.Teller and E.Teller, J. Chem. Phys. **21**, 1087(1953).

at a critical endpoint where distinction between gas and liquid disappears (see the figure on the right). At this point the phase transitions has changed its nature from a first order to a "*second order*" phase transition with intriguing universal features. The name "second order" stems from the fact that the first derivatives of the free energy are still continuous and only the second derivatives are discontinuous.

Universal behavior at second order phase transitions



In experiments in the late 19th century it was realized that the physical properties in the vicinity of such a second order critical point do not depend on the specific details of the system but are *universal*. When comparing measurements of physical properties, such as the compressibility, for a large number of liquids and gases it was found that, while the location of the critical point (the critical temperature and pressure) were different for each material, the *behavior in the vicinity of the critical point was the same for all materials!*

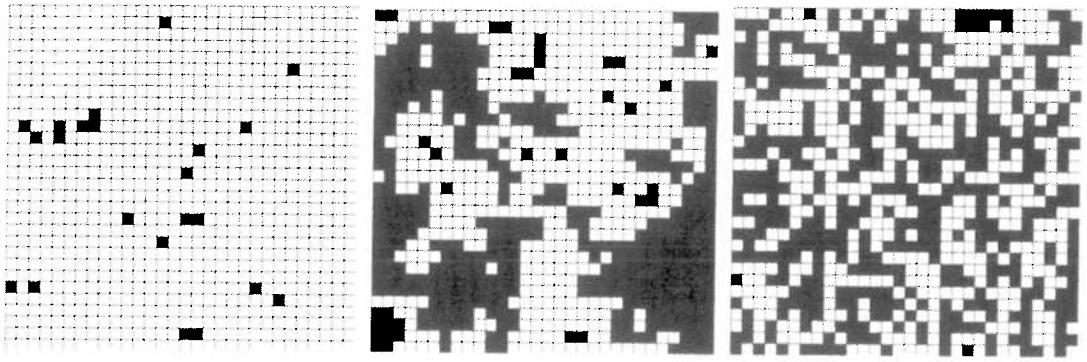
While this universal behavior was first discovered in the liquid-gas system it is much easier to investigate and more common in magnetic systems. In all magnets, including iron, nickel and others, the magnetization m vanishes in the same way as the temperature T is increased and approaches the critical temperature T_c, following a power law behavior (see the figure above):

$$m \propto (T_c - T)^{\beta} \qquad (1)$$

While the proportionality constant and T_c depend on the material, the "*critical exponent*" β is universal and does not depend on the material, but only on the dimensionality and on the symmetry of the magnetic order! When approaching the critical temperature from above, the magnet starts to order also in a universal way. Small locally ordered domains grow. Their size is given by the correlation length ξ, which diverges at the critical point again with a power law:

$$\xi \propto |T_c - T|^{-\nu} \qquad (2)$$

The three images below show snapshots of a simple Ising magnet at three different temperatures. At low temperatures (left) most local magnetic moments point in one direction (up, white color) and the system is magnetic. At high temperatures half point up (white) and half point down (black) with only small clusters of like color (small ξ). Close to T_c (middle) clusters of like color percolate (diverging ξ).



This universal behavior was a puzzle. The first theory was due to by L.D. Landau's mean-field theory of continuous phase transitions in 1937. At tat timethe only remaining problem seemed to be Landau's critical exponent $\beta=1/2$ was slightly larger than experimental measurements $\beta\approx 0.3$. This could initially be argued to be an experimental artifact, until in the late 1940's, Onsager's exact solution of the two-dimensional Ising model with an exponent $\beta=1/8$ clearly showed that Landau's theory is not enough. The breakthrough in understanding came with Wilson's *renormalization group* (RG) treatment[2] of continuous phase transitions. This led to an understanding of different universality classes, governed by fixed points of the RG flow. All models in the same universality class flow to the same fixed point under the RG transformation and show the same universal behavior close to the phase transition, governed by a non-analytic power-law behavior of the free energy, and thus have the same universal exponents β, and ν.

Numerical simulation of second order phase transitions

While the RG method is important in understanding universality, *numerical methods* are essential in determining the values of the critical exponents confirming the universality conjecture, and in finding its limitations. Numerical calculations were first performed using series expansion[3] techniques, and later with higher precision Monte Carlo methods. Nowadays the critical exponents are known for a large number of models and agree well with experimental measurements.

What makes these numerical simulations especially rewarding is that, because of the universality of properties in the vicinity of the critical point, simulations on the simplest models will give results which are valid also for more complicated models and realistic materials. There are very few fields in Computational Sciences and Engineering where toy model results apply directly to all experimental realizations!

The problem we face however is, that, as the correlation length ξ diverges close to the critical point, so does the necessary linear system size L, since we need $L >> \xi$. Fortunately the universal behavior extends also to finite size effects. In the vicinity of the critical point, where ξ diverges, the system size L can be interpreted as a cutoff to the correlation length ξ, and equations (1) and (2) combined to *finite size scaling* equations such as

$$m \propto L^{-\beta/\nu}. \tag{3}$$

The universal exponents can thus be calculated from the system size dependences. Still, large systems with linear dimensions $L\approx 100 \ldots 1000$ are needed to reach the asymptotic scaling given by equation (3).

This is where the next problem lurks. Standard Monte Carlo simulations proceed by local updates: the local magnetic moments are moved one by one. Clearly, as the domain size ξ grows (center picture above) these local updates are no longer efficient in updating the system and we see "*critical slowing down*": the time needed to obtain an independent configuration scales grows with L^2 – a slow-down by many orders of magnitude! This problem has been solved for classical Monte Carlo simulations for magnetic systems by cluster update algorithms.[4] Instead of updating single magnetic moments, cleverly chosen clusters are

[2] See e.g. K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[3] See the series "*Phase transitions and critical phenomena*", edited by C. Domb and M.S. Green (Academic Press).
[4] U. Wolff, Phys. Rev. Lett **62**, 361 (1989); R.H. Swendsen and J-S. Wang, Phys. Rev. Lett **58**, 86 (1987).

updated at once. These algorithms have been a breakthrough for classical simulations and have allowed very accurate investigations of phase transitions in classical systems.[5]

Quantum phase transitions

In our research group we focus on phase transitions in quantum systems. In a quantum system an ordered state can be destroyed either, like in a classical system, by increasing the temperature and thus thermal fluctuations. Alternatively, in a quantum system, the Heisenberg uncertainty principle leads to fluctuations even at zero temperature. In a quantum magnet the strength of these zero point fluctuations can be changed by, e.g. pressure or chemical doping. If we denote the strength of the quantum fluctuations by g, we get equations similar to (1) and (2), but now as a function of g instead of T:

$$m \propto (g_c - g)^{\beta} \quad \xi \propto |g_c - g|^{-\nu} \tag{4}$$

As in classical systems, analytical RG calculations help in understanding the universality at such quantum phase transitions, and numerical simulations are again essential for obtaining the universal exponents and for checking the scaling assumptions on which the RG theory is based. In order to perform Monte Carlo simulations for a quantum system we have to be able to calculate its partition function given by:

$$Z = \mathrm{Tr}\, e^{-\beta H}, \tag{5}$$

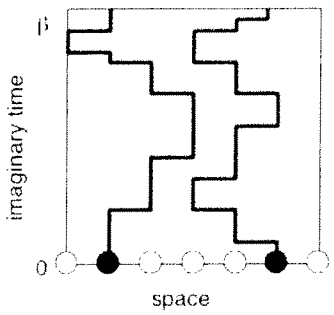
where H is the Hamilton operator of the system. Unlike a classical system, where the partition function is a sum over all configurations c with energy $E(c)$:

$$Z = \sum_c e^{-\beta E(c)}, \tag{6}$$

this cannot be evaluated directly. We thus have to map the quantum system (5) to a classical system (6) of classical configurations c with probability p_c:

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \sum_c p_c . \tag{7}$$

This can be done, e.g. in a path integral representation where each particle (or magnetic moment) is mapped to a world-line running along an imaginary time axis whose extent is the inverse temperature β, as sketched in the figure on the right. Dealing with these world-line objects is harder than a corresponding classical simulation, but efficient algorithms have been developed, including generalizations of the classical cluster algorithms to quantum systems.[6]



Parallelization

Despite having, in some cases, almost ideal algorithms, scaling linearly in the simulation volume these simulations pose a formidable challenge. Large systems of many thousand to million world lines are needed to see the correct asymptotic scaling behavior near a quantum phase transition. In addition, a large number of Monte Carlo steps have to be performed for a

[5] For a review over current work see the proceedings series "*Computer Simulation Studies in Condensed Matter Physics*" edited by D.P. Landau *et al.* (Springer Verlag Berlin).

[6] H. G. Evertz *et al.*, Phys. Rev. Lett. **70**, 875 (1993).

big range of system sizes, temperatures, and coupling strengths. While a single Monte Carlo step may take only a few seconds, the overall CPU need for an accurate simulation of the phase diagram of a is on the order of 50 CPU-years on the Asgard cluster.

Fortunately Monte Carlo simulations parallelize nearly perfectly. Simulations for different system sizes, temperatures and couplings are trivially independent and can run on the nodes of a cluster without the need for any communication. For all but the largest systems, a single CPU is sufficient for an individual simulation. These large simulations have to be further parallelized. This is trivially done in most cases by running copies of the same simulation but with different sequences of random numbers. The measurements collected by these copies are averaged at the end, which again requires almost no communication and scales nearly perfectly. Beowulf clusters are thus the ideal hardware platform for this type of simulations. The parallelization of these simulations is greatly simplified by an automatically parallelizing C++ Monte Carlo library that we have developed and used over the past eight years.[7]

Simulations of quantum phase transitions

Using these algorithms and large parallel computers, such as the Asgard cluster we could, for the first time, investigate the universal regime near quantum phase transitions with high accuracy.[8] First simulations were done on one-dimensional quantum magnets,[9] soon followed by a series of investigations of the critical behavior of two- and three-dimensional quantum magnets.[10] To highlight just a few findings, we could obtain highly accurate critical exponents of a quantum system and thus confirm that the universality class of the quantum phase transition a 2D quantum Heisenberg antiferromagnet is the same as that of the corresponding 3D classical one. In the presence of a magnetic field we could show that in a 2D quantum Heisenberg antiferromagnet close to the quantum phase transition even the critical temperature T_c can be universal, which has never been seen in another system before3. In the last two years new algorithms have been developed which allow us to extend these types of simulations to bosonic systems.[11] Again I want to mention two highlights: the first regards the existence of so-called supersolid phases, which are at the same time solid and superfluid. We could show that for hard-core bosons with nearest neighbor interactions the conjectured supersolid is actually just coexistence of a solid and a superfluid phase at a first order phase transition, while a stripe-like supersolid can exist with longer range interactions. An unusual feature was found near this first order phase transition: there the solid can melt – at fixed chemical potential – both when cooling or heating the system!

These algorithms can be used not only to study the universal behavior near phase transitions but also to quantitatively model real materials outside of the universal region. By doing fits of simulation data to experimental measurements or by combining our simulations

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[7] Matthias Troyer, Beat Ammon and Elmar Heeb, Lecture Notes in Computer Science **1505**, 191 (1998).

[8] For a review see H. G. Evertz, *The loop algorithm*, Advances in physics (to be published);

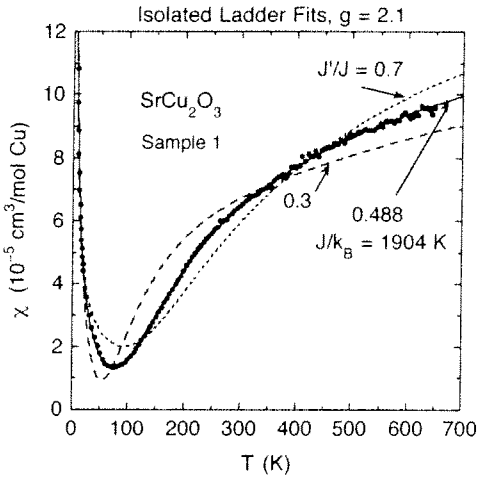
[9] B. Frischmuth *et al*, Phys. Rev. B **54**, 3714 (1996); T. Miyazaki, *et al.*, J. Phys. Soc. Jpn. **66**, 2590 (1997); B. Frischmuth, *et al.*, Phys. Rev. Lett. **82**, 835 (1999); F. Mila, *et al.*, Phys. Rev. Lett. **82**, 3697 (1999); B. Frischmuth, *et al.*, Phys. Rev. B **60**, 3388 (1999); V. A. Kashurnikov, *et al.*, Phys. Rev. B **59**, 1162 (1999)

[10] M. Troyer, *et al., Phys.* Rev. Lett. **76**, 3822 (1996); M. Troyer, *et al.*, Phys. Rev. B **55**, R6117 (1997); J.-K. Kim, *et al.*, Phys. Rev. Lett. **79**, 1583 (1997); M. Troyer, *et al.*, J. Phys. Soc. Jpn. **66**, 2957 (1997); J.-K. Kim and M. Troyer, Phys. Rev. Lett. **80**, 2705 (1998); K. Harada, *et al.*, J. Phys. Soc. Jpn. **67**, 1130 (1998); Lan Yin, *et al.*, Europhys. Lett. **42**, 559 (1998); M. Troyer and S. Sachdev, Phys. Rev. Lett **81**, 5418 (1998); S. Sachdev, *et al.*, Phys. Rev. Lett. **86**, 2617 (2001); K. Harada, *et al.*, Preprint submitted to Phys. Rev. Lett.; M. Troyer, Sup. Prog. Theor. Phys. (in press).

[11] F. Hebert, *et al.*, Phys. Rev. B **65**, 014513 (2002); A. Dorneich, *et al.*, Phys. Rev. Lett. **88**, 057003 (2002); K. Bernardet, *Get al.*, Phys. Rev. B **65**, 104519 (2002); G. Schmid, *et al.*, Phys. Rev. Lett. **88**, 167208 (2002); K. Bernardet, *et al.*, Phys. Rev. B **66**, 054520 (2002); G.G. Batrouni, *et al.*, Phys. Rev. Lett. **89**, 117203 (2002).

with ab-initio LDA+U methods, we could explain the unusual properties of a number of exotic quantum magnets.[12] The figure shows how well these quantitative comparisons to experiments work. I show a comparison of magnetic susceptibility measurements on SrCu2O3 to simulations. This material is well described by a ladder model, consisting of two couple chains. By fitting the exchange coupling on a chain J and the coupling on a rung of the ladder J' we get nearly perfect agreement of experiment (the black circles in the figure) with simulations at a ratio $J'/J \approx 0.488$ (solid line).

Remaining challenges



While algorithmic progress in the past decade has enabled us to simulate systems many orders of magnitude larger than before, there are still large classes of quantum systems for which no effective algorithm exists, and where more work is needed.

One problem occurs in disordered systems, like quantum glasses. As in classical glasses, or other complex systems such as protein folding, quantum there are a huge number of low-energy states. Sampling all these low-energy states, or finding the globai minimum is a formidable challenge, which in some cases can be shown to be *NP*-complete. Still, for finite but not too low temperatures, a new sampling scheme, Wang-Landau sampling was recently invented that promises to be much better than other existing schemes.[13]

The second formidable problem is the so-called "*negative sign problem*". While bosonic and unfrustrated magnetic systems can be simulated very efficiently, it happens in fermionic or frustrated quantum systems that in the mapping to a classical system [equation (7)] some of the probabilities p_c become negative. The consequence is a massive cancellation problem, and an exponential growth of the simulation time with the system volume. While for some special cases a solution to this sign problem is possible, we could show that there is at least one model in which a solution of the sign problem would give us a polynomial time algorithm for all the *NP*-complete problems.[14] While this makes a solution of the sign problem probably impossible (but also raises to stakes to include a nearly certain Nobel prize if one is found), other approaches can and need to be developed for these types of models.

Our strategy is to focus, at this time, on those systems where no sign problem occurs and where we have a chance of doing high-accuracy simulations. Planned for the near future are simulations of quantum spin glasses using a quantum version of Wang-Landau sampling, as well as the investigation of dissipation effects on quantum phase transitions.

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[12] S. Miyahara, *et al.*, J. Phys. Soc. Jpn. **67**, 3918 (1998); M. A. Korotin, *et al.*, Phys. Rev. Lett. **83**, 1387 (1999); D. Johnston, *et al.*, Phys. Rev. B **61**, 9558 (2000); R. Melzi *et al.*, Phys. Rev. Lett. **85**, 1318 (2000); D.C. Johnston *et al.*, Preprint, submitted to Phys. Rev. B.

[13] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001), Phys. Rev. E **64**, 056101 (2001); M. Troyer *et al*, preprint, submitted to Phys. Rev. Lett..

[14] M. Troyer and U.-J. Wiese, publication in preparation.

5
CSE Research Projects

Title: Topologically protected quantum bits

Researchers: D. Ivanov, M. Troyer, G. Blatter [*]
L. Ioffe [**]
M.V. Feigel'man, A. Ioselevich [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Rutgers University, USA
[***] Landau Institute, Moscow, Russia

Description:

We propose an implementation of a topologically protected quantum bit based on Josephson junction arrays. A topologically protected quantum bit has the huge advantage that no error correction is needed, since it is stable to disorder because of its topological nature. Unfortunately the implementation of a topologically protected quantum bit has remained unclear so far. Based on numerical investigations of strongly correlated systems, we show how their developing an isolated two-fold degenerate quantum dimer liquid groundstate can be used in the construction of topologically stable qubits and discuss their implementation using Josephson junction arrays

References:

- L. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter
Nature **415**, 507 (2002).

Title: Vortices in superconductors

Researchers: M. Bou-Diab, F. Mohamed, M. Troyer, G. Blatter [*]
I. Luk'yanchuk [**]

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

Description:

Vortices in type-II superconductors, caused by the intrusion of a magnetic field, form a new and unusual form of matter, so-called "vortex matter". Using numerical simulations we investigate two aspects in particular. The first are equilibrium ground state vortex configurations close to the quantum phase transition between type-I and type-II superconductors at $\kappa=1/\sqrt{2}$. The second project concerns the dynamics of vortex collisions, as a basis of a microscopic description of vortex lattice melting. Numerical simulations show that when two vortices collide, they recombine twice, and thus effectively cross.

References:

- M. Bou-Diab and G. Blatter, Phys. Rev. Lett. **86**, 5132 (2001).
- F. Mohamed, M. Troyer, G. Blatter and I. Luk'yanchuk, Phys. Rev. B **65**, 224504 (2002)

Title: Weather and Climate in the Alpine Region

Researchers: Huw C. Davies, Heini Wernli, Daniel Lüthi, Conny Schwierz, Michael Sprenger, Sandro Buss, Sebastien Dirren, Patrick Koch und Matthias Zillig

Institute/Group: Institut für Atmosphäre und Klima (IAC) ETH Zürich. Gruppe für Theoretische Meteorologie

Description:

The Theoretical Meteorology group is engaged in the study, analysis and simulation of atmospheric flow phenomena. A wide range of both time-scales ranging from decadal periods in climatological investigations to time-scales of a few minutes and spacial scales covering global scales to scales of a few km are hereby investigated. This requires also a variety of different analysis tools and simulation models that are appropriate for the phenomenon under investigation. We have a close cooperation with the group of Prof. Schär and with Meteo Schweiz and make use of the same models like the Canadian MC2-model and the operational Swiss high resolution model LM (both nonhydrostatic models suitable for resolutions higher than 10 km) or the CHRM-model (a hydrostatic model suitable for grid spacings > 10 km).
Even though special focus is given to processes related to Alpine meteorology the activities of the group cover a much wider area. Recent studies include the investigation of stratosphere-troposhere exchange and the formation of polar stratospheric clouds (both are relevant to the ozone problem), a study on the winter storm "Lothar", vortex dynamics and regional climate modelling. A complete list of recent publications is given in the references section.
The group is actively taking part in national and international programmes like NCCR Climate, MAP (Mesoscale Alpine Programme) and SOLVE/THESEO.

Title: Computational Solid State Electronics

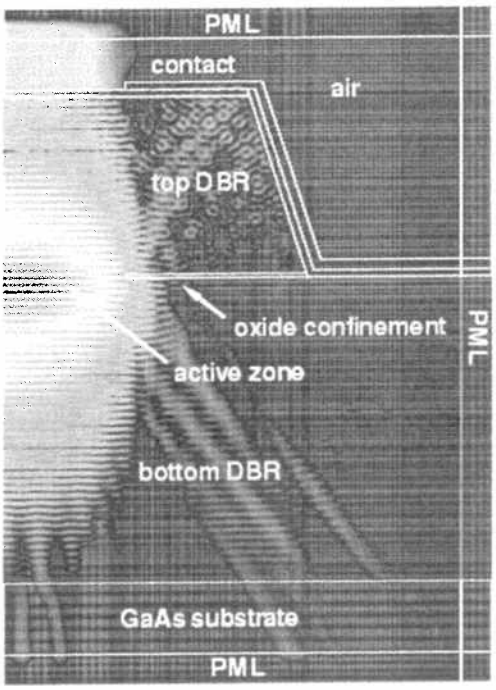
Researchers: Wolfgang Fichtner
Andreas Schenk
Andreas Witzig
Jens Krause
Eduardo Alonso
Dölf Aemmer

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

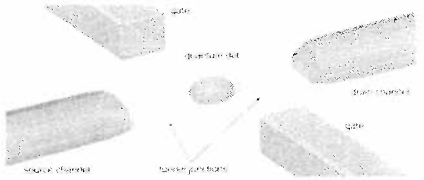
Description:

For the development of novel micro- and opto-electronic processes, devices and circuits, 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. As we are rapidly approaching nanoscale dimensions, effects at the atomistic or quantum-mechanical level are becoming dominant.

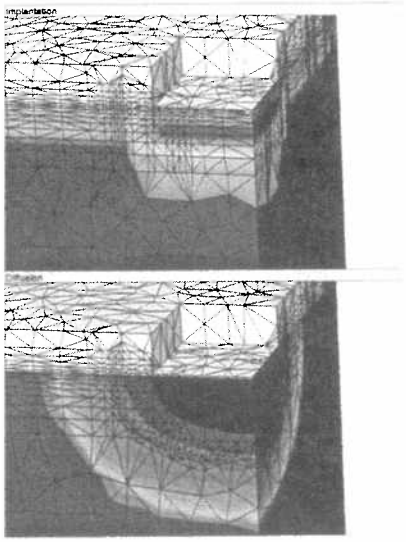
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulations tools for molecular dynamics studies in material diffusion, novel devices such as single-electron transistors, and optoelectronic devices such as LEDs and laser diodes. For all of our projects, the main emphasis lies in the exploration how accurate physical models can be pragmatically combined with state-of-the-art numerical algorithms. The following pictures illustrate some of our activities:



Optical simulation of a vertical-cavity surface-emitting laser (VCSEL).



Simulation of a electron transistor by the self-consistent solving of the Kohn–Sham equations.



Mesh generation for implantation and diffusion in semiconductor process simulation.

Title: Solitons in the nonlinear Hartree Equation

Researchers: W.H Aschbacher, J. Fröhlich, G. Interlandi, M. Troyer,

Institute/Group: Theoretische Physik, ETH Zürich

Description:

This project concerns minimizers (lowest energy eigenfunctions) of the Hartree energy functional with attractive Hartree interaction. Among the most important findings is a symmetry breaking of the ground state wave function when the interaction is sufficiently strong. We also investigate the time evolution of such soliton-like minimizers in an external potential. As a particular application of these results and as a motivation for the investigation of the Hartree functional, we propose a generalization of the Gross-Pitaevskii functional of Bose-Einstein condensation for *attractive* interatomic forces that overcomes the breakdown of this theory at the collapse point of the condensate.

References:

- W.H. Aschbacher, PhD Thesis (ETH Zürich, 2001)
- W.H. Aschbacher, J. Fröhlich, G.M. Graf, K. Schnee, M. Troyer, J. of Math. Phys. **43**, 3879 (2002)

CSE research project descriptions

Title:	The Jacobi–Davidson algorithm for solving large sparse symmetric eigenvalue problems
Researchers:	Roman Geus Peter Arbenz
Institute/Group:	Institute of Scientific Computing

Description:

The Maxwell equations for the strength of the electric field are solved by a mixed method with quadratic finite edge elements for the field values and corresponding node-based finite elements for the Lagrange multiplier. This approach avoids spurious modes that are introduced if the divergence-free condition for the electric field is not treated properly.
The Jacobi-Davidson (JD) algorithm has been implemented for solving the resulting large sparse symmetric matrix eigenvalue problem. A two-level hierarchical basis preconditioners are employed for the efficient solution of the correction equation that is at the heart of the JD algorithm. The solver is implemented stably and efficiently. It is able to handle very large eigenvalue problems of orders above 2 millions on a single-processor workstation.
The software is implemented as Python modules. The time-critical computations were realized as extension modules written in C.

References:

R. Geus
The Jacobi–Davidson algorithm for solving large sparse symmetric eigenvalue problems
ETH Zurich, PhD Thesis No. 14734, 2002.

CSE research project description

Title:	Jacobi–Davidson algorithms for the complex symmetric eigenvalue problem
Researchers:	Oscar Chinellato Peter Arbenz
Institute/Group:	Institute of Scientific Computing

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 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 hierarchical basis preconditioners based on Nédélec elements.

References:

P. Arbenz and M. Hochstenbach
Jacobi–Davidson Method for Solving Complex-Symmetric Eigenvalue Problems
ETH Zürich, Computer Science Department, Tech. Report 374, July 2002.
Available at URL `http://www.inf.ethz.ch/publications/`

CSE research project description

Title:	Parallel Smoothing for Multigrid with Sparse Approximate Inverses
Researchers:	Oliver Bröker* Marcus J. Grote†
Institute/Group:	*Institute of Scientific Computing † Department of Mathematics, University of Basel

Description:

The usefulness of SParse Approximate Inverses (SPAI) for multigrid (e.g. as smoothers) is investigated in this project. The convergence of standard multigrid for problems with discontinuous coefficients or complicated flow patterns can be improved by replacing the ubiquitous Gauss–Seidel iteration with approximate inverse smoothing. To attain even greater robustness in the presence of strong anisotropy, we combine the parallel SPAI smoother with the multigrid approach. The algebraic multigrid (AMG) procedure with SPAI smoothing is shown to yield robust multigrid convergence for a two–dimensional locally anisotropic problem. Advantages of SPAI smoothers over classical smoothers are inherent parallelism, possible local adaptivity, and improved robustness. We investigate the further incorporation of approximate inverses in the AMG iteration.

References:

Bröker, O. and M. J. Grote
Sparse approximate inverse smoothers for geometric and algebraic multigrid.
Applied Numerical Mathematics: Transactions of IMACS 41(1), 61–80.

Bröker, O., M. J. Grote, C. Mayer, and A. Reusken
Robust parallel smoothing for multigrid via sparse approximate inverses.
SIAM Journal on Scientific Computing 23(4), 1396–1417.

Grote, M. J. and T. Huckle
Parallel preconditioning with sparse approximate inverses.
SIAM Journal on Scientific Computing 18(3), 838–853.

Title: Structure-variant multi-body systems

Researchers: Prof. Dr. Ch. Glocker
Kerim Yunt
Christian Studer

Institute/ Group: Institute of Mechanical Systems
Research Group of Multibody Dynamics

Description:

The area of structure-variant multi-body systems is a relatively new field of research. The characteristics of those systems pose also new questions in the optimal control of such systems. As the number of D.O.F (Degrees of Freedom) increases, efficient numerical algorithms and computational speed becomes more and more important. The computational treatment of determining the optimal trajectory of such systems, requires the simultaneous solution of Linear Complementarity Problems within the optimization routine along with the direct collocation optimization method at every time step. Depending on the structure of the mechanical system as well as the structure of the equality and inequality equations, different computational schemes can be implemented. The floating point accuracy gets especially important as the D.O.F increases because the accumulation of numerical errors over the simulation must be prevented and corrected if possible.

References:

[1] GLOCKER, CH., Set-Valued Force Laws: Dynamics of Non-Smooth Systems. Springer Verlag, Berlin, Heidelberg 2001.

[2] PFEIFFER, F., GLOCKER, CH., Multibody Dynamics with Unilateral Contacts. John Wi-ley & Sons, New York 1996.

[3] BACHMANN, D, Optimale Impulssteuerung eines zweidimensionalen Mehrkörper-systems, Semesterarbeit am Zentrum für Mechanik, Institut für Mechanische Systeme, ETH Zürich, (2001)

[4] MEYER, K, Optimale Impulssteuerung eines unteraktuierten Roboters, Diplomarbeit am Zentrum für Mechanik, Institut für Mechanische Systeme, ETH Zürich, (2001/2002)

[5] GLOCKER, CH, Dynamik von Starrkörpersystemen mit Reibung und Stössen, Dissertation am Lehrstuhl B für Mechanik, Technische Universität München, (1995)

Title: Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L

Researchers: Alice Glättli
Xavier Daura
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

Different approaches to improve the simple point charge model for liquid water (SPC) were investigated. This led to a whole series of new water models with additional van der Waals interaction sites at the hydrogen atoms, modified partial charges and modified geometries. The properties of these models are analyzed and discussed. Particular emphasis has been put on the study of the dependence and sensitivity of water properties on the model parameters. We found that a simultaneous improvement of the dielectric permittivity and the diffusion coefficient is difficult to attain for a rigid, nonpolarizable three interaction site model. Nevertheless, two of the models presented here, SPC/A and SPC/L, show good agreement with experimental data on water and have been characterized in more detail. We conclude that SPC/L represents the overall properties of water better than SPC. Especially, it shows excellent dielectric properties, an improved shear viscosity and a slightly lower diffusion coefficient.

References: J. Chem. Phys. **116** (2002) 9811-9828

Title: Assessing equilibration and convergence in biomolecular simulations

Researchers: Lorna J. Smith*
Xavier Daura
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*OCMS, University of Oxford, Oxford, UK

Description:

If molecular dynamics simulations are used to characterise the folding of peptides or proteins a wide range of conformational states need to be sampled. This study reports an analysis of peptide simulations to identify the best methods for assessing equilibration and sampling in these systems where there is significant conformational disorder. Four trajectories of a β peptide in methanol and four trajectories of an α peptide in water, each of 5 ns in length, have been studied. Comparisons have also been made with two 50 ns trajectories of the β peptide in methanol. The convergence rates of quantities that probe both the extent of conformational sampling and the local dynamical properties have been characterised. These include the numbers of hydrogen bonds populated, clusters identified and main chain torsion angle transitions in the trajectories. The relative equilibrium rates of different quantities are found to vary significantly between the two systems studied reflecting both the differences in peptide primary structure and the different solvents employed. A cluster analysis of the simulation trajectories is identified as a very effective method for judging the convergence of the simulations. This is particularly the case if the analysis includes a comparison of multiple trajectories calculated for the same system from different starting structures.

References: Proteins **48** (2002) 487-496

Title: Molecular dynamics simulations of a double unit cell in a protein crystal: Volume relaxation at constant pressure and correlation of motions between the two unit cells

Researchers: Regula Walser
Philippe H. Hünenberger
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

Eight molecular dynamics simulations of a double crystal unit cell of ubiquitin were performed in order to investigate the effects of simulating at constant pressure and of simulating two unit cells compared to a single unit cell. To examine the influence of different simulation conditions, the constant-pressure and constant-volume simulations were each performed with and without counter ions, and using two different treatments of the long-ranged electrostatic interactions (lattice-sum and reaction-field methods). The constant-pressure simulations were analysed in terms of unit cell deformation and accompanying protein deformations. Energetic and structural properties of the proteins in the simulations of the double unit cell were compared to the results of previously reported one-unit-cell simulations. Correlation between the two unit cells was also investigated based on relative translational and rotational movements of the proteins, and on dipole fluctuations. The box in the constant-pressure simulations is found to deform slowly to reach convergence only after 5-10 ns. This deformation does not result from a distortion in the structure of the proteins, but rather from changes in protein packing within the unit cell. The results of the double-unit-cell simulations are closely similar to the results of the single-unit-cell simulations and little motional correlation is found between the two unit cells.

References: Proteins **48** (2002) 327-340

Title: An improved OPLS-AA force field for carbohydrates

Researchers: David Kony*
Wolfgang Damm
S. Stoll*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*CABE, University of Geneva, Geneva, CH

Description:

This work describes an improved version of the original OPLS-all atom (OPLS-AA) force field for carbohydrates (Damm et al., J Comp Chem 1997, 18, 1955). The improvement is achieved by applying additional scaling factors for the electrostatic interactions between 1,5- and 1,6-interactions. This new model is tested first for improving the conformational energetics of 1,2-ethanediol, the smallest polyol. With a 1,5-scaling factor of 1.25 the force field calculated relative energies are in excellent agreement with the *ab initio* derived data. Applying the new 1,5-scaling makes it also necessary to use a 1,6-scaling factor for the interactions between the C4 and C6 atoms in hexopyranoses. After torsional parameter fitting, this improves the conformational energetics in comparison to the OPLS-AA force field. The set of hexopyranoses included in the torsional parameter derivation consists of the two anomers of D-glucose, D-mannose and D-galactose, as well as of the methyl-pyranosides of D-glucose, D-mannose. Rotational profiles for the rotation of the exocyclic group and of different hydroxyl groups are also compared for the two force fields and at the *ab initio* level of theory. The new force field reduces the overly high barriers calculated using the OPLS-AA force field. This leads to better sampling which was shown to produce more realistic conformational behavior for hexopyranoses in liquid simulation. From 10-ns molecular dynamics (MD) simulations of α-D-glucose and α-D-galactose the ratios for the three different conformations of the hydroxymethylene group and the average $^{3}J_{H,H}$-coupling constants are derived and compared to experimental values. The results obtained for OPLS-AA-SEI force field are in good agreement with experiment whereas the properties derived for the OPLS-AA force field suffer from sampling problems. The undertaken investigations show that the newly derived OPLS-AA-SEI force field will allow simulating larger carbohydrates or polysaccharides with improved sampling of the hydroxyl groups.

References: J. Comput. Chem. (2002) in press

Title: Can one derive the conformational preference of a β-peptide from its CD spectrum?

Researchers: Alice Glättli
Xacier Daura
Dieter Seebach*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*Laboratory of Organic Chemistry

Description:

CD spectroscopy is often used to elucidate the secondary structure of peptides built from non-natural amino acids such as β-amino acids. The interpretation of such CD spectra is not always unambiguous. Here, we present a case where two β-hexapeptides, indicated as DM-BHP (**A**) and BHP (**B**) (figure 1), exhibit similar CD spectra, whereas they are expected to differ in secondary structure. The structural properties of both peptides were studied by molecular dynamics simulation and, from the resulting trajectories, the corresponding CD spectra were calculated. Starting from a fully extended conformation, BHP is observed to form a 3_{14}-helix, while DM-BHP remains unfolded. However, even though these two peptides hardly share any conformations, their calculated CD spectra are alike and close to the experimentally measured ones. Our results imply that a particular CD pattern can be induced by spatially different structures, which makes it difficult to derive the conformational preference of a peptide from its CD spectrum alone. In order to gain more insight into the relationship between the preferred conformation of a peptide and its CD spectrum more accurate methods to calculate the CD spectrum for a given conformation are required.

References: submitted to J. Am. Chem. Soc. (2002)

Title: β-peptides with different secondary structure preferences: How different are their conformational spaces?

Researchers: Riccardo Baron
Dirk Bakowies
Wilfred F. van Gunsteren
Xavier Daura*

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*Universitat Autònoma de Barcelona, Spain

Description:

The conformational spaces accessible to two β-hexapeptides in methanol solution at 298 K and 340 K are investigated by molecular dynamics simulation with an atomistic model of both solute and solvent. The structural properties of these peptides have been previously studied by NMR in methanol solution at room temperature. The experimental data could be fitted to a model P-12/10 helix for one of the peptides and a model hairpin with 10-membered hydrogen-bonded turn for the other. The goal of the present work is to determine whether the conformational space accessible to these two peptides of seemingly different conformational properties contain any common regions. In other words, to what extent the evident differences found at the macroscopic level are also present at the microscopic structural level. It is found, that for the two peptides studied the conformational spaces sampled in the respective simulations show significant overlap.

References: Helv. Chim. Acta (2002) in press

Title: A novel approach for designing simple point charge models for liquid water with three interaction sites

Researchers: Alice Glättli
Xavier Daura
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

A simultaneous improvement of the diffusion and dielectric properties of the simple point charge (SPC) model for liquid water appears to be very difficult with conventional reparametrization of the commonly used Lennard-Jones and Coulomb interaction functions and without including a self-energy correction in the effective pair-potential as is done in the SPC/E model. Here, a different approach to circumvent this problem is presented. A short-range interaction term, which corrects the oxygen-oxygen energy at small distances by small amounts of energy, was introduced in the non-bonded interaction function. This additional force-field term allows to derive new parameter sets for SPC-like water models that yield better agreement with experimental data on liquid water. Based on previous investigations of the force-field parameter dependence of the water properties of SPC-like models, the necessary parameter changes to obtain a lower diffusion coefficient and a larger dielectric permittivity were specified and accordingly six new models were developed. They all represent an improvement over SPC in terms of structural and diffusional properties, four of them show better dielectric properties too. One model, SPC/S, has been characterized in more detail and represents most properties of liquid water better than SPC while avoiding the larger discrepancies with experimental values regarding density, energy and free energy of the SPC/E model. We conclude that the use of a simple, short-ranged additional oxygen-oxygen interaction term makes a simultaneous improvement of the diffusion coefficient and the dielectric properties of water feasible.

References: submitted to J. Comput. Chem. (2002)

Title: Development of a simple, self-consistent polarizable model for liquid water

Researchers: Haibo Yu
Tomas Hansson
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

The Charge-On-Spring (COS) method is used to develop a rigid, three-site, polarizable water model, a non-iterative and a self-consistent version. In this method, the polarizability is taken into account by a variable separation of charges on selected polarizable centers. One of the pair of polarization charges resides on a polarizable center, while the other one is treated as an additional particle attached to the polarizable center by a parabolic restraint potential. The separation is calculated in response to the instantaneous electric field. We parametrized two models which are based on non-iterative and self-consistent versions of the method, respectively. We computed several liquid-phase and gas-phase properties and compared with data available from experiment and *ab initio* calculations. The condensed-phase properties of both models are in reasonable accord with experiment, apart from discrepancies in electrostatic properties consistent with a slightly too large liquid-state dipole.

References: submitted to J. Chem. Phys. (2002)

Title: A consistent potential energy parameter set for lipids: Dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field

Researchers: Indira Chandrasekhar
Mika Kastenholz
Roberto D. Lins
Chris Oostenbrink
Lukas D. Schuler
D. Peter Tieleman*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*University of Calgary, Canada

Description:

The performance of the GROMOS96 parameter set 45A3 developed for aliphatic alkanes is tested on a bilayer of dipalmitoylphosphatidylcholine (DPPC) in water in the liquid-crystalline L_α phase. Variants of the force-field parameter set as well as different sets of simulation conditions or simulation parameter sets are evaluated. In the case of the force-field parameters, the van der Waals constants for the non-bonded interaction of the ester carbonyl carbon and the partial charges and charge group definition of the phosphatidylcholine head group are examined. On the methodological side, different cut-off distances for the non-bonded interactions, use of a reaction-field due to long range electrostatic interactions, the frequency of removal of the centre of mass motion and the strength of the coupling of the pressure of the system to the pressure bath are tested. The area per lipid, as a measure of structure, the order parameters of the chain carbons as a measure of membrane fluidity and the translational diffusion of the lipids in the plane of the bilayer are calculated and compared with experimental values. An optimal set of simulation parameters for which the GROMOS96 parameter set 45A3 yields a head group area, chain order parameters and a lateral diffusion coefficient in accordance with the experimental data is listed.

References: submitted to Europ. Biophys. J. (2002)

Title: Putting titania shells in a polymer: which properties can be achieved?

Researchers: Ilya A. Karmilov
Andrei A. Gusev

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

Description:

In this work we have used a finite element based approach for predicting the overall elastic and dielectric properties of shell-egg-particle reinforced polymers. Multiscale tetrahedra-based meshes were employed for reproducing the morphology. The particles were approximated by core-shell spheres with the walls of different thickness. For the particles, typical titanium dioxide properties were assumed in calculations. We investigated the dependence of macroscopic properties on the inclusion volume fraction, thickness of the titanium dioxide walls, and aspect ratio of the spheroids. It appears that the core-shell-particle reinforced polymers exhibit a unique portfolio of technological properties that can be indispensable in various demanding weight-saving applications. The optimal wall thickness was found.

References: A.A. Gusev, I.A. Karmilov, *Macromol. Theory Simul.* **2002**, *11*, 247-249

Title: Finite element approaches to generation of complex morphological states in block copolymer systems.

Researchers: Ilya A. Karmilov[a]
Andrei A. Gusev[a]
Glen H. Fredrickson[b]
Frank S. Bates[c]
Hsuan-Yi Chen[d]

Institute/Group: [a]Institute of Polymers, Department of Materials, ETH
[b]Mitsubishi Chemical Center for Advanced Materials and Departments of Chemical Engineering & Materials, University of California, Santa Barbara
[c]Department of Chemical Engineering and Materials Science, University of Minnesota
[d]Department of Physics, National Central University of Taiwan

Description:

In this work we have developed and implemented a finite element based version of Self-Consistent Field Theory for predicting the morphologies of complex block copolymer systems. As a first application, we generated an ensemble of morphological states realizable in symmetric poly(styrene-*b*-isoprene-*b*-ethylene oxide) triblock copolymers, and compared the predicted mesoscopic crystals with experimental data. The principal objective of this study is to use a combination of experimental data and numerical predictions for gaining in-depth understanding of the morphologies realizable in this ABC triblock system.

References: A manuscript is in preparation.

Title: Numerical simulation of the effects of volume fraction, aspect ratio and fibre length distribution on the elastic and thermoelastic properties of short fibre composites

Researchers: Peter J. Hine[a]
Hans Rudolf Lusti[b]
Andrei A. Gusev[b]

Institute/Group: [a] IRC in Polymer Science and Technology, University of Leeds, Leeds. LS2 9JT, UK
[b] Institute of Polymers, Group of Polymer Chemistry, ETH-Zentrum, CH-8092 Zurich,Switzerland

Description:

The numerical procedure of Gusev is applied for predicting the elastic and thermoelastic properties of short fibre reinforced composites. Computer models, comprising 100 non-overlapping aligned spherocylinders, were generated using a Monte Carlo procedure to produce a random morphology. Periodic boundary conditions were used for all the generated structures. Where necessary, the generated microstructures were based on measurements of real materials: for example a measured fibre length distribution was used to seed the Monte Carlo generator to produce a computer model with an equivalent fibre length distribution (FLD). The generated morphologies were meshed using an intelligent 3 dimensional meshing technique, allowing the elastic and thermo-elastic properties of the microstructures to be calculated.
The numerical predictions were compared with those from three commonly used micromechanical models, namely those attributed to Halpin/Tsai, Tandon/Weng and Cox (shear lag). Firstly, the effect of volume fraction and aspect ratio were investigated, and the numerical results were compared and contrasted with those of the chosen models. Secondly, the numerical approach was used to investigate what effect a distribution of fibre lengths, as seen in real materials, would have on the predicted mechanical properties. The results were compared with simulations carried out using a monodispersed fibre length, to ascertain if the distribution of lengths could be replaced with a single length, and whether this length corresponded to a particular characteristic of the distribution, for example the first moment or average length.

References: Comp. Sci. Tech. **62** (2002) 1445-1453

Title: Direct numerical predictions for the elastic and thermoelastic properties of short fibre composites

Researchers: Hans Rudolf Lusti*
Peter J. Hine**
Andrei A. Gusev*

Institute/Group: * Institute of Polymers, Group of Polymer Chemistry, ETH-Zentrum, CH-8092 Zurich,Switzerland
** IRC in Polymer Science and Technology, University of Leeds, Leeds. LS2 9JT, UK

Description:

We compare the predictions of the thermoelastic properties of misaligned short glass fibre reinforced composites, calculated using the finite-element-based numerical approach of Gusev, with experimental measurements. Characterisation of the microstructure of the two injection moulded materials chosen for examination, in particular the fibre length and fibre orientation distributions, were used to ensure that the computer models were built with the same microstructure as the 'real' materials. Agreement between the measurements, in particular for the longitudinal Young's modulus E_{11} and the longitudinal and transverse thermal expansion coefficients, α_1 and α_2, and the numerical predictions was found to be excellent. A comparison was also made with the most commonly used micromechanical models available from the literature. The approaches of Tandon and Weng, Takao and Taya and McCullough were found to give good agreement with both the numerical and measured values, although only the numerical approach showed the same relationship between α_1 and the degree of orientation as shown by the real materials.

References: Comp. Sci. Tech. **62** (2002) in press

Title: Effect of particle agglomeration on the elastic properties of filled polymers

Researchers: Hans Rudolf Lusti
Ilya A. Karmilov
Andrei A. Gusev

Institute/Group: Institute of Polymers, Group of Polymer Chemistry, ETH-Zentrum, CH-8092 Zurich,Switzerland

Description:

We conducted a numerical finite-element-based study on the reinforcing effect of particle agglomeration on the stiffness of sphere filled polymers. Two different types of agglomerates were considered. The first type was made up of 10 non-overlapping identical spheres whereas the second type of 10 slightly fused spheres. Numerical results reveal that by using agglomerates with fused spheres one can significantly increase the composite stiffness while the use of non-fused agglomerates does not allow one to achieve any additional stiffness increase compared to a composite with evenly dispersed non-agglomerating spheres.

References: Soft Materials **1** (2002) in press

Title: Matching the thermal expansion of mica-polymer nanocomposites and metals

Researchers: Olga Guseva*
Hans Rudolf Lusti**
Andrei A. Gusev**

Institute/Group: * Department of Corrosion and Surface Protection, EMPA, Ueberlandstrasse 4, CH-8600 Dübendorf, Switzerland
** Institute of Polymers, Group of Polymer Chemistry, ETH-Zentrum, CH-8092 Zurich,Switzerland

Description:

It was found by numerical simulations that the dispersion of small amounts of exfoliated muscovite mica platelets in a polymer can dramatically reduce the mismatching of thermal expansion between metal and composite parts. The mismatch reduction can extend the service life of a metal-nanocomposite joint structure. For identification of the potential of mica-filled nanocomposites the finite-element-based numerical approach of Gusev was used. We studied computer models comprised of a random dispersion of parallel fully aligned muscovite mica platelets. A most remarkable finding is that the thermal expansion of platelet-filled nanocomposites is controlled by the product of the aspect ratio and the volume fraction of the mineral platelets. This universal design curve can help an engineer in finding a proper material for definite applications.

References: A manuscript is in preparation

Title: Solving the Poisson equation for solute-solvent systems using fast Fourier transforms.

Researchers: Christine Peter*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

An iterative algorithm based on fast Fourier transforms is proposed to solve the Poisson equation for systems of heterogeneous permittivity (*e.g.* solute cavity in a solvent) under periodic boundary conditions. The method makes explicit use of the dipole-dipole interaction tensor, and is thus easily generalizable to arbitrary forms of electrostatic interactions (*e.g.* Coulomb's law with straight or smooth cutoff truncation). The convergence properties of the algorithm and the influence of various model parameters are investigated in detail, and a set of appropriate values for these parameters is determined. The algorithm is further tested by application to three types of systems (a single spherical ion, two spherical ions, and small biomolecules), and comparison with analytical results (single ion) and with results obtained using a finite-difference solver under periodic boundary conditions. The proposed algorithm performs very well in terms of accuracy and convergence properties, with an overall speed comparable in the current implementation to that of a typical finite-difference solver. Future developments and applications of the algorithm will include: (*i*) the assessment of periodicity- and cutoff-induced artifacts in explicit-solvent simulations; (*ii*) the design of new electrostatic schemes for explicit-solvent simulations mimicking more accurately bulk solution; (*iii*) a faster evaluation of solvation free energies based on continuum electrostatics in cases where periodicity-induced artifacts can be neglected.

References: Peter, C., van Gunsteren W.F. & Hünenberger, P.H.
J. Chem. Phys. **116** (2002) 7434-4451.

Title: Protein-trehalose interactions in aqueous solution

Researchers: Roberto D. Lins*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

A variety of sugars are known to enhance the stability of biomaterials. Trehalose, a non-reducing disaccharide composed of two α-(1$\rightarrow$1)-linked glucopyranose units, appears to be one of the most effective protectant. It has been shown that this disaccharide efficiently protects biostructures such as proteins and membranes from dehydration- and heat-induced denaturation, and is used by several desert animals and plants for this purpose. However, despite the large amount of experimental data, no clear picture of the molecular mechanism responsible for this proctective action has emerged yet, although three alternative hypotheses (increase of the medium viscosity, water-trehalose hydrogen-bond replacement, and coating by trapped residual water) have been proposed. To investigate the nature of intermolecular interactions in a protein-trehalose-water system, we have carried out two two-nanosecond molecular dynamics simulations of the protein lysozyme in solution in the presence (0.5 M) and absence of trehalose. The results of these simulations can be summarized by the following observations : (*i*) when trehalose is present, the trehalose molecules progressively move towards the protein and cluster around it ; (*ii*) on the nanosecond timescale, water is not completely expelled from the protein surface, and a thin water layer is trapped between the protein and the trehalose cluster ; (*iii*) trehalose coating reduces the side chain fluctuations and positional deviations from the crystallographic structure, without affecting significantly the backbone deviations and fluctuations ; (*iv*) a detailed analysis of of the water molecules trapped by trehalose at the protein surface reveals that water-protein hydrogen bonds are being progressively replaced by water-trehalose hydrogen bonds. Thus, on the timescale of the simulations, trehalose slowly desolvates the protein surface by competing for the hydrogen bonds to water, rather than by removing water molecules. The observation that the protein backbone fluctuations are not damped by trehalose coating is not necessarily contradictory with the experimentally-observed damping of the fluctuations in dry protein-trehalose glasses, because the former observation is only pertinent to a concentrated trehalose solution (present simulation).

References: A manuscript is in preparation

Title: Comparison of the particle-particle–particle-mesh and reaction-field methods for the computation of electrostatic interactions in molecular dynamics simulations of highly-charged proteins

Researchers: Raimon Gargallo**
Philippe H. Hünenberger*
Francesc X. Avilés**
Baldomero Oliva**

Institute/ Group: * Laboratory of Physical Chemistry
** Departement of Analytical Chemistry, University of Barcelona

Description :

Molecular dynamics simulations of the activation domain of procarboxypeptidase B (ADBp) were performed in order to examine the effects of using the particle-particle–particle-mesh (P^3M) or the reaction-field (RF) methods for evaluating electrostatic interactions in molecular dynamics simulations of highly-charged proteins. The P^3M method uses an exact description of the electrostatic forces within the approximation of an exactly periodic system, while the RF method applies cutoff truncation together with a long-range correction approximating the medium beyond the cut-off distance as a homogeneous dielectric continuum with the same permittivity as the pure solvent. To compare the consequences of these two alternative approximations, two 2.5-nanosecond molecular dynamics simulations of ADBp were performed using either of the two methods to handle electrostatic interactions. Several structural and thermodynamical quantities were computed and compared, including the root-mean-square atomic positional deviation from the crystallographic structure, root-mean-square atomic positional fluctuations, essential dynamics, and estimates for the entropies and solvation free energies. Although the P^3M method leads to slightly higher atomic positional deviations and fluctuations during the simulations, the description of all other properties considered is found to be very similar when comparing the two electrostatic schemes.

References: A manuscript is in preparation.

Title: Inverse aerodynamic shape design for gas turbine components

Researchers: Rolf Jeltsch
Andrea Scascighini
Andreas Troxler

Institute: Seminar for Applied Mathematics
Group: Department of Mathematics

Description:

Computational fluid dynamics (CFD) has become a fundamental tool for the simulation of flow in turbomachinery devices such as diffusers, blade rows, etc. CFD is however still not being exploited as one would expect in the design process. In fact the 'trial and error' approach is the most used by designers.

In inverse design methods the distribution of a flow variable is prescribed (eg. the static pressure distribution along the sidewalls of a diffuser or the pressure loading of a blade), and the corresponding geometry is sought.

In this project we developed a code which can handle 2D and axis–symmetric inviscid flows following the approach of Keller (ZAMP, 49 (1998)). Current research is directed towards viscous and three–dimensional applications.

References: A manuscript entitled "A Numerical Method for Inverse Design Based on the Inverse Euler Equations" has been submitted to Numerical Methods for Fluids.

Title: Finite volume dynamical core for decadal-scale climate simulations

Researchers: William Sawyer*
Shian-Jiann Lin**
Kevin Yeh++
Rolf Jeltsch***

Institute/ Group: *Institute for Atmospheric and Climate Research, ETHZ

**Data Assimilation Office, NASA Goddard Space Flight Center
++Earth and Space Science Interdisciplinary Center, Univ. of Maryland
***Seminar for Applied Mathematics, ETHZ

Description:

A central component of numerical weather prediction and climate simulation is the solver of the equations of atmospheric motion, also known as the "dynamical core." Recent research indicates that the schemes which conserve physical quantities, such as mass and vorticity, consistently produce more accurate mid-term forecasts than non-conservative schemes. Several conservative dynamical cores have been proposed and implemented in recent years for atmospheric general circulation models employing orthogonal latitude-longitude grids. The finite-volume flux-form semi-Lagrangian scheme of Lin and Rood (2002) is a key example of such a dynamical core.

As a first step in our research we have parallelized the Lin/Rood dynamical core and inserted it successfully into the Community Climate System Model (CCSM2), which was released in May 2002 for public use (see `www.ccsm.ucar.edu`). Different techniques for data decomposition for the data-parallel and multithreaded-parallel implementation have been evaluated, e.g., distribution of latitudes and vertical levels simultaneously over the processors. Benchmarks on the NASA target platforms – an SGI Origin 3000 and a Compaq SC, both with 512 processors – have indicate excellent scalability and high performance (hundreds of simulated days per day at relatively high $1^o \times 1^o$ resolution).

In order to make our experiences in these supercomputers useful to the wider Earth Science community, we are also participating with numerous other institutions in the Earth Science Modeling Framework (see `www.esmf.ucar.edu`). The goal of this project is to isolate and implement key componentry for high-performance Earth Science applications. We have co-authored requirements documents for distributed grids and for (conservative) regridding components, among others.

We are now investigating the use of non-orthogonal grids for dynamical cores. This involved a thorough literature search on finite-difference and finite-volume techniques, as well as on the Method of Transport developed in the ETHZ Seminar for Applied Mathematics. We are in the process of implementing a mass- and vorticity-conserving shallow water model on the sphere which employs pentagonal-hexagonal grids.

References:

W. Sawyer and P. Messmer, "Parallel Grid Manipulations for General Circulation Models," LNCS 2328 (Springer Verlag, 2001): 564-571.

V. Balaji, Tom Bettge, Byron Boville, Tony Craig, Carlos Cruz, Arlindo da Silva, Cecelia DeLuca, Brian Eaton, Bob Hallberg, Chris Hill, Mark Iredell, Rob Jacob, Phil Jones, Brian Kauffman, Jay Larson, John Michalakes, David Neckels, Jim Rosinski, William Sawyer, Shepard Smithline, Max Suarez, Weiyu Yang, Mike Young, and Leonid Zaslavsky, "Earth Science Modeling Framework: ESMF Requirements". In preparation, see http://www.esmf.ucar.edu for details.

Title: Genuine Multidimensional, Divergence-free Numerical Methods for the Equations of Magnetohydrodynamics

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

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The equations of magnetohydrodynamics (MHD) describe the flow of plasmas in interaction with a magnetic field. MHD equations are relevant in investigations in several areas of engineering and astrophysical research.

The MHD equations form a system of hyperbolic partial differential equations, which will be solved in this project by use of genuine multidimensional numerical schemes. A major difficulty in solving the MHD equations arises from the fact that the divergence of the magnetic field has to be zero at any time. That is, an additional constraint has to be imposed on the solution in each time step. Fortunately, this constraint is inherent to the equations, i.e. once fulfilled at the initial data it is fulfilled for all times. Thus the constraint does not change the character of the equations, as in the case of the incompressible flow.

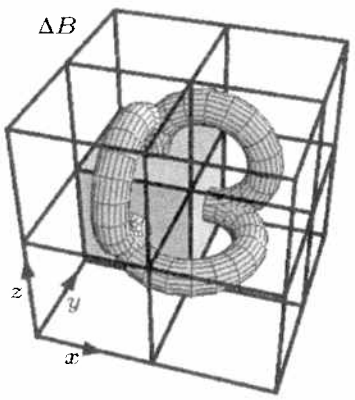


Figure 1: Divergence-preserving fluxes emerging from a grid cell in three dimensions. The fluxes have to approximate closed curves overstated as tubes in the figure.

It could be shown, that the additional constraint may be incorporated into the numerical method by special multidimensional flux formulations. This approach also has impacts on numerics in different fields where similiar constraints are present, like in electrodynamics, vorticity methods, meteorological flows and general relativity.

The large computations are parallelized and performed at the Beowulf cluster 'Asgard' at ETH Zürich.

References: M. Fey and M. Torrilhon, *A Constrained Transport Upwind Scheme for Divergence-free Advection*, Proc. 9. Intl. Conf. Hyperbolic Problems (2002), in press

Title: Theoretical and numerical study of axisymmetric triple flame.

Researchers: Marina Savelieva

Institute: Seminar for Applied Mathematics
Group: Department of Mathematics

Description:

Combination of both asymptotic analysis together with a perturbation theory methods are applied to the system of equations, describing reactive round jet. We get the analytical closed expressions for the propagation velocity of triple flamelet, formed on the base of lifted round jet flame. In these formulae explicit dependence of the velocity on mixture fraction gradient, flame curvature, as well as jet radius are presented. In order to validate these analytical results, numerical simulations are carried out. Full compressible Navier-Stokes equations are considered, and sixth-order finite-difference approximations are used in order to get high resolution, that is necessary for this multiscale problem. Big attention is payed to correct treatement of boundaries, as well as flow values on the inlet.

References:

Title: Numerical solution of high dimensional partial differential equations by the Feynman-Kac formula.

Researchers: F. M. Buchmann[1]
W. P. Petersen[1]

Institute/ Group [1] Seminar for Applied Mathematics

Description:

In many applications, for example finance or multiple species physics and chemistry applications, the underlying dimensionality of the space may be high. Unfortunately, the usual solution methods for solving partial differential equations (PDEs) describing these processes may become industrial tasks in dimensions higher than two. In this project, we are using Feynman-Kac formula to solve high dimensional PDEs by Monte-Carlo. Our experiments exceed dimension 64. The underlying simulations are of stochastic differential equations (SDEs). Although Monte-Carlo methods are subject to statistical errors, these are well understood and may be reduced by increasing the sample size N. The $N^{-1/2}$ statistical error behavior is independent of dimension. Our results show that the sensitivity to the simulation time step of our boundary finding algorithm actually decreases in higher dimensions.

Sub-samples may be computed independently, thus the ETH Beowulf cluster provides an excellent platform. Inter-CPU communication is small and sub-samples may be computed asynchronously. In consequence, simulations are easily parallelized, fault tolerant, and fairly simple to program.

This project is being funded by TH-Gesuch funds 0-20981-2, awarded in May 2002.

References

"Solving Dirichlet problems numerically using the Feynman- Kac representation," SAM Tech. Rep. 2002-01, Feb. 2002.
Submitted to *BIT*.

Title: A stochastically generated preconditioner for linear systems

Researchers: F. M. Buchmann[1]
W. P. Petersen[1]

Institute/ Group [1] Seminar for Applied Mathematics

Description:

When linear systems of the form $Ax = b$ are solved iteratively, preconditioning is often essential for good convergence. If an approximate inverse $M \approx A^{-1}$ is known, the transformed system $MAx = Mb$ is expected to have a smaller condition number, which yields faster convergence.

In this work, we construct M by simulating a Langevin equation, that is, a stochastic differential equation. The well known Ornstein-Uhlenbeck process (OUP) in n dimensions has an asymptotic invariant probability measure, namely, an n dimensional normal distribution with mean 0 and covariance matrix $(2A)^{-1}$. Simulating the trajectories of an OUP and approximating the covariance matrix is a promising *black box* for finding $M \approx (A)^{-1}$. We are investigating the performance of various numerical schemes for the system of stochastic differential equations and comparing the resulting condition numbers of the matrix MA. The number of iterations needed to solve the transformed system using iterative methods are also being studied.

The procedure to construct M will also work if A is not symmetric, when all the eigenvalues of A have positive real part. In that case, two n dimensional processes have to be simulated, using the same n stochastic increments for both of them.

References: "A stochastically generated preconditioner for linear systems," pre-print in preparation.

Title: Domain decomposition preconditioners for *hp* finite elements on anisotropically stretched meshes

Researchers: Dr. Andrea Toselli (Project Leader)
Dr. Xavier Vasseur

Institute: Seminar for Applied Mathematics
Group: Department of Mathematics

Description:

It is well-known that solutions of elliptic boundary value problems in polyhedral domains have corner and edge singularities. In addition, boundary layers may also arise in laminar, viscous, incompressible flows with moderate Reynolds numbers at faces, edges, and corners. Suitably graded meshes, geometrically refined towards corners, edges, and/or faces, are required in order to achieve a fast rate of convergence of hp finite element approximations.

In order to make the iterative solution of very large algebraic systems of finite element equations possible and efficient on parallel architectures, domain decomposition techniques (DD) have been used extensively in recent years. These methods are by now well-understood for standard equations (e.g., simple diffusion or viscous flow problems at moderate Reynolds number in regular 2-d or 3-d domains), with subdomains and meshes of regular shape. In this case, optimal or nearly optimal convergence of iterative solution techniques based on domain decomposition is by now well-established. This pertains to low order standard finite element discretizations as well as to high-order p-version or spectral element discretizations. However, their performance in general degrades drastically whenever anisotropic meshes or very thin subdomains are employed.

The purpose of this project is to extend some of the most popular and powerful DD methods to finite element approximations on anisotropic meshes of a wide class of equations. It consists of a theoretical part, where efficient methods are devised and analyzed, and a programming part, where these novel methods are implemented and tested on some real life problems.

This project is sponsored by the Swiss National Fund under Grant 20-63397.00.

Title: Numerical Schemes for Heat Conducting Colliding Astrophysical Flows

Researchers: Simin Motamen*
Jürg Marti*
Rolf Walder**

Institute/ *Seminar für angewandte Mathematik
**Institut für Astronomie
Group: Gruppe von Prof. Marti, ETHZ, Switzerland

Description:

We numerically investigate heat conducting colliding astrophysical flows. For ionized plasma the thermal diffusivity K depends on temperature ($K \propto T^{(5/2)}$). Such nonlinear heat conduction plays an important role, for example for X-ray emission.

The proposed numerical method is based on a splitting of the flow equations in an advective part, given by the Euler equations, and a diffusive part, given by the nonlinear heat conduction equation. For the calculation of the Euler equations in one dimension we use an existing code (AMRCART code, see http://www.astro.phys.ethz.ch/staff/walder/).

We have implemented several finite difference schemes for the nonlinear diffusion equation. The numerical scheme by Dai & Woodward with a fixed point method, the Crank-Nicolson scheme, and the L-stable TR-BDF2 method. The later two with the Newton method and the Thomas algorithm. We have performed several numerical simulations. From these we have found that in the absence of large density jumps the TR-BDF2 method allows for much larger time steps than the Crank-Nicolson scheme. However, in the presence of large density jumps comparable time steps have to be used in both methods. Hence, it is more efficient to use the Crank-Nicolson scheme as it requires less operations.

References: S. M. Motamen, PhD Thesis, to appear.

Institut für Hydromechanik und Wasserwirtschaft (IHW), ETH Hönggerberg Arbeitsgruppe W. Kinzelbach

Abstracts of projects involving computational science:

1.) Particle methods for the solution of transport equations and their application to nonlinear problems

This contribution investigates a novel particle method for solute transport in groundwater using a Lagrangian scheme. The grid-free character of particle methods and the straightforward physical interpretation distinguishes them from established methods such as finite differences or finite elements. The interest in particle methods is big due to the fact that accurate solutions not suffering from numerical dispersion and spurious oscillations can be obtained at competitive computational expense. The numerical scheme used, originally developed for viscous fluid flow carrying vorticity, is applied for the 2D and 3D simulation of non-reactive solute transport in groundwater.
We treat the advection-dispersion-equation by means of the Particle Strength Exchange method (PSE) describing the diffusive-dispersive process. The key idea of the method is the approximation of the differential diffusion operator by an integral operator, which is discretized using as quadrature points the locations of the particles. The distorted particle field must be occasionally remeshed onto a new structured field in order to maintain stability and accuracy.
The goal of the work is to develop a particle code, which is capable to calculate the phenomena of density fingering with variable fluid density. For the validation of the method, exact solutions, standard benchmark problems and the application to a field study concerning density instabilities will be utilized. The work is embedded in a joint ETH project between the Institute of Computational Science (Prof. P. Koumoutsakos, ICOS), the Laboratory for Thermodynamics in Emerging Technologies (Prof. D. Poulikakos, LTNT), and the Institute of Hydromechanics and Water Resources Management (Prof. W. Kinzelbach, IHW). The aim of the joint effort is to develop a fast "billion particle code" that would be modular and useful for a number of applications.

Contacts:

Stephanie Zimmermann, IHW, ETH Zürich; Jens Walther, ICOS, ETH Zürich; Wolfgang Kinzelbach, IHW, ETH Zürich; Petros Koumoutsakos, ICOS, ETH Zürich

Publications:

S. Zimmermann, P. Koumoutsakos, W. Kinzelbach, Simulation of Pollutant Transport Using a Particle Method, Journal of Computational Physics **173**, 322-347, 2001

2.) Stochastic modelling of well catchments

The project is part of the European Project W-SAHaRA (2000-2003) on 'Stochastic Analysis of Well Head Protection and Risk Assessment' comprising nine partners. Wellhead protection zones serve as an effective protection of groundwater against pollution by regulating human activities in areas around drinking wells. Stochastic computational methods are developed for the delineation of well catchments in aquifers of random heterogeneity, which may be conditioned on available measurements. The main task is to quantify the uncertainty in the extent of the well catchments. The methods comprise numerical Monte Carlo techniques, alternative methods of particle tracking, analytical stochastic approximations, as well as stochastic inverse modelling. The methodologies are applied to benchmarks and selected real-world cases. The results are conceived to serve as a basis to delineate wellhead protection zones. Furthermore, the methods will be used to develop a strategy for reducing the uncertainty of the results.

Contacts:

Harrie-Jan Hendricks Franssen, IHW ETH Zürich; Fritz Stauffer, IHW,ETH Zürich; Wolfgang Kinzelbach, IHW ETH Zürich.

Publications:

Stauffer F., S. Attinger, S. Zimmermann, and W. Kinzelbach, Uncertainty estimation of well head protection zones: A Lagrangian approximation. Proc. Int. Groundwater Symp. "Bridging the gap between measurement and modeling in heterogeneous media", March 25-28, 2002, Lawrence Berkeley National Laboratory, Berkeley, California, Editor A.N. Findikakis, p. 63-66, 2002.

Hendricks Franssen H.-J., F. Stauffer, and W. Kinzelbach, Impact of spatio-temporally variable recharge on the characteristics of well capture zones. Proc. 4th Int. Conf. on "Calibration and Reliability in Groundwater Modelling", ModelCARE 2002, June 17-20 2002, Prague, Czech Republic, Editors K. Kovar and Z. Hrkal, p. 472-476, 2002.

Hendricks Franssen H.-J., F. Stauffer, and W. Kinzelbach, Reducing the uncertainty of well capture zones by inverse conditioning. Proc. XIV. Int. Conf. on "Computational Methods in Water Resources", June 23-28, 2002, Delft, The Netherlands, Vol. 2, Editors, S.M. Hassanizadeh, R.J. Schotting, W.G. Gray, and G.F. Pinder; publ. in Series Developments in Water Science 47, Elsevier, Amsterdam, p. 1403-1410, 2002.

Stauffer F., S. Attinger, S. Zimmermann, and W. Kinzelbach, Uncertainty estimation of well catchments in heterogeneous aquifers. Accepted for publication in Water Resour. Res., 2002.

3.) Reactive transport in heterogeneous porous media

Many solutes transported by groundwater are not inert but undergo chemical reactions. Most commonly, one encounters adsorption resulting in an exchange of solute between the mobile fluid and immobile regions of the solid matrix. In the case of non-linear equilibrium adsorption the adsorbed concentration is a non-linear function of the dissolved concentration. This usually intensifies its influence on the transport behaviour compared to linear adsorption. At the same time the mathematical treatment becomes more difficult. Transport processes through heterogeneous porous media are usually investigated with stochastic models, which incorporate the heterogeneous structure of the medium. The stochastic theory is well established and linear transport phenomena have been studied using analytical and numerical methods. In the framework of this project we focus on transport processes with a non-linear Freundlich isotherm in a heterogeneous porous medium. Using methods of statistical physics such as perturbation theory and homogenisation theory we investigate the large-scale behaviour of the effective transport parameters. For strongly heterogeneous media, the semi-analytic approach fails and extensive Monte Carlo simulations are required to obtain ensemble properties of the medium. In the framework of a project of the Gesellschaft für Reaktorsicherheit, (Germany) a fast computation code is developed together with the Institute für Wissenschaftliches Rechnen in Heidelberg, the Institut of Mathematics of Bonn University and the Institut of Mathematics at the University of Freiburg. This code allows to compute ensembles on 3D heterogeneous media in a reasonable discretization. The results are of interest to nuclear waste repository planning.

Contacts:

Jiva Dimitrova, IHW, ETH-Zürich, Sabine Attinger, ICOS, ETH-Zürich, Wolfgang Kinzelbach, IHW, ETH-Zürich

Publications:

P. Bauer, S. Attinger, W. Kinzelbach, 2001, Transport of a decay chain in homogenous porous media: analytical solutions. J. Cont. Hydr., 49(2001)217-239
J. Dimitrova, S. Attinger, W. Kinzelbach, 2001, Large Scale Transport Behaviour of a Nonlinear Absorbing Solute in Heterogeneous Porous Media. Submitted to Water Resour. Res.
J. Dimitrova, S. Attinger, W. Kinzelbach, 2002, A Study of Nonlinear Multi-Scale Subsurface Transport: Numerical Results. Submitted to SIAM MMS.
J. Dimitrova, S. Attinger, W. Kinzelbach, 2002, A Study of nonlinear Multi-Scale Subsurface transport: Explicit Results. Submitted to SIAM MMS.

4.) Modelling of Density Driven Flows in Porous Media

Density driven flow is of interest in situations of seawater intrusion or up-coning of salt water from deep saline aquifers. The latter is the case in Brandenburg, Germany. In arid environments such as Botswana or Uzbekistan freshwater lenses form around ephemeral rivers and represent the only year-long available drinking water resource, the surrounding groundwater being saline or brackish. In this situation the exploitation of the freshwater lens by pumping must be well planned in order to avoid the attraction of saline water into drinking water wells. When a salt water layer forms on top of the aquifer, a phenomenon observed under saltpans or swamp islands in the arid tropics, fingering phenomena may develop and constitute an important mechanism of transporting salt water downward. We simulate density driven flow, which is quite demanding as far as discretization is concerned. Especially the unstable fingering situation is very sensitive to numerical artefacts. We start out to investigate the onset of instability by network models in 2D and 3 D. We also employ an algorithm based on the method of characteristics and a novel algorithm, which is developed in an ETH-project described above.

The work is embedded in the EU SALTRANS project involving the Weitzmann Institute, Israel, the Politechnical University of Catalonia, Barcelona, the Institute de Physique du Globe, Paris, and the universities of Rennes, Edinburgh and Leeds. Further means are made available through the INTAS framework together with Moscow University and scientists in Uzbekistan.

Contacts:

Rudolf Held, IHW ETH Zürich; Wolfgang Kinzalbach, IHW,ETH Zürich

Publications:

K. Johannsen, W. Kinzelbach, S. Oswald, and G. Wittum, Numerical simulation of density driven flow in porous media, Advances in Water Resources, 25(3), 335-348, 2002.

S.E. Oswaldand W. Kinzelbach, Three-dimensional physical benchmark experiments to test variable-density flow models, submitted to J. of Hydology 2002

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

Researchers: Nikolaus A. Adams, Andreas Jocksch, Leonhard Kleiser, Sebastian Müller, Benjamin Rembold, Philipp Schlatter, Steffen Stolz, Roland von Känel

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

Description:

Most engineering and geophysical flows occur at high Reynolds numbers. Due to their wide range of length and time scales such turbulent flows are not amenable to Direct Numerical Simulations (DNS). In Large-Eddy Simulations (LES), one only resolves the large scales, while their interaction with the non-resolved subgrid scales is modeled. Unlike solutions of the Reynolds-averaged Navier-Stokes equations (RANS), which are the workhorse for present-day industrial flow computations, LES are also able to provide information about the large-scale unsteady flow field that can be crucial for many problems such as fluid-structure interactions or noise generation. In addition, LES can be expected to yield much more reliable results for the mean flow and turbulence statistics than RANS.
In our recently developed 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. LES using ADM have already been demonstrated to give excellent results for a range of flows including isotropic turbulence, incompressible channel flow, supersonic compression ramp flow and rectangular jet flow, all at a fraction (order one percent) of the cost that would be needed for a DNS of the same flows.
The behavior of this novel approach has been studied further for the idealized case of homogeneous isotropic turbulence. The relation between ADM and the traditional eddy-viscosity approach was investigated. At the same time, application of the model is being extended to physically more complex flow cases involving transition, massive separation and swirl. Results obtained so far indicate that it is well possible to simulate transitional wall-bounded and free shear flows on the basis of the ADM approach. Large-scale simulations have been started for supersonic compression ramp flows at higher Reynolds numbers for which experimental data are available for comparison. Another recently started activity is the evaluation of DNS and LES data for subsonic jet flow with respect to noise radiation.
After successful demonstration of the power of ADM in high-order research codes, this approach was also implemented in an industrial-type finite volume code. Following successful test computations for a compressible turbulent channel flow, the more challenging case of turbulent shock-boundary-layer interaction was tackled. Results obtained to date are encouraging.

References: See separate list.

Title: Simulation of Particle-laden Flows

Researchers: Thorsten Bosse
Carlos Härtel
Leonhard Kleiser
Anna Kubik
Eckart Meiburg*
Frieder Necker

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser
*Dept. of Mechanical and Environmental Engineering,
University of California, Santa Barbara, CA, USA

Description:

In a first investigation we studied the dispersion of a suspension of small particles in a plane channel filled with clear fluid. In addition the case of a suspension volume deeply submerged in clear fluid has been studied. We consider dilute flows, i.e. flows with small particle concentrations where the particle-fluid interaction is the dominant process while particle-particle interactions may be neglected. The case of small particle Stokes numbers is considered which allows us to use a Eulerian approach also for the treatment of the particulate phase. High-resolution two- and three-dimensional simulations were performed to study issues such as the propagation speed of the suspension, the deposition of particles at the bottom wall, the mixing with ambient fluid, and the energy budget of the flow.
Ongoing work aims at an improved numerical modeling of turbulent particulate flows. The case of dilute two-way coupled flows is considered where the particles have a significant effect on the dynamics of the carrier fluid. Here the particulate phase is treated in a Lagrangian fashion by tracking each particle along its trajectory. A simplified one-dimensional test case, the settling of a suspension drop in a viscous fluid under gravity, has been employed to investigate effects of numerical model choices and parameters such as interpolation techniques, resolution, box size, Reynolds and Stokes numbers.
The behaviour of particles in a separated backward-facing step flow is being studied taking into account particle-wall interactions. Furthermore, the problem of turbulence modification by particles in a three-dimensional homogeneous isotropic setting is addressed. Simulation results will be assessed by comparison with experimental data.

References: See separate list.

Title: Large-scale Multi-agent Transportation Simulations

Researchers: N. Cetin,* B. Raney,* K. Nagel,* M. Vrtic,** K. Axhausen**

Institute/ Group: * Institute for Scientific Computing, Dept. of Computer Science, ETHZ
** Inst. of Transportation, Traffic, Highway- and Railway- Engineering (IVT), ETHZ

Description:

Traffic modeling is a challenging subject since not only the flow of the traffic through the city needs to be modeled, but also what causes traffic in the first place, i.e. the human decisions leading to travel. Our approach is *agent-based*, which means that we resolve each traveler individually throughout all modules of the simulation package. In contrast to physics particles, agents have more interal complexity. Since a metropolitan area can have of the order of 10^7 travelers, this poses a considerable computing challenge.

Our overall approach consists of separating a physical simulation layer, where the agents have very limited capabilities such as collision avoidance and lange changing, from a tactical/strategic layer, in which the agents compute decisions such as route or destination choice. – The physical simulation layer is represented by the traffic micro-simulation. We use parallel computing to achieve satisfactory computing speeds. The hardware is a 128-CPU Beowulf cluster with Ethernet communicatin; 64-CPUs are also connected via Myrinet. We reach simulation speeds of up to 300 times faster than real time for 10^6 particles in the simulation; this corresponds to doing a simulation of all car traffic in all of Switzerland during a full 24-hour day within 5 min of computing time.

The tactical/strategic layer currently consists of activities generation (what do people do during a day and where?), and route planning (how do people get to their destinations?). Since these modules interact, it is necessary to iterate between them, meaning that the computing burden increases even further. We also use a so-called agent database where the agents keep track of their strategies and the scores of those strategies. In the case of traffic simulation, a strategy is a specific activity plan and an associated route plan, and a score is the travel time required to complete that plan.

Our future plans go in two directions: (1) Real-world case studies. (2) A distributed plug-and-play implementation, where additional modules can be added on an arbitrary CPU of the cluster, and the framework will take care of using them for the simulation.

Selected references:

[1] N. Cetin and K. Nagel. Parallel queue model approach to traffic microsimulations, submitted. See www.inf.ethz.ch/personal/nagel/papers. Earlier version presented at Swiss Transportation Research Conference (STRC), Monte Verita, 2002.

[2] B. Raney, N. Cetin, A. Völlmy, and K. Nagel. Large scale multi-agent transportation simulations. In *Proceedings of the annual congress of the European Regional Science Association (ERSA)*, Dortmund, Germany, Aug 2002. Also see www.inf.ethz.ch/~nagel/papers.

[3] B. Raney and K. Nagel. Iterative route planning for modular transportation simulation. In *Proceedings of the Swiss Transport Research Conference*, Monte Verita, Switzerland, March 2002. See www.strc.ch.

See also `http://www.inf.ethz.ch/~nagel/projects/traffic`.

Title: Planning with Virtual Alpine Landscapes and Autonomous Agents

Researchers: C. Gloor,* K. Nagel*, D. Cavens**, E. Lange**, W. Schmid**

Institute/ Group: * Inst. for Scientific Computing, Dept. of Computer Science, ETHZ
** Institute for National, Regional, and Local Planning (ORL), ETHZ

Description:

The visual quality of the landscape is an important but often neglected factor in landscape and environmental planning. Especially for the recreation potential, the quality of the visual landscape plays a key role.

Up to now, the judgement of human preferences about the landscape and landscape elements is based on the existing landscape, either by placing people into or monitoring people in the real environment, or by exposing test persons to visual surrogates such as photographs of the real landscape.

Recent developments in the virtual representation of landscapes suggest that it might be possible to reliably observe the behaviour and deduct landscape preferences of people in a more controlled laboratory environment as it is provided through new developments in computer and projection technology. Such visualizations permit to show the visual landscape both at present and at potential future situations, giving a tool to systematically investigate how people react to changes in the landscape.

Such a visualization of a changed landscape would be unpopulated, since no data about human behaviour existed for this changed landscape. Autonomous agents modeling enables one to populate the virtual world with rule-driven agents which can act as surrogates for real humans.

The two main modules that we need are a visualization and a simulation. The visualization is both useful for standalone applications (for example fly-overs over the investigated landscape) and for animation of the simulation (for example populating the landscape with autonomous agents; showing the landscape from one particular agent's view).

The simulation is responsible for moving the hiking agents through the area of interest. Besides low-level path following and pedestrian interaction rules, this also includes modules for tactical and strategic decisions, such as route finding and destination choice. The different decision levels are implemented via different, interacting modules. The different pieces of software are coupled via protocols.

See also `http://www.inf.ethz.ch/~nagel/projects/alpsim/`
or `http://www.orl.arch.ethz.ch/~Lange/research_NFP48.html`.

Title: The influence of the muscle fiber orientation on the mechanical behavior of the human ventricles: A finite element model approach

Researchers: Peter Niederer[*]
Paul P. Lunkenheimer[**]
Farshad Dorri[*]

Institute: [*] Institute of Biomedical Engineering
University and ETH, Zürich, Switzerland
[**] Exp, Thorax, Heart and Vessel surgery
University of Münster, Germany

Description:

An important aspect of cardiodynamics (*i.e.*, the mechanics of the human heart) is related to the architecture of the ventricular muscle fibers. Although there are presently no methods to determine the fiber orientation in the human myocardium under *in vivo* conditions and nonivasively, advanced clinical imaging methods allow for an analysis of the deformation pattern of the heart with a high resolution in space and time.

Mathematical models of the human heart are intended to facilitate an in-depth understanding of cardiodynamics, particularly as it relates to the left ventricle. For this purpose, we develop a finite-element model to analyse the contraction and relaxation processes of the left ventricle by including the anisotropy associated with the fibrous structure of the myocardium and by prescribing the active fiber contraction pattern. The results of the simulation are assessed primarily by comparison with MRI imaging and tagging data. Under pathologic conditions such as hypertrophy or infarction, furthermore, the fiber structure will be changed, and computer modelling of these pathologies is intended to be of help in the diagnosis and treatment of these diseases.

Title: A mathematical model of the human kidney for use in trauma research.

Researchers: Mehdi Farshad[*]
Peter Niederer[**]
Franz Schmidlin[***]
Jess Snedeker[**]

Institute/ Group:
[*] EMPA Duebendorf, Switzerland
Abt. Kunstoffe/Composites
[**] University and ETH Zurich, Switzerland
Institute of Biomedical Engineering
[***] University Hospital, Geneva, Switzerland
Department of Urology

Description:

A model of the human kidney has been constructed that is based on a continuum mechanics approach whereby the Finite Element method is applied. The current model encompasses a realistic gross anatomy (including the effects of the inhomogeneous structure of the kidney), the nonlinear, viscoelastic characteristics of the constituent tissues, as well as considerations for the fluidic structures such as blood vessels and the urine collection system. Ultimately, the boundary conditions of the model will reflect the complicated mechanical environment in which the kidney is embedded within the human body. The completed model can then be subjected to typical loading patterns derived from accidental impact situations, and exploited to analyze injury mechanisms with the ultimate goal of advancing injury protection strategies.

Reference:

JG Snedeker, M Bajka, JM Hug, G Székely, P Niederer
The Creation of a High-Fidelity Finite Element Model of the Kidney for Use in Trauma Research.
J Visualization and Computer Animation, **13** (2002) 53 - 64

CSE research project description

Title: *Ab initio* molecular dynamics-based assignment of the protonation state of pepstatin A/HIV-1 protease cleavage site

Researchers: Stefano Piana*
Daniel Sebastiani**
Paolo Carloni*
Michele Parrinello***

Institute/ Group: *Scuola Internazionale Superiore di Studi Avanzati and Istituto di Fisica della Materia, Trieste, Italy
**Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
***Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

A recent ^{13}C NMR experiment (Smith et al. *Nature Struct. Biol.* **1996**, *3*, 946-950) on the Asp 25-Asp25' dyad in pepstatin A/HIV-1 protease measured two separate resonance lines, which were interpreted as being a singly protonated dyad. We address this issue by performing *ab initio* molecular dynamics calculations on models for this site accompanied by calculations of ^{13}C NMR chemical shifts and isotopic shifts. We find that already on the picosecond time-scale the model proposed by Smith et al. is not stable and evolves toward a different monoprotonated form whose NMR pattern differs from the experimental one. We suggest, instead, a different protonation state in which both aspartic groups are protonated. Despite the symmetric protonation state, the calculated ^{13}C NMR properties are in good agreement with the experiment. We rationalize this result using a simple valence bond model, which explains the chemical inequality of the two C sites. The model calculations, together with our calculations on the complex, allow also the rationalization of ^{13}C NMR properties on other HIV-1 PR/inhibitor complexes. Both putative binding of the substrate to the free enzyme, which has the dyad singly protonated (Piana, S.; Carloni, P. *Proteins: Struct. Funct. Genet.* **2000**, 39, 26-36), and pepstatin A binding to the diprotonated form are consistent with the inverse solvent isotope effect on the onset of inhibition of pepsin by pepstatin and the kinetic iso-mechanism proposed for aspartic proteases (Cho, T.-K.; Rebholz, K.; Northrop, D.B. *Biochemistry* **1994**, 33, 9637-9642).

References: J. Am. Chem. Soc. **123** (2001) 8730

Title: Dehydroxylation and silanization of the surfaces of _-cristobalite silica: an *ab initio* simulation

Researchers: S. Iarlori*
D. Ceresoli*
M. Bernasconi*
D. Donadio*
M. Parrinello**

Institute/ Group: *Pirelli Cavi e Sistemi, Istituto Nazionale per la Fisica della Materia and Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, Italy
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

Dehydroxylation and silanization processes on the silica surface are studied by *ab initio* molecular dynamics. The (100) and (111) surfaces of _-cristobalite are used as two possible models of the hydroxylated amorphous surface. The activation energy and latent heat for the dehydroxylation reactions of the (100) surface computed by constrained *ab initio* molecular dynamics are in reasonable agreement with experimental data on the amorphous surface. Adhesion reactions of silanes are simulated, aiming at elucidating the binding mechanism of organosilanes used for instance as silica-polymer coupling agents. The simulations have provided insights into the occurrence of multiple silica-silane bonds and on the role of hydrolization of silane by physisorbed water in the adhesion on the wet surface.

References: J. Phys. Chem. B **105** (2001) 8007

Title: Medium effects on ^{51}V NMR chemical shifts: a density functional study

Researchers: Michael Bühl*
Michele Parrinello**

Institute/ Group: *Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

Car-Parrinello molecular dynamics simulations were performed for $[H_2VO_4]^-$, $[VO_2(OH_2)_4]^+$, and $[VO(O_2)_2(OH_2)]^-$ in periodic boxes with 30, 28, and 29 water molecules, respectively, employing the BLYP density functional. On the timescale of the simulations, up to 2 ps, well-structured first solvation spheres are discernible for $[H_2VO_4]^-$ and $[VO(O_2)_2(OH_2)]^-$ containing, on average, eight and ten water molecules, respectively. One of the four water molecules directly attached to the metal in $[VO_2(OH_2)_4]^+$ is only loosely bound, and the average coordination number of vanadium in aqueous VO_2^+ is between five and six. ^{51}V chemical shifts were evaluated at the B3LYP level for representative snapshots along the trajectories, including the water molecules of the solvent by means of point charges. The resulting averaged _(^{51}V) values are proposed to model the combined effects of temperature (dynamic averaging) and solvent (charge polarization). Both effects are shown to be rather small, of the order of a few dozen ppm. The observed shielding of ^{51}V in the bis(peroxo) complex with respect to the vanadate species is not reproduced computationally.

References: Chem. Eur. J. **20** (2001) 4487

Title: Accurate total energies without self-consistency

Researchers: David M. Benoit*
Daniel Sebastiani**
Michele Parrinello*

Institute/ Group: * Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland
**Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Description:

We present a new way of calculating approximate but accurate total energies within the framework of density functional theory. Our technique is based on an expansion of the energy functional to second order and does not require self-consistent iterations of the total density. The functional can be minimized by using the same techniques as developed for variational density functional perturbation theory. The method is ideally suited to systems composed of weakly interacting fragments, but it can also be applied to semi-conductors and insulators. We show the versatility of our approach in a variety of examples exhibiting different types of chemical bonding.

References: Phys. Rev. Lett. **87** (2001) 226401

Title: Role of conformational fluctuations in the enzymatic reaction of HIV-1 protease

Researchers: Stefano Piana*
Paolo Carloni*
Michele Parrinello**

Institute/ Group: * Scuola Internazionale Superiore di Studi Avanzati and Istituto Nazionale di Fisica della Materia, Trieste, Italy
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

The emergence of compensatory drug-resistant mutations in HIV-1 protease challenges the common view of the reaction mechanism of this enzyme. Here we address this issue by performing classical and *ab-initio* molecular dynamics simulations (MD) on a complex between the enzyme and a peptide substrate. The classical MD calculation reveals large-scale protein motions involving the flaps and the cantilever. These motions modulate the conformational properties of the substrate at the cleavage site. The *ab-initio* calculations show in turn that substrate motion dramatically modulates the activation free energy barrier of the enzymatic reaction. Thus, the catalytic power of the enzyme does not arise from the presence of a pre-organized active site but from the protein thermal fluctuations. The implications of this finding for the emergence of drug resistance are discussed.

References: J. Mol. Biol. **319** (2002) 567

Title: Structure and chemical activity of point defects on $MgCl_2$ (001) surface

Researchers: Karine Costuas*
Michele Parrinello*

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

$MgCl_2$ is a support of choice for industrial production of polyolefins in Ziegler-Natta catalysis. Recent experiments have shown that the inert (001) $MgCl_2$ surface can be activated by electron irradiation. To better understand this process, we have studied the properties of point defects on the (001) surface and their interaction with $TiCl_4$. We have used density functional theory and Car-Parrinello methods and calculated mono- and di-vacancies of Cl and Cl^-. Particularly interesting is the case of Cl di-vacancy, which is heavily reconstructed and forms with $TiCl_4$ a structure where the Ti atom is bonded with a Mg atom.

References: J. Phys. Chem. B. **106** (2002) 4477

Title: Anharmonic Raman spectra in high-pressure ice from *ab initio* simulations

Researchers: Anna Putrino*
Michele Parrinello**

Institute/ Group: *Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

We calculate from *ab initio* molecular dynamics the Raman scattering of high-pressure ice. To this effect we apply a new method based on the Berry phase theory of polarization. Our results are in agreement with recent and difficult experiments and are compatible with a picture in which ice VII is a proton-disordered system and in ice X the hydrogen bond is symmetric.

References: Phys. Rev. Lett. **88** (2002) 176401

Title: Classical polarizable force fields parametrized from *ab initio* calculations

Researchers: Gloria Tabacchi*
Christopher J. Mundy**
Jürg Hutter***
Michele Parrinello****

Institute/ Group: *Dipartimento di Scienze Chimiche, Fisiche e Matematiche, Università dell'Insubria, Como, Italy
**Chemistry and Materials Science L-231, Lawrence Livermore National Laboratory, Livermore, California, USA
***Physical Chemistry Institute, Universität Zürich, Zürich, Switzerland
****Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

A computationally efficient molecular dynamics implementation of a polarizable force field parametrized from *ab initio* data is presented. Our formulation, based on a second-order expansion of the energy density, models the density response using Gaussian basis functions derived from density functional linear response theory. Polarization effects are described by the time evolution of the basis function coefficients propagated via an extended Lagrangian formalism. We have devised a general protocol for the parametrization of the force field. We will show that a single parametrization of the model can describe the polarization effects of LiI in the condensed phase.

References: J. Chem. Phys. **117** (2002) 1416

Title: *Ab-initio* study of NMR chemical shifts of water under normal and supercritical conditions

Researchers: Daniel Sebastiani*
Michele Parrinello**

Institute/ Group: *Max Planck Institute for Polymer Research, Mainz, Germany
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

We present a theoretical investigation of the hydrogen nuclear magnetic resonance (NMR) chemical shift and the magnetic susceptibility of normal and supercritical water using a recently developed *ab initio* approach in the framework of density functional perturbation theory. The results are in very good agreement with experiment. The shifts can be used to determine whether the atomic configurations, taken from a first principles simulation, give a good description of the system on a microscopic scale. In particular, the hydrogen chemical shifts are very sensitive to the character of the hydrogen bond network, which plays a crucial role in the macroscopic properties of liquid water under normal and supercritical conditions.

References: ChemPhysChem **3** (2002) 675

Title: *Ab-initio* X-ray scattering of liquid water

Researchers: Matthias Krack*
Alfredo Gambirasio*
Michele Parrinello*

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

A direct calculation of the coherent X-ray scattering spectrum of liquid water under ambient conditions is presented using *ab-initio* density functional theory (DFT). The experimental data are compared with the calculated X-ray scattering spectra retrieved from the trajectories of two Car-Parrinello molecular dynamics (CPMD) runs of about 10 ps with 32 and 64 water molecules in the simulation cell, respectively. Furthermore, the X-ray spectra obtained from MD runs of 20 ps for 128 water molecules using empirical water models are presented. All calculations were performed with the QUICKSTEP code, which includes an all-electron implementation of the Gaussian augmented plane wave (GAPW) method. It is shown that by this approach one can assess how well different models describe the structural properties of water.

References: A manuscript has been submitted to J. Chem. Phys. (2002, in press)

Title: Action-derived molecular dynamics in the study of rare events

Researchers: Daniele Passerone*
Michele Parrinello*

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

We present a practical method to generate classical trajectories with fixed initial and final boundary conditions. Our method is based on the minimization of a suitably defined discretized action. The method finds its most natural application in the study of rare events. Its capabilities are illustrated by non-trivial examples. The algorithm lends itself to straightforward parallelization, and when combined with *ab initio* molecular dynamics it promises to offer a powerful tool for the study of chemical reactions.

References: Phys. Rev. Lett. **87** (2001) 108302

Title: Efficient k.p method for the calculation of total energy and electronic density of states

Researchers: Marcella Iannuzzi*
Michele Parrinello*

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

An efficient method for calculating the electronic structure in large systems with a fully converged BZ sampling is presented. The method is based on a k.p-like approximation developed in the framework of density functional perturbation theory. The reliability and efficiency of the method are demonstrated in test calculations on Ar and Si supercells.

References: Phys. Rev. B **64** (2001) 233104

Title: Quantum-classical simulation of proton transport via a phospholipid bilayer

Researchers: Dirk Zahn*
Karl F. Schmidt**
Stefan M. Kast**
Jürgen A. Brickmann**

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland
**Institut für Physikalische Chemie, Universität Darmstadt, Germany

Description:

The protonation of N-methylacetamide by a hydronium ion is investigated by means of *ab initio* methods and statistical-mechanical integral equation theory. The proton transfer reaction is treated as a function of a two-dimensional coordinate. It is monitored in terms of the distance of the transferred proton to the amide oxygen atom and the distance of the oxygen atoms of the amide and the hydronium. The energy profile of the reaction is calculated for the isolated system as well as for the reaction in aqueous solution. The reaction in vacuum is investigated by *ab initio* calculations. The solvent effect is modeled on the basis of a classical approach using the reference interaction site model (RISM) integral equation theory. Therein reactant and product states are described by classical force fields. A smooth transition between both states is modeled using a continuous switching function. The proton transfer potential was calculated for the average solvent effect. As a result, the minimum energy path for amide protonation is determined as a function of a one-dimensional reaction coordinate.

References: J. Phys. Chem. A., **106** (2002), 7807-7812

Title: Theory of quantum annealing of an Ising spin glass

Researchers: Giuseppe E. Santoro*
Roman Martoňák**
Erio Tosatti***
Roberto Car****

Institute/ Group: *SISSA, Trieste, Italy
**Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland
***INFM/SISSA/ICTP, Trieste, Italy
****Department of Chemistry and Princeton Materials Institute, Princeton University, New Jersey, USA

Description:

Quantum annealing was recently found experimentally in a disordered spin 1/2 magnet to be more effective than its classical, thermal counterpart. Comparing classical and quantum Monte Carlo annealing protocols on the random two-dimensional Ising model we confirm the superiority of quantum relative to classical annealing. We also propose a theory of quantum annealing, based on a cascade of Landau-Zener tunneling events, which rationalizes these findings. For both classical and quantum annealing, the residual energy after annealing decreases only as a logarithm, to an exponent $-\zeta$, of the annealing time τ, but the quantum case has a larger value for ζ which makes it faster.

References: Science **295** (2002) 2427

Title: Bending strain-driven modification of surface reconstructions: Au(111)

Researchers: U. Tartaglino*
Erio Tosatti**
Daniele Passerone***
F. Ercolessi****

Institute/ Group: *INFM/SISSA, Trieste, Italy
** INFM/SISSA/ICTP, Trieste, Italy
***Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland
****Dipartimento di Fisica, Università di Udine, Italy

Description:

Strain can affect the morphology of a crystal surface, and cause modifications of its reconstruction even when weak, as in the case of mechanical bending. We carried out calculations of strain-dependent surface free energy and direct bending simulations demonstrating the change of incommensurate reconstruction in Au(111) under strain, in good agreement with recent data. Time-dependent strain should cause a sliding of the topmost layer over the second, suggesting an interesting case of nanofriction. Bending strain could also be used to fine tune the spacing of selectively absorbed nanoclusters.

References: Phys. Rev. B **65** (2002) 241406

Title: Molecular dynamics study of water pores in a phospholipid bilayer

Researchers: Dirk Zahn*
Jürgen A. Brickmann**

Institute/ Group: *Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland
**Institut für Physikalische Chemie, Unversität Darmstadt, Germany

Description:

A molecular dynamics study of a hydrated phospholipid bilayer is reported. Therein the stability of initially formed water pores in phospholipid membranes is investigated by means of computer experiments based on a microscopic membrane model. The pore lifetimes were found to be in the range of 100 ps. The probability of finding water molecules in the hydrophobic interior of the membrane is discussed. Our results give evidence for the existence of water pores in phospholipid membranes which are sufficiently thin.

References: Chem. Phys. Lett. **352** (2002), 441

Title: The nature and transport mechanism of hydrated hydroxide ions in aqueous solution

Researchers: Mark E. Tuckerman*
Dominik Marx**
Michele Parrinello***

Institute/ Group: *Dept. of Chemistry, New York University, New York, USA
**Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Fakultät für Chemie, Bochum, Germany
***Swiss Center for Scientific Computing (CSCS/ETH), Manno, Switzerland

Description:

Compared to other ions, protons (H^+) and hydroxide ions (OH^-) exhibit anomalously high mobilities in aqueous solutions. On a qualitative level, this behaviour has long been explained by 'structural diffusion' – the continuous interconversion between hydration complexes driven by fluctuations in the solvation shell of the hydrated ions. Detailed investigations have led to a clear understanding of the proton transport mechanism at the molecular level. In contrast, hydroxide ion mobility in basic solutions has received far less attention, even though bases and base catalysis play important roles in many organic and biochemical reactions and in the chemical industry. The reason for this may be attributed to the century-old notion that a hydrated OH^- can be regarded as a water molecule missing a proton, and that the transport mechanism of such a 'proton hole' can be inferred from that of an excess proton by simply reversing hydrogen bond polarities. However, recent studies have identified OH^- hydration complexes that bear little structural similarity to proton hydration complexes. Here we report the solution structures and transport mechanisms of hydrated hydroxide, which we obtained from first-principles computer simulations that explicitly treat quantum and thermal fluctuations of all nuclei. We find that the transport mechanism, which differs significantly from the proton hole picture, involves an interplay between the previously identified hydration complexes and is strongly influenced by nuclear quantum effects.

References: Nature **417** (2002) 925

Title: Scale-Space Techniques for Feature Extraction in Flow Data

Researchers: Dr. Ronald Peikert
Dirk Bauer
Mie Sato

Institute/ Group: Institute of Scientific Computing
Computer Graphics Laboratory

Description:

Scale-space techniques have become popular in computer vision for their capability to access the multi-scale information inherently contained in images. Recently, the use of these techniques has been extended to the field of scientific visualization. When applied to feature extraction problems, this results in more coherent features and less sensitivity to both numerical artifacts and irrelevant large-scale features. We implemented scale-space computation for unstructured hexahedral grids using finite elements[4] and demonstrated that performance is sufficient for computing a scale-space of time-dependent CFD data. The problem of feature tracking arises when data from either multiple scales or multiple time steps have to be analyzed. For a specific application, the extraction of vortex cores from velocity and/or pressure fields, we obtained an implicit tracking by extending a class of feature extraction schemes from three to four dimensions[1]. Further processing of the extracted features can be the computation of vortex hulls from vortex cores[3], or the selective visualization of the flow within data-guided regions of interest[2].

References:

1. D. Bauer, R. Peikert, Vortex Tracking in Scale-Space, In: *Data Visualization 2002, Proceedings of Joint Eurographics - IEEE TCCG Symposium on Visualization,* May 2002, ACM SIGGRAPH Press.
2. D. Bauer, R. Peikert, M. Sato, M. Sick, A Case Study in Selective Visualization of Unsteady 3D Flow, To appear in: *Proceedings of IEEE Visualization '02*, IEEE Computer Society Press, pp. 1-4, October 2002.
3. M. Sato, R. Peikert, Core-Line Based Vortex Hulls in Turbomachinery Flows, submitted (2002) to *IEICE Trans. Fundamentals*.
4. F. Sadlo, Glättung in unstrukturierten Hexaedergittern mittels Finiter Elemente, *Semesterarbeit im Computer Graphics Laboratory, ETH Zürich*, 2001.

Title: Use of structure generators for automatic structure elucidation and database search

Researchers: Patrick Fontana
Martin Badertscher
Pius Portmann
Ernö Pretsch

Institute/ Group: Laboratory of Organic Chemistry
Group of Prof. E. Pretsch
In cooperation with
Prof. M.E. Munk, Arizona State University
Pius Portmann, Upstream Solutions, Zürich

Description:

The structure generator, Assemble 2.1, has been successfully used as a versatile structure search system with features presently not available in any of the publicly accessible programs. It can be adapted to any database having structures in a standard format (e.g., SD file). The results can be exported or used as input for further searches.

A program has been developed that automatically extracts structural information from infrared, ^{1}H and ^{13}C NMR spectra. The resulting substructures required to be present or absent as well as other structural constraints can be edited by the user or directly processed by the structure generator, Assemble 2.1. Tests with over 100 sets of spectra have shown a high reliability in that not a single incorrect interpretation has occurred. The automatic spectra interpretation allows the number of possible isomers given by the molecular formula alone to be reduced to 1.5% on average. After ranking the resulting isomers based on their ^{1}H and ^{13}C NMR chemical shifts and multiplicities, the correct structure in each case has been found as the best or within the few best solutions.

References:

M. Badertscher, K. Bischofberger, M.E. Munk, and E. Pretsch
A novel formalism to characterize the degree of unsaturation of organic molecules
J. Chem. Inf. Comput. Sci. **41** (2001) 889–893

P. Fontana and E. Pretsch
Automatic spectra interpretation, structure generation and ranking
J. Chem. Inf. Comput. Sci. **42** (2002) 614–619

Title: Dynamics of Ferromagnets and Liquid Crystals

Researcher: Andreas Prohl*
Martin Kružík**

Institute/ Group: *Department of Mathematics, ETH Zürich
Seminar of Applied Mathematics
**Center of Advanced European Studies and Research (CAESAR), Bonn

Description:

Ferromagnetic materials are widely used as recording media. Their magnetic patterns are described by the well-accepted model of Landau and Lifshitz. Over the last years, different strategies have been developed to tackle the related non-convex minimization problem: direct minimization, convexification, and relaxation by using Young measures. Nonstationary effects are considered in the extended models of Landau, Lifshitz and Gilbert for (electrically conducting) ferromagnets. Finally, new nonstationary macroscopic models to understand hysteresis phenomena are studied.

The objective of this project is a numerical analysis of these models. Convergence behavior of different finite element schemes for solving the stationary problem is discussed. Then, numerical analyses of different penalization/projection strategies in nonstationary micromagnetism are provided; further results include the analysis, numerical analysis, and scientific computation for nematic liquid crystals.

References: A. Prohl, *Computational Micromagnetism*, Teubner (2001)
M. Kružík, A. Prohl, *Macroscopic modeling of magnetic hysteresis*, Preprint (2002).

Title: Gas Phase Kinetics, Encyclopedia of Chemical Physics and Physical Chemistry, Chapter A.3.4

Researchers: D. Luckhaus
M. Quack

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

Description:

Experimental and theoretical including computational work on gas phase kinetics is reviewed.

References:

D. Luckhaus and M. Quack
Encyclopedia of Chemical Physics and Physical Chemistry Vol. 1 (Fundamentals), Chapter A.3.4, pages 653–682 (IOP publishing, Bristol 2001, ed. by J. H. Moore and N. D. Spencer)

Title: Energy Redistribution in Reacting Systems

Researchers: R. Marquardt
M. Quack

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

Description:

Experimental and theoretical including computational work on energy redistribution is reviewed.

References:

R. Marquardt and M. Quack
Encyclopedia of Chemical Physics and Physical Chemistry Vol. 1 (Fundamentals), Chapter A.3.13, pages 897–936 (IOP publishing, Bristol 2001, ed. by J. H. Moore and N. D. Spencer)

Title: Gas Phase Kinetics Studies

Researchers: D. Luckhaus
M. Quack

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

Description:

Experimental and theoretical including computational gas phase kinetics studies are reviewed.

References:

D. Luckhaus and M. Quack
Encyclopedia of Chemical Physics and Physical Chemistry Vol. 2 (Methods), Chapter B.2.5, pages 1871–1904 (IOP publishing, Bristol 2001, ed. by J. H. Moore and N. D. Spencer))

Title: Analytical three-body interaction potentials and hydrogen bond dynamics of hydrogen fluoride aggregates $(HF)_n$, $n \geq 3$

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

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

Description:

Oligomeric aggregates of hydrogen fluoride are important prototype molecules for a detailed understanding of the structure, energetics, spectroscopy and dynamics of hydrogen bonding. The pairwise additive description of these oligomers is known to be inadequate. We have sampled the three-body potential for HF at 3000 $(HF)_3$ configurations selected by various classical and quantum sampling techniques, including dynamic sampling based on Voronoi step representation. The counterpoise-corrected Møller-Plesset second-order three-body energies using a double zeta gaussian basis set with polarization functions (DZP+MP2) at these configurations are fitted by analytical 12-dimensional potentials. Cooperative effects are found to be sizeable and predominantly stabilizing in hydrogen fluoride ring aggregates. Test calculations with larger basis sets and for larger HF aggregates show that in combination with available high quality pair potentials, the analytical three-body terms give an excellent description of the $(HF)_3$ surface in the hydrogen bonding region and a good approximation for clusters up to at least the hexamer. Multidimensional vibrational quantum Monte Carlo calculations indicate that degenerate HF stretch excitation in $(HF)_3$ (3712 cm^{-1}) is in close coincidence with $(HF)_3 \rightarrow 3$ HF dissociation channels at low HF angular momentum, whereas degenerate DF stretch excitation in $(DF)_3$ (2725 cm^{-1}) falls slightly below any $(DF)_3 \rightarrow (DF)_2 + DF$ dissociation channels. The $(HF)_3$ potential surface, its stationary points, possible interconversion tunneling pathways, zero point energies, adiabatic channels, unusual isotope effects, fully centrifugal rotational states and the harmonic infrared spectrum are discussed in detail and compared to ab initio calculations and experiment.

References:

[1] M. Quack, J. Stohner and M. Suhm, J. Mol. Structure **599**, 381–425 (2001)
[2] M. Quack and M.A. Suhm, in "Conceptual Perspectives in Quantum Chemistry", p. 415-463, E.S. Kryachko and J.L. Calais eds., Kluwer, Dordrecht 1997
[3] M. Quack and M.A. Suhm, in "Advances in Molecular Vibrations and Collision Dynamics, Vol. III, Molecular Clusters", p. 205-248, Z. Bacic & J. Bowman eds., JAI press, Stamford, Conn. and London, England 1998 (ISBN: 1-55938-790-4)

Title: High resolution analysis of the complex symmetric stretching chromophore absorption in CF_3I

Researchers: Y. He*
H. Hollenstein*
M. Quack*
E. Richard*
M. Snels**
H. Bürger***

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Istituto per Materiali Speciali, CNR, Potenza
*** Anorganische Chemie, Bergische Universität, Wuppertal

Description:

Very high resolution spectra of CF_3I have been measured by slit jet diode laser and FTIR techniques and are analyzed theoretically. Extensive numerical calculations are carried out in the simulations of the spectra.

References:

[1] Y. He, H. Hollenstein, M. Quack, E. Richard, M. Snels and H. Bürger J. Chem. Phys **116**, 974–983 (2002)
[2] H. Hollenstein, M. Quack and E. Richard, Chem. Phys. Lett. **222**, 176-184 (1994)
[3] M. Quack, Annual Rev.Phys. Chem. **41**, 839-874 (1990)

Title: Molecules in Motion

Researchers: M. Quack

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

Description:

We investigate the fundamental physical-chemical primary processes of chemical reactions. We have developed a conceptually new approach to derive these primary processes of intramolecular kinetics on time scales leading into the femtosecond and subfemtosecond domain on the basis of infrared spectroscopy with high frequency resolution but without short-time resolution. Selected applications include intramolecular wavepacket dynamics of chemical functional groups of isolated, individual molecules and IR-laser chemistry of molecules under infrared multiphoton excitation, hydrogen bond tunneling dynamics in hydrogen fluoride clusters $(HF)_2$ and the tunneling stereomutation of prototypical chiral molecules. One of the greatest current challenges is the elucidation of the influence of the parity violating weak interaction mediated by the Z-Boson of high energy physics on the dynamics of chiral molecules.
Experimental and theoretical work including computational work is reviewed.

References:

[1] M. Quack, Chimia **55**, 753–758 (2001)
[2] M. Quack, chapter 27 in: "Femtosecond Chemistry", J. Manz and L. Woeste eds., Proc. Berlin Conf. Femtosecond Chemistry, Berlin (March 1993), Verlag Chemie, Weinheim (1994), p. 781-818

Title: Parity violation dominates the Dynamics of Chirality in Dichlorodisulfane

Researchers: R. Berger**
M. Gottselig*
M. Quack*
M. Willeke*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Institut für Chemie, TU Berlin (present address)

Description:

According to the traditional point of view on the structure and dynamics of chiral molecules, parity violation would be too small to be of any real importance. Enantiomers would thus exist as symmetry related structures, which are *de facto* stable because of very long tunneling times. We present here with ClSSCl the first example of a chiral molecule, where electroweak and tunneling dynamics calculations demonstrate that the *de lege* asymmetry arising from the parity-violating energy difference ΔE_{pv} between the two enantiomers (about $1.5 \cdot 10^{-11}$ J mol^{-1}/N$_A$ with time for parity violation $t_{pv} \simeq 30$ s) dominates by far over the tunneling splitting $\Delta E_{\pm} \ll 10^{-70}$ J mol^{-1}/N$_A$ in the symmetrical case, with tunneling time $t_{\pm} \gg 10^{60}$ s. These results are of fundamental interest for our concept on molecular chirality as well as for potential experiments on parity violation in molecules.

References:

[1] R. Berger, M. Gottselig, M. Quack and M. Willeke, Angew. Chem. **113**, 4342–4345 (2001), Angew. Chem. Intl. Ed. (English) **40**, 4195–4198 (2001)
[2] M. Quack, Nova Acta Leopoldina **81**, Neue Folge (No. 314) 137-173 (1999)
[3] M. Quack, Angewandte Chemie (Intl.Ed.) **28**, 571-586 (1989)

Title: Molecular chirality and the fundamental symmetries of physics: Influence of parity violation on rovibrational frequencies and thermodynamic properties

Researchers: M. Quack
J. Stohner

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

Description:

We introduce the topic of fundamental symmetries of physics in relation to molecular chirality by a brief review of the development and current status of the theory for parity violation in chiral molecules. We then discuss in some detail CHBrClF (bromochlorofluoromethane) as a test case, to which the work of André Collet has contributed importantly. For this molecule and its isotopomers we report here the first detailed theoretical calculations of the influence of parity violation on statistical thermodynamic properties.

High quality *ab initio* calculations (RPA, random phase approximation and CASSCF, complete-active-space self-consistent-field) are performed to determine the small energy difference between R- and S-enantiomers of H and D isotopomers of bromochlorofluoromethane (CHBrClF, CDBrClF), and fluorooxirane $^{1}H_3C_2OF$) introduced by the parity violating weak interaction. Together with vibrational and rotational frequency shifts caused by parity violation these are used to determine the statistical thermodynamic quantities from the corresponding partition functions within the separable harmonic and in part also anharmonic adiabatic approximation. Temperature dependent equilibrium constants for the stereomutation are calculated and discussed in relation to biochemical homochirality.

References:

M. Quack and J. Stohner, Chirality, **13**, 745–753 (2001)

Title: Spectroscopy and dynamics of the isolated sp^2 CH chromophore in trideuteroacetaldehyde CD_3CHO as derived from extrapolated SDCI ab initio calculations

Researchers: T.K. Ha
M. Quack
J. Stohner

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

Description:

Ab initio CI potential energy (PES) and dipole moment (DMS) surfaces have been calculated with singles and doubles excitation configuration interaction (SDCI) for the two-dimensional isolated sp^2 CH chromophore subspace of trideuteroacetaldehyde CD_3CHO. Different extrapolation schemes to full-CI have been applied after the extrapolation to full-SDCI. Vibrational band centers and absolute intensities are determined variationally on six extrapolated surfaces. The band centers are analyzed within the effective Hamiltonian model for isolated CH chromophores and the effective spectroscopic parameters are compared for the different extrapolation schemes. Time-dependent population evolution for vibrational quantum motion with a pure CH stretching state being initially populated is calculated for some of the extrapolated surfaces within the effective Hamiltonian model.

References:

T.K. Ha, M. Quack, J. Stohner, Mol. Phys. **100**, 1797–1805 (2002)

Title: Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses

Researchers: G.S. Tschumper*
M.L. Leiniger**
B.C. Hoffmann**
E.F. Valeev**
H.F. Schaefer III**
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Center for Computational Quantum Chemistry,
University of Georgia, Athens

Description:

Ab initio calculations of very high level on the title compound are carried out.

References:

G.S. Tschumper, M.L. Leiniger, B.C. Hoffmann, E.F. Valeev, H.F. Schaefer III and M. Quack, J. Chem. Phys. 116, 690–701 (2002)

Title: High-resolution FTIR and cw-diode laser cavity ring-down spectroscopy of the $\nu_2 + 2\nu_3$ band of methane near 7510 cm^{-1} in slit jet expansions and at room temperature

Researchers: M. Hippler
M. Quack

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

Description:

The $\nu_2 + 2\nu_3$ combination band of $^{12}CH_4$ near 7510 cm^{-1} was studied with the recently introduced technique of cavity ring-down spectroscopy employing a cw-diode laser in a pulsed supersonic slit jet expansion and with Doppler-limited Fourier-transform infrared spectroscopy at room temperature. $\nu_2 + 2\nu_3$ is the strongest absorption band in the high-wavenumber region of the $N = 2.5$ icosad of methane. First assignments of the combination band are provided. The vibrational origin of $\nu_2+2\nu_3$ at 7510.3378 ± 0.0010 cm^{-1}, the integrated band strength $G = (1.3 \pm 0.2)\times10^{-4}$ pm^2 and the vibrational transition moment $|\langle\mu_v\rangle| = (1.0 \pm 0.1)\times10^{-3}$ D have been determined. The values represent benchmarks to test effective vibrational Hamiltonians and *ab initio* calculations for methane. Although an isolated band analysis was possible at low J-values, the influence of strong perturbations becomes evident at higher rotational excitation. The F_1-component of $\nu_2 + 2\nu_3$ interacting by a strong Coriolis resonance with the IR-active F_2-component appears to be a dominant perturber.

Extensive numerical calculations are carried out in the simulations of the spectra.

References:

M. Hippler and M. Quack, J. Chem. Phys. **116**, 6045–6055 (2002)

Title: Nonlinear intensity dependence in the infrared multiphoton excitation and dissociation of methanol preexcited to different energies

Researchers: O.V. Boyarkin**
T. R. Rizzo**
D.S. Rueda**
M. Quack*
G. Seyfang*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Laboratory of Physical Chemistry, EPF Lausanne

Description:

We report quantitative dissociation yields for the reaction $CH_3OH(v_{OH}) \xrightarrow{nh\nu} CH_3 + OH$ induced by infrared multiphoton excitation of methanol preexcited to various levels of the OH stretching vibration (v_{OH} = 0, 1, 3, 5) by detecting OH using laser induced fluorescence. It is demonstrated that for low levels of preexcitation (v_{OH} = 0, 1, 3) there is a substantial nonlinear intensity dependence, as a higher yield is found for self mode-locked CO_2 laser pulses (with higher peak intensity) as compared to single mode pulses of the same laser fluence, but lower peak intensity. In contrast, at high levels of preexcitation (v_{OH} = 5) this nonlinear intensity dependence is absent. Quantitative model calculations are carried out using a case B/case C master equation approach that takes nonlinear intensity dependence into account. The calculations are consistent with the experimental results and confirm the prediction that an important part of the selectivity of the CO_2 laser excitation step in IRLAPS (Infrared laser assisted photofragment spectroscopy) of CH_3OH is due to this nonlinear intensity dependence. We discuss further consequences of these experimental observations and theoretical predictions, which are also extended to IR multiphoton excitation of C_2H_5OH. Infrared (C–O) chromophore band strengths are reported for CH_3OH and C_2H_5OH.

References:

[1] O.V. Boyarkin, T.R. Rizzo, D.S. Rueda, M. Quack and G. Seyfang, J. Chem. Phys. in press (2002)
[2] M. Quack in "Encyclopedia of Computational Chemistry", Vol. 3, p. 1775-1791, P. von Ragué Schleyer, N. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III and P.R. Schreiner eds., John Wiley and Sons, 1998

Title: High resolution FTIR spectra and analysis of the ν_{11} fundamental band of $^{13}C_6H_6$

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

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Istituto di Fisica dell' Atmosfera, Area di Ricerca di Roma Tor Vergata

Description:

A high resolution FTIR (apodized instrumental bandwidth 0.004 cm^{-1} FWHM) spectrum has been measured for the isotopically pure benzene molecule $^{13}C_6H_6$ in the range 600-850 cm^{-1}. Accurate molecular constants have been obtained for the fundamental vibration ν_{11} (Wilson's notation, which is used here: ν_4 according to Herzberg's notation) of $^{13}C_6H_6$ with band center at 672.12930(5) cm^{-1}. Several hot-bands have been analyzed as well. Improved ground state constants have been deduced from a fit of ground state combination differences.
Extensive numerical calculations are carried out in the simulations of the spectra.

References:

M. Snels, H. Hollenstein, M. Quack, Chem. Phys. Lett. 350, 57–62 (2001)

Title: High resolution FTIR spectra and analysis of the ν_{11} fundamental and of the $\nu_2 + \nu_{11}$, $\nu_5 + \nu_{12}$ and $\nu_7 + \nu_{16}$ combination bands of $^{12}C_6D_6$

Researchers: M. Snels**
H. Hollenstein*
M. Quack*
E. Cané***
A. Miani***
A. Trombetti***

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Istituto per Materiali Speciali, CNR, Potenza
*** Dip. di Chimica Fisica ed Inorganica, Università di Bologna

Description:

We report results from measurements of the high resolution FTIR spectrum for the fully deuterated benzene molecule C_6D_6 in the range 450-3500 cm^{-1}. Accurate spectroscopic constants have been obtained for the fundamental vibration ν_{11} at 496.208 cm^{-1} and improved ground state constants have been deduced from a fit of ground state combination differences. The J structure of the combination parallel bands $\nu_2 + \nu_{11}$ (at 2798.1 cm^{-1}), $\nu_5 + \nu_{12}$ (1802.5 cm^{-1}) and $\nu_7 + \nu_{16}$ (2619.3 cm^{-1}) of C_6D_6 has been analysed as well, from which improved values of the band origin and of the B and D_J constants of the excited states have been obtained. The strongest hot bands accompanying these parallel transitions have been assigned by means of published anharmonic force fields. In particular $(\nu_{11} + \nu_{16}) - \nu_{16}$ is assigned to the band at 492.4 cm^{-1} even though its shape is typical of a perpendicular transition (PAPE). New values for the ν_5, ν_{12} and ν_{16} band origins are determined from the band origins of combination bands and from calculated anharmonic constants. Numerous anharmonic constants are derived from the assignment of hot band and combination transitions. Extensive numerical calculations are carried out in the simulations of the spectra.

References:

[1] M. Snels, H. Hollenstein, M. Quack, E. Cané, A. Miani, and A. Trombetti, Mol. Phys. 100, 981–1001 (2002)
[2] M. Snels, A. Beil, H. Hollenstein and M. Quack, Chem. Phys. 225, 107-130 (1997)
[3] M. Snels, H. Hollenstein and M. Quack, Chem. Phys. Lett. 350, 57–62 (2001)
[4] E. Riedle, A. Beil, D. Luckhaus and M. Quack, Mol. Phys. 81, 1-15 (1994)
[5] H. Hollenstein, S. Piccirillo, M. Quack and M. Snels, Mol. Phys. 71, 759-768 (1990)
[6] M. Quack, Annu. Rev.Phys. Chem. 41, 839-874 (1990)

Title: Analysis of the $\nu_3 + \nu_7$ combination band of CF_2Cl_2 from spectra obtained by high resolution diode laser and FTIR-supersonic jet techniques

Researchers: G. D'Amico**
M. Snels**
H. Hollenstein*
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Istituto per Materiali Speciali, CNR, Potenza

Description:

High resolution (0.0011 cm^{-1} full width half maximum) diode laser spectra have been measured for mixtures of CF_2Cl_2 in Ne, expanded in a supersonic planar jet. In addition interferometric Fourier transform infrared (FTIR) spectra have been recorded with a resolution of about 0.004 cm^{-1} (FWHM, Hamming apodization) for neat CF_2Cl_2, expanded through a circular 200 μm nozzle. We present the analysis of the $\nu_3 + \nu_7$ combination band of ($CF_2{}^{35}Cl_2$ [$(\tilde{\nu}_0)$ = 888.49689(10) cm^{-1}] and ($CF_2{}^{35}Cl{}^{37}Cl$) [$\tilde{\nu}_0$ = 883.20389(12) cm^{-1}]. Absolute band strengths have been measured for all bands falling in the atmospheric window ($\nu_3 + \nu_7$, ν_6, ν_1 and ν_8) and thus being important for monitoring CF_2Cl_2 in the lower troposphere and stratosphere. A Fermi resonance coupling constant W = (15± 2) cm^{-1} is estimated for the resonance between $\nu_3 + \nu_7$ and ν_6 in both isotopomers. Extensive numerical calculations are carried out in the simulations of the spectra.

References:

G. D'Amico, M. Snels, H. Hollenstein, M. Quack, Phys.Chem.Chem.Phys., **4**, 1531–1536 (2002)

Title: High resolution spectroscopy of the ν_3 band of WF_6 and ReF_6 in a supersonic jet

Researchers: V. Boudon**
M. Rotger**
Y. He*
H. Hollenstein*
M. Quack*
U. Schmitt*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Laboratoire de Physique de l'Université de Bourgogne, Dijon

Description:

We have recorded the Fourier-transform infrared (FTIR) spectrum of the ν_3 fundamental band of WF6 in a continuous supersonic jet expansion with an instrumental bandwidth of 0.0024 cm^{-1} (FWHM, full width at half maximum, unapodized), using a Bomem DA.002 spectrometer. Some parts of this band have also been recorded with 0.0007 cm^{-1} bandwidth using a diode laser spectrometer combined with a pulsed slit jet expansion. A multiple-pass arrangement has been used for the slit jet to observe low-intensity lines. In each case, we have used a WF_6:He mixture with a seeding ratio 1:3 leading to a rotational temperature of ca. 50 K. This work extends the previous investigation of Takami and Kuze [J. Chem. Phys. 80, 5994 (1984)] to much higher J transitions. In both P and R branches, rotational lines have been recorded for J up to 46-48. We have used a tensorial Hamiltonian adapted to the group chain $O(3) \subset O_h$ and developed to the third order for the analysis of the spectra. A least-squares fit for each of the four main isotopic species: $^{182}WF_6$, $^{183}WF_6$, $^{184}WF_6$, and $^{186}WF_6$ results in band centers (in this order) 714.538 19, 714.214 06, 713.895 44, and 713.266 21 cm^{-1}. We report furthermore first results on the high-resolution spectra of ν_3 of ReF_6, which exhibits a fourfold degenerate electronic ground state of G_g' species in the O_h^S group. Supersonic jet-FTIR spectra show a moderately structured relatively broad band, whereas the diode laser spectroscopy of the seeded jet in the range 708-733 cm^{-1} results in line resolved spectra of high complexity. A preliminary analysis is discussed, while a complete analysis still represents an appreciable challenge. Extensive numerical calculations are carried out in the analysis and simulations of the spectra.

References:

V. Boudon, M. Rotger, Y. He, H. Hollenstein, M. Quack and U. Schmitt, J. Chem. Phys **117**, 3196–3207 (2002)

Title: How Important is Parity Violation for Molecular and Biomolecular Chirality?

Researchers: M. Quack

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

Description:

Parity violation leads to energy differences $\Delta_{pv}H_0^{\ominus} = N_A\Delta_{pv}E$ of enantiomers in the Femtojoule to Picojoule per mole range. Recently introduced methods of electroweak quantum chemistry predict such energy differences to be one to two orders of magnitude larger than previously accepted -- but still very small. How can such small energies be measured and what are the consequences for our understanding of molecular chirality, biomolecular homochirality, and perhaps fundamental physics? The essay gives some tentative answers to these questions. We discuss the current status of theory and some of the current experimental approaches.

References:

[1] M. Quack, Angewandte Chemie (2002), in press
[2] A. Bakasov, T.K. Ha and M. Quack, in Proc. of the 4th Trieste Conference (1995), *Chemical Evolution: Physics of the Origin and Evolution of Life*, 287-296, J. Chela-Flores and F. Rolin eds, Kluwer Academic Publ. Dordrecht, 1996
[3] A. Bakasov, T.K. Ha and M. Quack, J. Chem. Phys. **109**, 7263-7285 (1998), Erratum: J. Chem. Phys. **110**, 6081 (1999)
[4] M. Quack, Nova Acta Leopoldina **81**, Neue Folge (No. 314) 137-173 (1999)
[5] M. Quack and J. Stohner, Phys. Rev. Lett. **84**, 3807-3810 (2000)
[6] M. Quack and J. Stohner, Z. Physik. Chem. **214**, 675-703 (2000)
[7] R. Berger and M. Quack, ChemPhysChem. **1**, 57-60 (2000)
[8] R. Berger and M. Quack, J. Chem. Phys. **112**, 3148-3158 (2000)
[9] R. Berger, M. Quack and G. Tschumper, Helv. Chim. Acta **83**, 1919–1950 (2000)
[10] R. Berger, M. Quack and J. Stohner, Angew. Chemie **113**, 1716–1719 (2001); Angew. Chem. Intl. Ed. (Engl.) **40**, 1667–1670 (2001)
[11] M. Quack and J. Stohner, Chirality, **13**, 745–753 (2001)
[12] M. Quack, Angewandte Chemie **101**, 588-604 (1989), Angewandte Chemie (Intl.Ed.) **28**, 571-586 (1989)

Title: Tunneling Dynamics of the NH Chromophore in NHD_2 During and After Coherent Infrared Excitation

Researchers: R. Marquardt**
M. Quack*
I. Thanopulos***
D. Luckhaus****

Institute/Group:
* Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Laboratoire de Chimie Théorique, Université de Marne-la-Vallée
*** Weizmann Institute of Science, Rehovot (present address)
**** Institut für Physikalische Chemie, Universität Göttingen (present address)

Description:
The time dependent quantum dynamics of the large amplitude motion of the NH stretching chromophore in NHD_2 is investigated during and after coherent multiphoton excitation by calculation of the wave packet evolution using global analytical potential energy and electric dipole hypersurfaces of ammonia derived from *ab initio* calculations. Intramolecular vibrational redistribution (IVR) between the NH stretching and bending motion and coupling to the radiation field induces a diffusion of probability density into the NH chromophore space, which includes the inversion coordinate. But inversion remains essentially dominated by a tunneling process, even at average energies well above the inversion barrier.

References:
R. Marquardt, M. Quack, I. Thanopulos, and D. Luckhaus, J. Chem. Phys. in press (2002)

Title: Application of Stochastic Simulations to problems in forming technology

Researchers: A. Unterkircher
P. Hora
J. Reissner

Institute: Institute of Virtual Manufacturing

Description:

In order to predict real life behaviour of forming processes uncertainties of severeral process parameters have to be included into finite element simulations. Thus a deterministic simulation has to be replaced by a stochastic simulation. We achieve this goal by using Monte Carlo techniques. If the distributions of significant process parameters are known one can generate a series of input files reflecting the statistical characteristics of these parameters. Thus one simulation is being replaced by a series of simulations. The computations may be carried out in parallel. As a result one receives the statistical behaviour of the process which in turn may be used to predict the robustness of the proposed manufacturing technique. In cooporation with industrial partners we have already investigated several processes including deep drawing of sheet metal and a 9-step bulk forming process demanding very narrow tolerances.

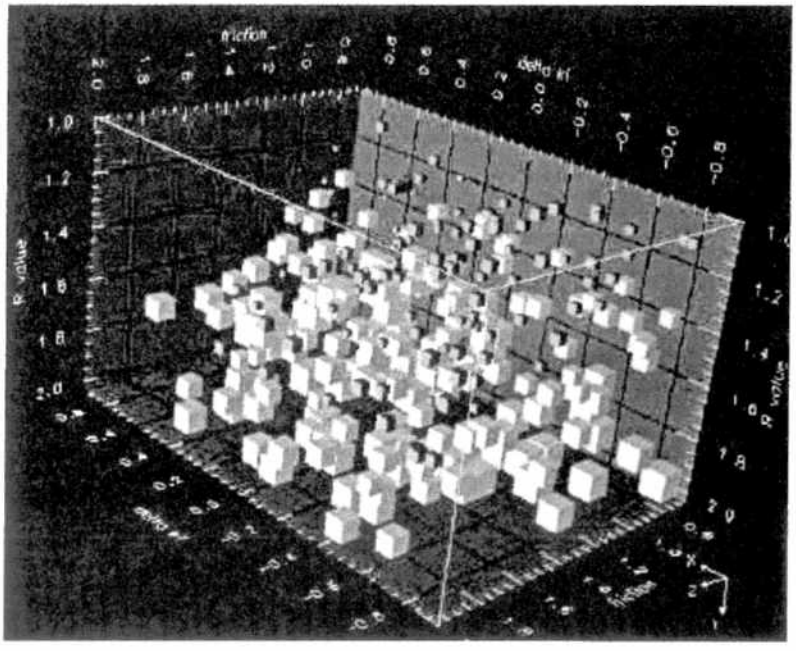


Figure: Sheet thickness depending on 3 material parameters (with given statistics).

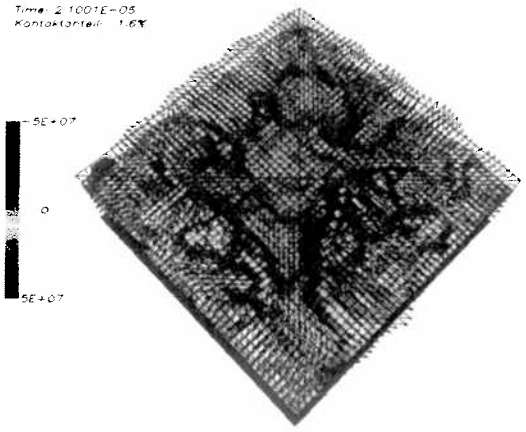
Title: Simulations for tribology on different length scales

Researchers: Thomas Bonner
Reto Grüebler

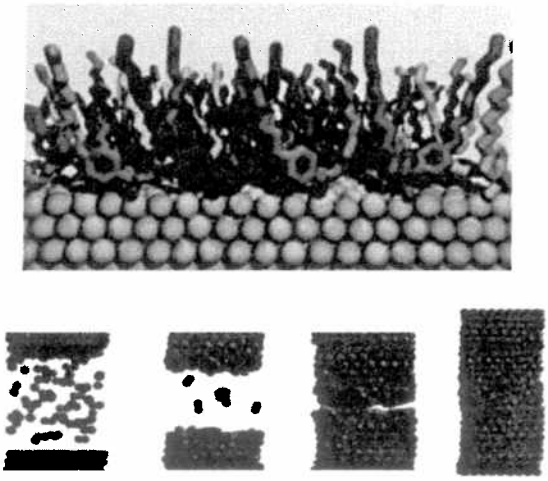
Institute/ Group: Institute for virtual manufacturing
Institut für virtuelle Produktion

Description:

For the simulation of tribological systems relevant to the industrial manufacturing praxis different length scales are considered: While the hydrodynamic part of the friction, which is influenced mostly by the lubricant and the surface roughness, is modeled by means of finite element methods, molecular dynamics simulations are employed for the places where boundary lubrication occurs. For the latter three different regimes are identified: First a thin layering regime is reached, where the discretization by single molecules becomes apparent and the remaining layers inbetween show a solid-like behavior. Next, anti-wear (AW) additives with special head groups, to favor the adsorption onto the surface, are building up carpet-like protective layers on the surface. Finally, under severe conditions, extreme pressure (EP) additives come into play to react at the points with elevated temperatures (under optimum conditions this happens only at the asperities where friction is taken place) and to form very hard, protective EP-layers. They may be bad lubricants, but their function is to protect the surface against microwelding between the two surfaces.



FEM simulation with surface roughness and lubricant.



Top: MC/MD minimization of the AW/EP-additive Irgalube 211, bottom: forming of aluminum oxide interface as EP-model during sliding (modeled with charge equilibration method).

References:

J. Reissner, R. Grüebler, Th. Bonner. Tribosimulation. in: Umformtechnik 2000 Plus, S. 245 - - 254, Festschrift zu Ehren von Professor Kurt Lange, Herausgeber: M. Geiger.

Title:	Evolving virtual microstructures: simulation of the evolution of microstructures of metals including concurrent deformation, recovery, recrystallization, grain growth and precipitation.
Researchers:	K. G. F. Janssens* F. Vanini* E. Kozeschnik**
Institute / Group:	* Institute for virtual Manufacturing Prof. J. N. Reissner ETH Zurich ** Institute for Materials Science, Welding and Forming Graz University of Technology

Description:

Driven by cost reduction needs, metal working industry is investing in research and development of virtual processing. In order to predict the mechanical properties of a finished product, one needs to compute the evolution of the properties of the metal along the virtual process. As the mechanical properties of a metal are governed by its microstructure, this implies one needs to be able to simulate the evolution of the microstructure given the boundary conditions set by the thermo-mechanical process. In addition one needs to be able to predict the mechanical properties from the virtual microstructure. This project concerns the further development and implementation of a semi-physical model, which allows simulation of the microstructure under thermo-mechanical processing, as well as the prediction of particular mechanical properties from the simulated microstructure.

The objective of this project is to develop and implement a methodology allowing the prediction of the mechanical properties of cold and hot formed metal products.

The approach used to solve the problem described is to divide the process into small time steps, in each of which the processes of deformation, recovery-recrystallization-grain growth and precipitation are computed in sequence, taking into account the influence they may have on one another. The model for deformation is Taylor-model based one, modified to include the interaction of the work hardening and texture development with obstructions (such as particles) in the metal. For recovery, recrystallization and grain growth a new cellular automaton is developed, taking into account misorientation dependence of grain boundary energy and mobility and their interaction with precipitation particles. The process of precipitation simulation using MatCalc, a set of algorithms developed at the University of Graz.

References: Manuscripts have been submitted to Advanced Engineering Materials and to Modelling and Simulation in Materials Science and Engineering

Title: Electronic Structure of Strongly Correlated Materials

Researchers: T.M. Rice, M. Sigrist [*]
V.I. Anisimov [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Inst.of Metal Physics, Russian Academy of Sciences, Yekaterinburg

Description:

Modifications of standard density functional theory are needed to calculate the electronic structure in the presence of strong correlations among the electrons. One method known as LDA+U, allows the treatment of broken symmetries in spin and orbital degrees of freedom. A second method combines the local density approximation with the dynamical mean field theory to describe systems without a broken symmetry. These methods are applied to materials of high current interest.

References:

- V.I. Anisimov, I.A. Nekrasov, D. Ekondkov, T.M. Rice and M. Sigrist, Eur. J. Phys. B **25**, 191 (2002)
- V. I. Anisimov, R. Hlubina, M.A. Korotin, V.V. Mazurenko, T. M. Rice, A.O. Shorikov and M. Sigrist, Phys. Rev. Lett. (in press)

Title: Multiparticle ring exchange in the Wigner glass

Researchers: K. Völker [*]
S. Chakravarty [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California at Los Angeles, USA

Description:

The two-dimensional electron gas (2DEG) occurs in a variety of systems, such as semiconductor heterostructures, the Copper-Oxide layers of high-temperature superconductors, or on liquid-Helium surfaces. Potential applications are in nanotechnology and spintronics. From a theoretical point of view, it provides an opportunity to study the rich and often novel physics arising from strong electron interactions. One example is the unexpected metal-insulator transition (MIT) in two dimensions. At very low densities, and zero temperature, the 2DEG is expected to freeze into a crystalline state, the so-called Wigner crystal (or a Wigner glass in the presence of disorder), which is an insulator. Under certain conditions (in very clean systems) the Wigner glass can melt into a metal. The nature of this metallic state is at present not understood. An important part of the problem is to determine the magnetic properties of the 2DEG close to the MIT. From a numerical point of view, the determination of magnetic interactions involves the minimization of the action functional, which is represented as a function of about 1000 variables. Minimization is performed by a variable metricalgorithm (Broyden-Fletcher-Goldfarb-Shanno, BFGS).

References:

- K. Völker and S. Chakravarty, Phys. Rev. B **64** 235125 (2001)

Title: Numerical investigation of strongly correlated systems

Researchers: A. Läuchli, C. Honerkamp, Th. Siller, M. Indergand, S. Wessel, M. Sigrist, M. Troyer, T.M. Rice [*]
S.R. White [**]
M. Salmhofer [***]
D. Poilblanc [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California at Irvine, USA
[***] Theoretische Physik, Universität Leipzig, Germany
[****] Université Toulouse, France

Description:

The physics of strongly correlated electrons is one of the most active research fields in condensed matter physics. Next to technologically relevant developments such as high-temperature superconductors and colossal magnetoresistance materials, the field raises many important and difficult questions to basic research such as new exotic states of matter and the breakdown paths of the more conventional metallic or ordered states. We analyze the latter issue by means of extensive numerical renormalization group calculations for two-dimensional electron systems. Furthermore novel correlation phenomena like the binding of holes or magnetic excitations with impurity sites are investigated using modern numerical techniques such as density matrix renormalization group and exact diagonalization.

References:

- C. Honerkamp, M. Salmhofer, N. Furukawa, and T.M. Rice, Phys. Rev. B **63**, 035109 (2001)
- C. Honerkamp, Euro. Phys. J. B 21, 81 (2001)
- C. Honerkamp and M. Salmhofer, Phys. Rev. Lett. 87, 187004 (2001)
- Th. Siller, M. Troyer, T.M. Rice and S.R. White, Phys. Rev. B **63**, 195106 (2001).
- Th. Siller, M. Troyer, T.M. Rice and S.R. White, Phys. Rev. B **65**, 205109 (2002).
- J. Riera and D. Poilblanc , Phys. Rev. B **63**, 241102 (2001)
- P. Maurel, M.-B. Lepetit and D. Poilblanc , Eur. Phys. J. B (2001)
- K. Tsutsui, D. Poilblanc and S. Capponi, Phys. Rev. B (2001).
- A. Läuchli, D. Poilblanc, T.M. Rice and S.R. White, Phys. Rev. Lett. **88**, 257201 (2002)
- S. Wessel, M. Indergand, A. Läuchli, U. Ledermann ,M. Sigrist, submitted to Phys. Rev. B
- U. Schollwöck, S. Chakravarty, J.O. Fjærestad, J. B. Marston ,M. Troyer, submitted to Phys. Rev. Lett.

Title: Structural and Dynamical Characterization of Dizinc DF1, a Biomimetic Compound of Diiron Proteins via ab initio and Hybrid (QM/MM) Molecular Dynamics

Researchers: Alessandra Magistrato[a],
William F. DeGrado[c]
Ursula Röthlisberger[b]
Michael L. Klein[a]

Institute/Group: [a]Center for Molecular Modeling, University of Pennsylvania, Department of Chemistry, Philadelphia, PA, 19104-6323, USA
[b]Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland
[c] Department of Biochemistry and Biophysics, University of Pennsylvania, School of Medicine, Philadelphia, PA, 19104-6054, USA

Description:

A systematic study of structural and dynamical properties of a four-helix bundle biomimetic complex (Due Ferri 1, DF1) of diiron proteins has been performed through density functional theory (DFT) based calculations and hybrid QM/MM (Car-Parrinello) molecular dynamics simulations.
Four different quantum mechanical models of the active site have been employed in order to systematically assess the role of first and second shell interactions: (a) a 66 atom model comprising only first shell interactions, (b) two larger models (78 and 86 atoms) containing different second shell hydrogen bond networks and (c) a 98 atom model including both first and second shell interactions. The geometrical constraints and electrostatic stabilization provided by the full four-helix bundle have been explicitly considered by performing mixed QM/MM molecular dynamics simulations. Two different QM/MM models have been chosen: (a) a model in which only the first shell ligands (54 QM atoms) are described at the quantum mechanical (DFT) level while the rest of the protein and the solvation water molecule are taken into account at the MM level (using the Amber force field) and (b) a model in which a second shell hydrogen bond network in addition to the first shell ligands (68 QM (DFT) atoms) is included in the QM region.
Our results demonstrate the importance of the second shell interactions and the whole protein environment in stabilizing the hydrogen bond networks that surround the active site. The calculations confirm the high flexibility of the carboxylate bridged binuclear motif. The present systematic approach enables to identify stability/reactivity-governing factors and provides unique insights for the future tailoring of new highly selective biomimetic compounds.

References: submitted to PNAS

Title: Structure-based thermodynamic analysis of caspases reveals key residues for dimerization and activity.

Researchers: Stefano Piana
Marialore Sulpizi
Ursula Röthlisberger

Institute/Group: Institute of Molecular and Biological Chemistry. Federal Institute of Technology, EPFL, 1015 Lausanne. Switzerland

Description:

Caspases are a family of enzymes which play a crucial role in apoptosis. They are accumulated in eukaryotic cells in the form of low-activity proenzyme precursors. Proteolytic cleavage of specific sites triggers conformational changes that lead to full activation and thus to the initiation of the process of apoptosis. Several experimental observations suggest that dimerization is essential for the activity and regulation of caspases. In this work, we have used a structure-based thermodynamic analysis method [Edgcomb, S.P. and Murphy, K. P. *Curr. Opin Biotechnol.*, **11**, 62-66 (2000)] to calculate the free energy of association and folding for all the caspases and procaspases whose structures are known up to date. In all cases, analysis of the single residue contributions to the dimerization energy shows that 30 to 50% of the dimer stability originates from the highly specific interaction of 12-14 residues located on the N- and C-termini of the large and small subunit, respectively. Our calculations indicate that these residues are particularly critical for stabilising the conformation of the active site loops for binding substrates and inhibitors. Our results are in good agreement with the available experimental data and help to rationalize the relation between dimerization and activity in this important class of enzymes.

References: submitted to J. Mol. Biol

Title: Multiple steering molecular dynamics applied to water exchange at alkali ions

Researchers: Michele Cascella+
Leonardo Guidoni°
Amos Maritan+
Ursula Röthlisberger°
Paolo Carloni+

Institute/Group: + International School of Advanced Studies (SISSA/ISAS) and Istituto Nazionale di Fisica della Materia; Via Beirut 2-4, 34014 - Trieste, Italy
° Department of Chemistry, ETH Zürich, CH-8093 - Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The novel fast-growth or multiple steering molecular dynamics (MSMD) technique has been recently developed by Jarzynski to calculate the free energy profiles along general transformation pathways. Here, we apply this approach to calculate free energy barriers involved in the water exchange reaction of Na^+ and K^+ in aqueous solution. We investigate the influence of the key parameters of the MSMD simulations – the steering velocity, the sampling of the initial configurations and the force constant – on the free energy. Furthermore, we use this approach to describe energetical and structural features of the water exchange reaction of Na^+ and K^+ in aqueous solution. The MSMD technique turns out to be an efficient and fastly convergent tool to enhance the sampling of rare chemical events with the help of nonequilibrium forces.

References: submitted to J. Phys. Chem. B

Title: Molecular Dynamics Studies of Caspase-3 Dimer

Researchers: M. Sulpizi[1,2]
U. Röthlisberger[3]
P. Carloni[1,2,4]

Institute/Group: [1]SISSA, International School for Advanced Studies, via Beirut 2-4, 34013 Trieste, Italy
[2]INFM, Istituto Nazionale di Fisica della Materia, Italy.
[3]Laboratory of Inorganic Chemistry, ETH Hönggerberg - HCI, CH-8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland
[4]ICGB, International Centre for Genetic Engineering and Biotechnology, AREA Science Park, Padriciano 99, 34012, Trieste, Italy

Description:

Caspases are fundamental targets for pharmaceutical interventions in a variety of diseases involving disregulated apoptosis. Here, we present the first molecular dynamics study of a member of this family, the executioner caspase-3 in complex with the pentapeptide substrate DEVDG. Our study provides a characterizaion of the dynamic properties of the active dimeric form in aqueous solution. In particular, we focus on the mobility of the active site regions and possible dynamic correlation effects between the two monomer units that could influence the enzymatic activity upon dimerization. The flexibility of the catalytic residues and their mutual position is analyzed and compared to other well-studied cysteine proteases such as papain. At difference to the latter, the substrate mobility is rather low indicating a distinct preorganization effect of the Michaelis complex. An analysis of the global motion of the protein indicates a coupling between the two monomer units, occurring not only in terms of collective motions such as intermonomer flapping, twists and rotations, but also at the level of the two active sites. An essential dynamics analysis shows that the movements of the loops surrounding the substrate in one monomer are correlated with loop displacements in the other monomer suggesting that dimerization has a distinct effect on the dynamic properties of the active site regions.

References: submitted to Biophys. J.

Title: Oxidation of Nitrite by Peroxynitrous Acid

Researchers: Patrick Maurer[a]
Chris F. Thomas[a]
Reinhard Kissner[a]
Heinz Rüegger[a]
Oswald Greter[b]
Ursula Röthlisberger[a]
Willem H. Koppenol[a]*

Institute/Group: [a]Laboratorium für Anorganische Chemie and [b]Laboratorium für Organische Chemie, Eidgenössische Technische Hochschule Zürich, ETH Hönggerberg, CH-8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The kinetics of the oxidation of nitrite to nitrate by peroxynitrous acid at pH 5.2 is best described by the rate law: $k_{obs} = k_{iso} + k'[NO_2^-] + k''[NO_2^-]^2$, in which the peroxynitrous acid isomerization rate constant $k_{iso} = (1.10 \pm 0.05)\ s^{-1}$, $k' = (3.2 \pm 0.1)\ M^{-1}s^{-1}$ and $k'' = (4.2 \pm 0.3)\ M^{-2}s^{-1}$. Ab initio calculations indicate that there is only a small intrinsic barrier to the net transfer of HO^+ from peroxynitrous acid to the nitrogen atom of nitrite. A similar transfer to either of the two oxygens of nitrite produces the reactants, and would not lead to an increase in the rate of disappearance of peroxynitrous acid, as observed. The low rate constant is most likely due to stringent orientational constraints. Formal transfer of HO^+ to $^{15}NO_2^-$ results in formation of $^{15}NO_3^-$, as experimentally observed.

References: submitted to J. Phys. Chem. B

Title: Molecular Dynamics Simulations of Structural Changes During Procaspase-3 Activation

Researchers: Stefano Piana
Ursula Röthlisberger

Institute/Group: Department of Chemistry, ETH Zürich, Wolfgang Pauli Strasse 10, 8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

Molecular dynamics (MD) simulations of the initial structural rearrangements on the pathway leading to procaspase-3 activation are presented that suggest a molecular mechanism for the pH dependent activation of caspase-3 mediated by the 'safety catch'. In particular, the 'safety catch' binds to a protein region that appears to be critical for the stability of the active site loop conformation and thus could be potentially exploited as a target for the rational design of selective caspase-3 inhibitors. In the free active enzyme, the selectivity loop is already preorganized to accomodate the substrate. Such a preorganization is not present neither in monomeric caspase-3 nor in procaspase-3 dimer thus suggesting that the structure of the selectivity loop is highly sensitive to perturbations and of importance for caspase activity regulation. A simple kinetic model for the activation of caspase-3 from the zymogen precursor is proposed.

References: submitted to Biochemistry

Title: Early Steps of the Intramolecular Signal Transduction in Rhodopsin Explored by Molecular Dynamics Simulations

Researchers: Ute F. Röhrig
Leonardo Guidoni
Ursula Röthlisberger

Institute/Group: Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technology, CH-8093 Zürich, Switzerland
Current address: Laboratory of Computational Chemistry and Biochemistry, Swiss Federal Institute of Technology, CH-1015 Lausanne, Switzerland

Description:

We present molecular dynamics simulations of bovine rhodopsin in a membrane mimetic environment based on the recently refined X-ray structure of the pigment. The interactions between the protonated Schiff base and the protein moiety are explored both with the chromophore in the dark adapted 11-cis and in the photoisomerized all-trans form. Comparison of simulations with Glu181 in different protonation states strongly suggests that this loop residue located close to the 11-cis bond bears a negative charge. Restrained molecular dynamics simulations also provide evidence that the protein tightly confines the absolute conformation of the retinal around the C12-C13 bond to a positive helicity. 11-cis to all-trans isomerization leads to an internally strained chromophore, which relaxes after a few nanoseconds by a switching of the ionone ring to an essentially planar all-trans conformation. This structural transition of the retinal induces in turn significant conformational changes of the protein backbone, especially in helix VI. Our results suggest a possible molecular mechanism for the early steps of intramolecular signal transduction in a prototypical G-protein-coupled receptor.

References: Biochemistry (ASAP article)

Title: The Dialkyl Effect on Enantioselectivity: π-Stacking as a Structural Feature in P,N Complexes of Pd(II)

Researchers: Pascal Dotta[1]
Alessandra Magistrato[1]
Ursula Röthlisberger[1,2]
Paul S. Pregosin[1]
Alberto Albinati[3]

Institute/Group: [1]Laboratory of Inorganic Chemistry, ETHZ, 8093 Zürich, Switzerland
[2]Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, 1015 Lausanne, Switzerland
[3]Chemical Pharmacy, University of Milan, I-20131 Milan, Italy

Description:

A phosphino,oxazoline P,N-bidentate ligand, 4, containing 3,5-di-t-butyl phenyl groups has been prepared. In the Heck arylation of dihydrofuran, 4 is shown to afford higher ee's than either 2 or 3 the, unsubstituted and m-dimethylphenyl analogs, respectively. Several Pd(0)-complexes of 4 are reported. The X-ray structure for $PdCl_2$(4), 8, was determined by X-ray diffraction methods and comparison data with $PdCl_2$(2), 9, and $PdCl_2$(3), 10 suggest that differing amounts of π-π stacking strongly influence the structures of these relatively simple Pd complexes, with 9 and 10 revealing the strongest π-π interactions. An estimation of the van der Waals energies involved in the interaction supports a ca. 4 kcal/mol stabilization via π-π stacking.

References: Organometallics 21, 3033-3041 (2002)

3
CSE Case Studies Seminar

Title: Accelerating Rare Reactive Events by Means of a Finite Electronic Temperature

Researchers: Joost VandeVondele
Ursula Röthlisberger

Institute/Group: Laboratory of Inorganic Chemistry, ETH Zürich, 8092 Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The range of chemical problems that are directly accessible to first-principles molecular dynamics simulations based on density functional theory is extended with a novel method apt to accelerate rare reactive events.
The introduction of a finite electronic temperature within the Mermin formalism leads to a lowering of chemical activation barriers and thus to an exponential enhancement of the rate at which these reactions are observed during a first-principles molecular dynamics simulation.
The method presented here makes direct use of the intrinsic chemical information encoded in the electronic structure, and is therefore able to lower selectively chemically relevant activation energies even in systems where many competing low-energy pathways for conformational transitions or diffusive motions are present.
The performance of this new approach is demonstrated for a series of prototypical chemical reactions in gas and in condensed phase. These tests show that the activation barriers can be lowered substantially while the locations of the stationary points remain essentially unchanged with respect to the zero Kelvin potential energy surface.
The electronic temperature is the only tunable parameter of this electronic bias potential and the thermodynamic properties of the original ground state system can be recalculated on-the-fly from the trajectory of an accelerated molecular dynamics simulation via a linear perturbation approach.

References: J. Am. Chem. Soc. 124, 8163-8171 (2002)

Title: Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions

Researchers: Maria Carola Colombo,
Leonardo Guidoni
Alessandro Laio
Alessandra Magistrato
Patrick Maurer
Stefano Piana
Ute Röhrig
Katrin Spiegel
Marialore Sulpizi
Joost VandeVondele
Martin Zumstein
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Institute/Group: Laboratorium für Anorganische Chemie
Eidgenössische Technische Hochschule
ETH Hönggerberg, Wolfgang Pauli Str. 10, CH-8093 Zürich
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

First-principles molecular dynamics (Car-Parrinello) simulations based on density functional theory have emerged as a powerful tool for the study of physical, chemical and biological systems. At present, using parallel computers, systems of a few hundreds of atoms can be routinely investigated. By extending this method to a mixed quantum mechanical – molecular mechanical (QM/MM) hybrid scheme, the system size can be enlarged further. Such an approach is especially attractive for the *in situ* investigation of chemical reactions that occur in a complex and heterogeneous environment. Here, we review some recent applications of hybrid Car-Parrinello simulations of chemical and biological systems as illustrative examples of the current potential and limitations of this promising novel technique.

References: CHIMIA 56, 11-17 (2002)

Title: D-RESP: Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/ Molecular Mechanics Simulations

Researchers: Alessandro Laio
Joost VandeVondele
Ursula Röthlisberger

Institute/Group: Laboratory of Inorganic Chemistry, ETH Hönggerberg-HCI, 8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

A scheme is proposed for calculating electrostatic potential (ESP) derived charges from mixed Quantum Mechanics/ Molecular Mechanics (QM/MM) molecular dynamics simulations. These charges are fitted to the electrostatic field due to the quantum charge density evaluated on the MM atoms close to the QM system and are restrained to the corresponding Hirshfeld value by a quadratic penalty function. The D-RESP charges estimated by this procedure reproduce the field due to the charge density polarized by the environment and can be obtained as a function of time along a finite temperature molecular dynamics trajectory with essentially no computational overhead with respect to a standard QM/MM calculation. The fluctuation of the D-RESP values in a finite temperature run provide information about the importance of polarization effects and thus allow for a direct comparison of the relative performance of polarizable versus non polarizable point charge models.
Moreover, the D-RESP charges estimated by this procedure can be used as a simple and straightforward indicator of the chemical state of the system.

References: References: J. Phys. Chem. B 106, 7300-7307 (2002)

Title: The Role and Perspective of *Ab-initio* Molecular Dynamics in the Study of Biological Systems

Researchers: Paolo Carloni[1]
Ursula Röthlisberger[2]
Michele Parrinello[3]

Institute/Group: [1]International School for Advanced Studies (SISSA/ISAS) and Istituto Nazionale per la Fisica della Materia (INFM), via Beirut 4, I-34014, Trieste, Italy
[2]Department of Chemistry, ETH-Hönggerberg HCI, CH-8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland
[3]CSCS-Centro Svizzero di Calcolo Scientifico, Via Cantonale, CH-6928 Manno, Switzerland

Description:

Ab initio molecular dynamics (MD) allows realistic simulations to be performed without adjustable parameters. In recent years, the technique has been used on an increasing number of applications to biochemical systems. Here, we describe the principles on which ab initio MD is based. We focus on the most popular implementation, based on density functional theory and plane wave basis set. By a survey of recent applications, we show that despite the current limitations of size and time scale, ab initio MD (and hybrid ab initio MD/MM approaches) can play an important role for the modeling of biological systems. Finally, we provide a perspective for the advancement of methodological apporaches which may further expand the scope of ab initio MD in biomolecular modeling.

References: Acc. Chem. Res. 35, 455-464 (2002)

Title: Drug Resistance in HIV-1 Protease: Flexibility-Assisted Mechanism of Compensatory Mutations

Researchers: Stefano Piana[§]
Paolo Carloni[‡]
Ursula Röthlisberger[§]

Institute/Group: [‡]Scuola Internazionale Superiore di Studi Avanzati and Istituto Nazionale di Fisica della Materia. Via Beirut 2-4, 34014 Trieste, Italy
[§]Laboratory of Inorganic Chemistry, ETH Hönggerberg - HCI, Wolfgang Pauli Strasse 6, 8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The emergence of drug-resistant variants is a serious side effect associated with AIDS therapies based on inhibition of HIV-1 protease (HIV-1 PR). In these variants, compensatory mutations, usually located far from the active site, are able to affect the enzymatic activity via molecular mechanisms that have been related to differences in the conformational flexibility, although the detailed mechanistic aspects have not been clarified so far.
Here, we perform multi-nanosecond molecular dynamics simulations on the L63P HIV-1 PR, corresponding to the wild type, and one of its most frequently occurring compensatory mutations, M46I, complexed with the substrate and an enzymatic intermediate. The quality of the calculations is established by comparison with the available NMR data. The molecular dynamics simulations indicate that the dynamical fluctuations of the mutated enzyme differ from those in the WT. These differences in the dynamic properties of the adducts with the substrate and with the gem-diol intermediate might be directly related to variations in the enzymatic activity (Piana, S; Parrinello, M and Carloni, P J. Mol. Biol. 2002 in press) and therefore offer an explanation of the observed changes in catalytic rate between WT and mutated enzyme. We anticipate that this "flexibility-assisted" mechanism might be effective in the vast majority of compensatory mutations, which do not change the electrostatic properties of the enzyme.

References: Protein Science (in press)

Title: A Hamiltonian Electrostatic Coupling Scheme for Hybrid Car-Parrinello Simulations

Researchers: A. Laio
J. VandeVondele
U. Röthlisberger

Institute/Group: Laboratory of Inorganic Chemistry, ETH Hönggerberg - HCI, Wolfgang Pauli Strasse 6, 8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

We present a fully Hamiltonian and computationally efficient scheme to include the electrostatic effects due to the classical environment in a Car-Parrinello mixed Quantum Mechanics/ Molecular Mechanics (QM/MM) method. The polarization due to the MM atoms close to the quantum system is described by a Coulomb potential modified at short range. We show that the functional form of this potential has to be chosen carefully in order to obtain the correct interaction properties and to prevent an unphysical escape of the electronic density to the MM atoms (the s-called spill-out effect). The interaction between the QM system and the more distant MM atoms is included by a Hamiltonian term explicitly coupling the multipole moments of the quantum charge distribution with the classical point charges. Our approach remedies some of the well known deficiencies of current electrostatic coupling schemes in QM/MM methods, allowing molecular dynamics simulations of mixed systems within a fully consistent and energy conserving approach.

References: J. Chem. Phys. 116, 6941-6948 (2002)

Title: Hybrid Car-Parrinello/Molecular Mechanics Modelling of Transition Metal Complexes: Structure, Dynamics and Reactivity

Researchers: Leonardo Guidoni
Patrick Maurer
Stefano Piana
Ursula Röthlisberger

Institute/Group: Department of Chemistry, ETH Zürich
Wolfgang Pauli Str. 10, 8093 Zürich, Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The theoretical modelling of chemically active transition metal (TM) centres is a notoriously difficult task. The metal-ligand interactions in these complexes are often highly directional and the concoction of suitable analytic interaction potentials can be far from trivial. The situation is rendered even more difficult by the fact that at finite temperature, the system might switch dynamically between different bonding situations or exhibit several energetically-close lying spin states which are all characterized by different coordination numbers and geometries. In this article, we describe the structural, dynamical and reactive properties of complex TM-containing systems with the help of a mixed quantum mechanical/molecular mechanical (QM/MM) molecular dynamics approach, in which the TM centre is described with generalized gradient corrected density functional theory embedded in a classical force field description. The power of such a combined Car-Parrinello/molecular mechanics approach is illustrated with a number of representative examples ranging from enantioselective TM catalysts to radiopharmaceuticals and metalloenzymes.

References: References: Quant. Struct.-Act. Rel. 21, 119-127 (2002)

Title: Canonical Adiabatic Free Energy Sampling (CAFES): A Novel Method for the Exploration of Free Energy

Researchers: Joost VandeVondele
Ursula Röthlisberger

Institute/Group: Laboratory of Inorganic Chemistry, ETH Zürich, 8092 Switzerland
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

We present a novel method, canonical adiabatic free energy sampling (CAFES) that allows for the efficient exploration of the free energy surface of a subsystem (S) embedded in an environment (E) using molecular dynamic simulations. The dynamics of S is decoupled from the environment by introducing fictitious masses that ensure that S evolves slowly and adiabatically on the potential of mean force generated by E. In addition, the decoupling enables the use of different temperatures for the two parts of the system without introducing an irreversible heat flow. Using a higher temperature for the subsystem, a high efficiency for the sampling of rare events on the physical free energy surface is obtained. The performance of this approach is demonstrated with a conformational analysis of a Gly-Ala dipeptide in aqueous solution. Rare conformational transitions, which naturally occur on a millisecond time scale, are observed within a few nanoseconds of a classical molecular dynamics simulations. The same method has also been applied in a hybrid Car-Parrinello/classical molecular dynamics investigation of the proton-catalyzed conversion of 2-bromoethanol to dibromoethane in water. Using CAFES, the anchimeric assistance of the bromine atom and the occurrence of a bromonium ion intermediate, a process which involves a barrier of ca. 23 kcal/mol, is observed spontaneously on the subnanosecond time scale.

References: References: J. Phys. Chem. B 106, 203-208 (2002)

Title: The mechanism of catalytic enantioselective fluorination: Computational and experimental studies.

Researchers: Stefano Piana
Ingrid Devillers
Antonio Togni
Ursula Rothlisberger

Institute/Group: Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technology, ETH Hönggerberg, 8093 Zürich (Switzerland)
Current address: Institute of Molecular and Biological Chemistry, Swiss Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Description:

The synthesis of stereoactive organofluorine compounds is particularly challenging. Recently, the first catalytic enantioselective fluorination of β-ketoesters with F-TEDA in the presence of 5% of $TiCl_2$(TADDOLato) complexes as catalysts was presented. The enantioselectivity reaches 90%.
Here, we present a DFT-based QM/MM study of the reaction in acetonitrile solution. Our calculations elucidate the source of the observed enantioselectivity and provide a description of the reaction mechanism that allows to rationalize a large number of experimental data.
Furthermore, comparison with the same calculations in vacuo indicates that the interaction between the solvent and the reactants plays a crucial role in modulating the reaction pathway. Low-cost and accurate QM/MM schemes are nowadays readily available, thus we expect that the simulation of quantum reactants in a classical solvent will soon become the method of choice for the theoretical study of a large number of chemical reactions.

References: References: Angew. Chem. Intl. Ed. 41, 979 (2002)

Title: Modelling Weather and Climate on European and Alpine scales

Researchers: Christoph Schär, Robert Benoit, Olivier Fuhrer, Jan Kleinn, Daniel Leuenberger, Daniel Lüthi, Jürg Schmidli, Pier Luigi Vidale, Andre Walser

Institute/Group: Institute for Atmospheric and Climate Science (IAC) ETH, Zürich, Switzerland

Description:

Our research revolves around the study of continental and Alpine-scale weather and climate, with special focus on the water cycle. Regional climate processes are investigated with the help of our Regional Climate Model (RCM), the Climate High Resolution Model (CHRM); the dynamics of dry and moist atmospheric flow past complex topography are investigated with the help of a hierarchy of atmospheric models, including some non-hydrostatic ones (e.g. MC2, LM); hydrological processes in intermediate and major catchments in the Alpine region are investigated with the help of hydrological models (e.g. WASIM).

For the simulation of European regional climate, multiple state of the art, general circulation models (GCMs) are currently run at high resolution (grid spacing equivalent down to 100 km) by the European climate community in the context of two major research projects which will be active for the next few years, one funded by the Swiss NFS (NCCR Climate), the other by the European Commission (PRUDENCE). These current and future (scenario) simulations, together with the re-analyses provided by the European Center for Middle-Range Weather Forecasts (ECMWF, ERA-15 and ERA-40) are used to drive RCMs, which serve as dynamical downscaling tools. Our own CHRM, which we have extensively applied and verified in the past (using ERA-15 forcing data), in cooperation with the same community, is forced at the boundaries (nudged) with global data provided by the Hadley Center (HadCM) and the Max Planck Institut (ECHAM) GCMs. These simulations, both at grid spacings of 56 and 14 km (using a nested grid approach), cover a 30 year period under current climate conditions and also a 2071-2100 period, corresponding to standard SRES scenarios. The 14 km simulations are also used to drive the WASIM hydrological model, for impacts studies.

The principal focus of the PRUDENCE project is the production of regional climate change scenarios, and the assessment of their reliability and variability, (as related to climate but also to model formulations), together with the estimate of local impacts and risks. The NCCR project has broader scientific focus and also covers climate processes such as the moisture cycle (and relative feedbacks) within the soil, the land surface and the atmosphere. NCCR concurrently addresses research topics related to the debate on the ability of the GCMs to credibly represent tropospheric moisture dynamics and thermodynamics within different scenarios, together with consequences for precipitation estimation (and higher order statistics thereof) over the North Atlantic-European domain.

The purpose of the Mesoscale Alpine Project (MAP) is to declaredly improve the understanding of orographically influenced precipitation events and related flooding episodes involving deep convection, frontal precipitation and runoff. This includes the numerical prediction of moist processes over and in the vicinity of complex topography; the understanding and forecasting of the life-cycle of Foehn-related phenomena; the study of three-dimensional gravity wave breaking and associated wave drag; and the production of data sets for the validation and improvement of high-resolution numerical weather prediction, hydrological and coupled models in mountainous terrain. These research goals are pursued by exercising a hierarchy of numerical models, also applied in weather forecasting, and applying them at very high resolution to case studied of relevant weather events, which were amply documented by the MAP datasets.

Title: Fast deterministic pricing of options on Levy driven assets

Researchers: Ana-Maria Matache*
Christoph Schwab**

Institute: *Seminar for Applied Mathematics and RiskLab, ETH Zürich
**Seminar for Applied Mathematics, ETH Zürich

Funding: Research supported by Credit Suisse Group, Swiss Re and UBS AG through RiskLab.

Description: The fast numerical valuation of assets whose prices are driven by Brownian motion has become standard practice worldwide. In a Black-Scholes setting, this reduces to the numerical solution of a parabolic advection-diffusion equation with various initial/boundary conditions and possibly constraints. When closed form solutions are not available, numerical methods must be employed; methods for handling such numerical problems have been well developed. General Lévy processes have been advocated in recent years for models in option pricing. They offer more flexibility than Brownian motion and appear superior e.g. for modelling short-term asset returns whose distributions are heavy-tailed. Lévy models lead to parabolic integro-differential equations with nonlocal integro-differential operators which, in general, cannot be evaluated explicitly.

The objective of this project is to develop computational methodology for the fast numerical solution of pricing problems driven by general Lévy processes, based on wavelet techniques co-developed by Ch. Schwab. Our deterministic algorithm gives optimal convergence rates (up to logarithmic terms) for the computed solution in the same complexity as finite difference approximations of the standard Black-Scholes equation.

We plan to extend the types of contracts that can be priced: we allow American puts for jump-diffusion as well as pure jump processes, and also Asian contracts.

References: A.-M. Matache, T. von Petersdorff, C. Schwab, *Fast Deterministic Pricing of Options on Lévy Driven Assets*, submitted; available also as Research Report 2002-11 Seminar für Angewandte Mathematik, ETH Zürich
`http://www.sam.math.ethz.ch/reports/details/2002/2002-11.shtml`

Title: Generalized *hp*-FEM for Lattice Structures

Researchers: A. W. Rüegg, A.-M. Matache, Ch. Schwab

Institute/Group: Seminar for Applied Mathematics

Description:
Progress in manufacturing techniques allows the production of *lattice materials* of increasing complexity that are of growing importance in mechanical engineering, optoelectronics, etc.
Typically, when trying to characterize the physical properties of such materials, one has to take into account *three different length scales*: the macroscopic size l of the material block, the microscopic scale of the heterogeneities ε and finally the thickness of the bars δ. Taking the limit $\delta \to 0$, the remaining dimensionally reduced structures can be modeled by *networks* consisting of one-dimensional curves periodically arranged in a higher dimensional space.
A high order *generalized Finite Element Method* (gFEM) is developed to solve numerically elliptic *partial differential equations* (PDE's) on periodic lattice structures (see [3]). The standard polynomial spaces are replaced by conforming function spaces that are adapted to the micro-scale dependent coefficients of the differential operator, i.e. information much smaller than the macro mesh size $H \gg \varepsilon$ is built into the shape functions. These two-scale FE-spaces are obtained by augmenting the standard piecewise polynomial FE spaces with non-polynomial, periodic micro shape functions that are solutions of suitable unit cell problems on the reference network.
Taking into consideration the periodicity of the micro shape functions, the computation of the stiffness matrices to solve the discrete two scale problem can be realized with *work independent of the micro scale length* ε.
This method is implemented in C++ within the programming framework described in [2].

This Research is supported under the project "Homogenization and multiple scales" HMS2000 of the EC (HPRN-CT-1999-00109), by the Swiss Federal Government under Grant BBW 01.0025-01 and by the Swiss National Science Foundation under Project "Hierarchic FE-Models for periodic lattice and honeycomb materials" with Number SNF 21-58754.99.

References:

[1] A.-M. Matache, *Sparse Two-Scale FEM for Homogenization Problems*, Journal of Scientific Computing, (2002) **17**, 659–669

[2] A.W. Rüegg, *Implementation of Generalized Finite Element Methods for Homogenization Problems*, Journal of Scientific Computing, (2002) **17**, 671–681

[3] A.W. Rüegg. A. Schneebeli, R. Lauper, *Generalized hp-FEM for Lattice Structures*, in preparation

Title: Design of an *hp*-adaptive FE code for general elliptic problems in 3D

Researchers: Philipp Frauenfelder
Kersten Schmidt
Christoph Schwab

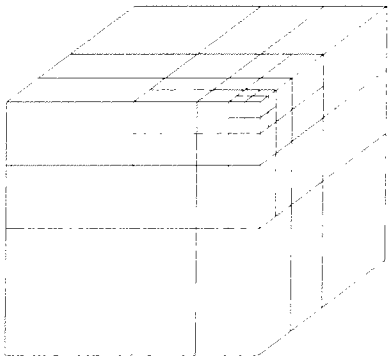
Institute/ Group: Seminar for Applied Mathematics
Departement of Mathematics

Description:

Many problems of engineering interest cannot be solved by applying a FEM based upon uniform meshes. To resolve boundary layer effects by a uniform mesh in a shell problem would make the numerical method prohibitively expensive and it would not be possible to obtain any solution of good quality. It is also advantageous if the meshsize as well as the polynomial degree can be adapted to account for boundary layer effects.

The project is design of a 3D *hp* FEM code that incorporates tetrahedral as well as hexahedral, prismatic and pyramidical elements. Based upon an existing C++ class library for fully *hp*-adaptive 2D FEM, 3-d classes in the library are developed.

On hexahedral meshes, the code is able to deal with non-conforming meshes resulting from element subdivisions. Anisotropic subdivisions are possible: into two, four or eight new elements. This allows for anisotropic refinements (see figure) and scale resolution. The mesh in the figure is non-conforming, ie. there are so-called *hanging nodes* which have to be treated carefully. Hanging nodes are eliminated by constraining the associated degrees of freedom by the degrees of freedom of the parent element (recursively if necessary). The approximation order (polynomial degree of the shape functions) can be chosen anisotropically and element by element.



Using the code, we are solving Maxwell equations in the frequency domain using weighted regularization (Costabel, Dauge). Other problem classes will follow.

References:

P. Frauenfelder, C. Lage. *Concepts—An Object Oriented Software Package for Partial Differential Equations* in press in M2AN Math. Model. Numer. Anal., SAM report 2002-09 (`http://www.sam.math.ethz.ch/reports/details/2002/2002-09.shtml`).

P. Houston, C. Schwab and E. Süli. *Discontinuous hp–Finite Element Methods for Advection–Diffusion Problems*, SIAM J. Numer. Anal., **39** (2002), no. 6, 2133–2163.

Title: Fast algorithms for the boundary element method

Researchers: Gregor Schmidlin[1]
Christoph Schwab

[1] supported under the TMR network (BBW 97.0404)

Institute/ Group: Seminar for Applied Mathematics

Description:

Many three-dimensional problems in possibly unbounded domains can be reduced to integral equations on the boundary of the domain. The discretization of these equations by finite elements on the boundary leads to the so-called Boundary Element Method (BEM) which has, in recent years, become a widely used tool in engineering for example in the loss computation within a transformer (ABB CRC Germany). Its competitiveness has, however, been moderate through the substantial quadrature work necessary to generate the dense stiffness matrices. The recently developed fast algorithms, such as *multipole*, *panel clustering* and also *wavelet-based methods* allow to decrease the computational complexity of BEM by several orders of magnitude. While the *panel clustering* is more resistant to complex geometries than the *wavelet-based methods* but the latter allow better preconditioning. With a new Haar wavelet basis (Figure 1) constructed by agglomeration we combine the robustness of the *panel clustering* with the advantage of the *wavelet-based methods*. This leads to a fast up to polylogarithmic factors linear algorithm.

Figure 1: Agglomerated wavelet basis

References:

[1] G. Schmidlin and C. Schwab, *Wavelet Galerkin BEM on Unstructured Meshes by Aggregation*, Lecture Notes in Computational Science and Engineering **20**, Multiscale and Multiresolution Methods, Theory and Applications, T. Barth, T. Chan, R. Haimes, Springer 2002, 359-378.

[2] G. Schmidlin, C. Lage and C. Schwab, *Rapid solution of first kind boundary integral equations in* $\mathbb{R}^3$, to appear in Engineering Analysis with Boundary Elements.

Title: Quantum Antiferromagnetism in Quasicrystals

Researchers: S. Wessel [*]
A. Jagannathan [**]
S. Haas [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of Southern California , Los Angeles, USA

Description:

Quantum magnetic phases of low-dimensional antiferromagnetic Heisenberg systems show various degrees of disorder caused by zero-point fluctuations. In our study we explore how non-perodic environments, such as provided in quasicrystal structures, further affect the magnetic properties of quantum magnets. In particular we study the Heisenberg model on a two-dimensional bipartite quasiperiodic lattice. The distribution of local staggered magnetic moments is determined, using the stochastic Series Expansion Quantum Monte Carlo method. A non-trivial inhomogeneous ground state is found. For a given local coordination number, the values of the magnetic moments are spread out, reflecting the fact that no two sites in a quasicrystal are identical. A hierarchical structure in the values of the moments is observed which arises from the self-similarity of the quasiperiodic lattice. Furthermore, the computed spin structure factor shows antiferromagnetic modulations that can be measured in neutron scattering and nuclear magnetic resonance experiments. Our generic model is a first step towards understanding magnetic quasicrystals such as the recently discovered Zn-Mg-Ho icosahedral structure.

References:

- S. Wessel, A. Jagannathan and S. Haas, Preprint submitted to Phys. Rev. Lett.

Title: New Quantum Monte Carlo Algorithms

Researchers: M. Troyer [*]
A. Dorneich [**]
F. Alet [*]
S. Wessel [*]

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

Description:

Great algorithmic progress for quantum Monte Carlo simulations has been achieved in the past years, shadowing the growth of processor power by many orders of magnitude. Still, many problems remain intractable and further algorithmic progress is needed. We have developed an algorithm to measure offdiagonal and time-dependent Green's function in the Stochastic Series Expansion (SSE) Quantum Monte Carlo algorithm.

A possible break-through was achieved by an adaptation of Wang-Landau sampling to quantum systems. This algorithm has the potential of overcoming the problems associated with tunneling through energy barriers at first order transitions and for disordered and glassy systems.

References:

- M. Troyer, S. Wessel and F. Alet, Preprint, submitted to Phys. Rev. Lett.
- A. Dorneich and Matthias Troyer, Phys. Rev. E **64**, 066701 (2001)

Title: Quantum Monte Carlo Study of Randomness-Driven Quantum Phase Transitions in Two-Dimensional Antiferromagnets

Researchers: Synge Todo*
Chitoshi Yasuda, Munehisa Matsumoto, Hajime Takayama **
Shigeru Koikegami***

Institute/Group: * Theoretische Physik, ETH Zürich
** ISSP, University of Tokyo, Japan
*** AIST Tsukuba, Tsukuba, Japan

Description:

We investigate effects of randomness, such as site dilution and bond randomness, on the ground state of two-dimensional Heisenberg antiferromagnets and also the nature of randomness-driven quantum phase transitions by means of the quantum Monte Carlo method.

References:

- C. Yasuda, S. Todo, M. Matsumoto, and H. Takayama, Phys. Rev. B. **64**, 092405 (2001).
- C. Yasuda, S. Todo, K. Harada, N. Kawashima, S. Miyashita, and H. Takayama, Phys. Rev. B **64**, R140415 (2001).
- S. Todo and K. Kato, Phys. Rev. Lett. **87**, 047203 (2001).
- S. Todo, M. Matsumoto, C. Yasuda, and H. Takayama, Phys. Rev. B **64**, 224412 (2001)
- M. Matsumoto, C. Yasuda, Synge Todo, and Hajime Takayama, Phys. Rev. B **65**, 014407 (2002)
- Chitoshi Yasuda, Synge Todo, Munehisa Matsumoto, and Hajime Takayama, J. Phys. Chem. of Solids, **63**, 1607 (2002)
- Masaaki Nakamura and Synge Todo, Phys. Rev. Lett. **89**, 077204 (2002)
- S. Koikegami, S. Todo, and H. Takayama, submitted to Solid State Commun.

Title: Quantum criticality

Researchers: M. Troyer [*]
M. Vojta [**]
S. Sachdev [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Universität Augsburg, Germany
[***] Yale University, USA

Description:

In low dimensional systems, such as layered materials quantum fluctuations are especially strong. They can lead to a destruction of an ordered ground state, just as thermal fluctuations can destroy order at finite temperatures. In the vicinity of a quantum critical point (a continuous phase transition in the ground state of a quantum system at zero temperatures) universal quantum critical behavior can be observed. This is similar to classical critical behavior observed near classical phase transitions at finite temperatures. Universal here means that the behavior does not depend on details of the system, material, lattice structure, but only on the symmetries of the phases and on the dimensionality. Simulations on simple models can thus provide results valid for a large class of materials. In the determination of universal classical critical behavior (characterized by universal critical exponents and amplitude ratios) numerical simulations were essential. The biggest challenge for these simulations is that the relevant length scales diverge at the phase transition, requiring extremely large lattices for accurate and reliable results. Recent breakthroughs in algorithmic developments for quantum systems now allow similar calculations to be performed near quantum critical points.

References:

- Subir Sachdev, M. Troyer and M. Vojta. Phys. Rev. Lett. **86,** 2617 (2001)
- K. Harada, N. Kawashima and M. Troyer, Preprint, submitted to Phys. Rev. Lett.
- M. Troyer, Sup. Prog. Theor. Phys. (in press)

Title: Quantitative modeling of quantum magnets

Researchers: A. Läuchli, M. Troyer [*]
D.C. Johnston [**]
A. Honecker [***]
F. Mila [****]

Institute/Group: [*]Theoretische Physik, ETH Zürich
[**] Ames Laboratories, Ames, Iowa
[***] Universität Braunschweig, Germany
[****] Université de Lausanne

Description:

Unusual behavior is observed in materials where quantum effects are strong. These materials typically consist of low-dimensional structures, such as weakly coupled chains or planes. The most prominent examples are the high temperature superconductors, which consist of doped copper oxide layers. While we are still far from a complete understanding of these doped systems, we could make rapid progress on the undoped parent compounds, which are quantum magnets. Modern quantum Monte Carlo algorithms allow quantitative comparisons between models and experimental measurements on these quantum magnets. These comparisons allow the determination of microscopic coupling constants and the explanation of unusual magnetic properties of low-dimensional quantum magnets, such as copper and vanadium oxide materials.

References:

- D.C. Johnston, Matthias Troyer, S. Miyahara, D. Lidsky, K. Ueda, M. Azuma, Z. Hiroi, M. Takano, M. Isobe, Y. Ueda, M.A. Korotin, V.I. Anisimov, A.V. Mahajan, and L.L. Miller, Preprint, submitted to Phys. Rev. B
- A. Honecker and A. Läuchli, Phys. Rev. B **63**, 174407 (2001)

Title: Phase Diagrams of 2D Bosonic Systems

Researchers: G. Schmid, S. Todo, M. Troyer [*]
G.G. Batrouni, K. Bernardett, F. Hebert [**]
A. Dorneich, W. Hanke [***]
R.T. Scalettar [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Nice, France
[***] Universität Würzburg, Germany
[****] University of California, Davis

Description:

The behavior of bosons in two dimensions is of major current interest for several reasons. Such systems describe, for example, Helium adsorbed on surfaces. They can also be mapped (approximately) to models for Josephson junction arrays, which can be manufactured and studied experimentally. In addition, a Hamiltonian describing a system of hardcore bosons, can be mapped exactly onto models of spin-1/2 Heisenberg quantum antiferromagnets. Such quantum spin models are of great theoretical and experimental interest: There are several recently discovered materials, exhibiting a variety of interesting properties such as magnetization plateaus, which are very well described by these Hamiltonians. In addition, such bosonic models can be used as effective models for fermionic systems where the bosonic Cooper pairs are well formed. In several extensive simulations we could determine the ground state and finite temperature phase diagram of the bosonic hardcore Hubbard model. Previously conjectured supersolid phases turned out to be phase separation instead. Unusual reentrant behavior and ordering upon *increasing* the temperature have been found.

References:

- K. Bernardet, G. G. Batrouni, Matthias Troyer, A. Dorneich, Phys. Rev. B **66**, 054520 (2002)
- G.G. Batrouni *et al.*, Phys. Rev. Lett. **89**, 117203 (2002)
- K. Bernardet, G.G. Batrouni, J.-L. Meunier, G. Schmid and M. Troyer, Phys. Rev. B **65**, 104519 (2002).
- G. Schmid, S. Todo, M. Troyer and A. Dorneich , Phys. Rev. Lett. **88**, 167208 (2002).
- F. Hebert, *et al*, Phys. Rev. B **65**, 014513 (2002).
- A. Dorneich, *et al.*,Phys. Rev. Lett. **88**, 057003 (2002).

Title: Frustrated Quantum Spin Systems

Researchers: A. Läuchli, G. Schmid, S. Wessel, M. Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:

Frustrated quantum spin systems offer the possibility to study the appearance of unusual quantum phases, driven by competing interactions and large fluctuations. In recent experiments on insulating cuprate materials evidence for substantial cyclic four-spin exchange interactions was accumulated. Higher order spin interactions are poorly understood in general. We investigated the overall phase diagrams of systems with such interactions and witnessed a surprisingly rich phase diagram already on the simple ladder structure. Among the different phases we discover the long sought staggered spin current phase.
We are also interested in the phase diagram of the generalized Shastry-Sutherland model (which seems to be realized in $SrCu_2(BaO_3)_2$). Our results indicate that the phase between the usual Neel order and the exact dimmer phase is actually a Valence Bond Crystal with a plaquette covering.

References:

- A. Läuchli, G. Schmid and M. Troyer, submitted to Phys. Rev. Lett.
- A. Läuchli, S. Wessel and M. Sigrist, Phys. Rev. B 66, 014401 (2002)
- A. Honecker and A. Läuchli, Phys. Rev. B 63 174407 (2001)

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

Researchers: Martin Wild
Andreas Roesch
Peter Tschuck
Atsumu Ohmura

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

Description:

Climate dynamics has attained much scientific and public attention in recent years due to the possibility of human-induced global change. Particularly, the increasing concentration of greenhouse gases and their potential to modify the climate of the Earth has raised much concern. This project is dedicated to the use of coupled atmosphere-ocean models to study the natural variability of the global atmosphere-ocean system and its response to anthropogenic forcing.
For this purpose the coupled atmosphere-ocean-seaice model ECHAM5/HOPE has been installed at the Swiss Center for Scientic Computing (CSCS) during summer 2001. This step represents a major upgrade of the atmospheric model component, which has already been successfully running at CSCS, to a comprehensive model of the entire global climate system, including atmosphere-ocean and seaice interactions. The model has been integrated in test simulations to ensure the correct installation of the system.
Multi-decadal integrations are performed with the coupled model under present day forcings, to assess its ability to simulate the present day climate. This provides the basis for subsequent climate change experiments based on various IPCC (Intergovernmental Panel on Climate Change) emissions scenarios.
In terms of research, special emphasis is placed on the simulation of the exchanges of energy fluxes at the interface between the components of the atmosphere, land/vegetation, and oceans, which are critical in terms of a successful coupling and the representation of the feedbacks between the subsystems. A key component thereby is the radiation, which forms the largest of these fluxes, and which is most directly responding to human or naturally induced alterations in the atmospheric composition. Typically, as much as 40% of the total CPU time of a climate simulation is devoted to the calculation of radiative fluxes. The accurate representation of these fluxes is a prerequisite for a realistic simulation of the response of the climate system to human-induced and natural radiative perturbations.
Further research areas include the evolution of global sea level due to mass balance changes of ice sheets and glaciers, as well as the simulation of regional scale climate dynamics, with a focus on the European and Alpine areas.

References:

See separate list

Title: Automated NMR structure determination using the new software CANDID and the torsion dynamics algorithm DYANA.

Researchers: Torsten Herrmann
Peter Güntert
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
The new software CANDID (Combined Automated NOE Assignment and Structure Determination Module) for efficient NMR structure determination of proteins performs automated NOE assignment of NOESY spectra using - in the present implementation - the fast DYANA torsion angle dynamics algorithm for the protein structure calculation. In 2001/2002 the software CANDID was used for *de novo* structure determinations of about a dozen proteins (see following project descriptions).

Reference: Herrmann, T., Güntert, P. and Wüthrich, K.
J. Mol. Biol. **319** (2002), 209–227

Title: Structural studies of prion proteins

Researchers: Luigi Calzolai
Vicent Esteve
Thorsten Lührs
Dominik Lysek
Christian Schorn
Nivon Lucas
Ralph Zahn
Christine von Schroetter
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik, ETH Zürich

Description:
The prion protein (PrP) is an indispensable 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. The prion protein is a highly conserved glycoprotein in mammals, where it is predominantly expressed in neuronal tissue, and which has also been found in birds and reptiles. We have solved 3-dimensional structures of the normal recombinant form of a selection of mammalian prion proteins, and are analyzing similarities and differences that might bear on the species barrier for infectious transmission of TSEs. Further we are extending these studies to birds and reptiles in search of new insight into the physiological role of normal PrPs. With the same goal in mind we have recently started a program of studies of intermolecular interactions with PrPs to extend and supplement the structure determinations. An important part of these projects is the cloning and expression of wild-type and variant prion proteins with and without isotope labeling for NMR studies.

Reference: Several manuscripts about the 3D structure determination of different species are in preparation.

Title: Structural studies of the pheromone-binding protein from *bombyx mori* (BmPBP).

Researchers: Fred Damberger*
Reto Horst*
Donghan Lee*
Peter Lüginbühl*
Peter Güntert*
Guihong Peng**
Larisa Nikonova**
Walter S. Leal**
Kurt Wüthrich*

Institute/Group: * Institut für Molekularbiologie und Biophysik, ETH Zürich, Switzerland
** National Institute of Agrobiological Sciences, Tsukuba, Ibaraki, Japan

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 ($BmPBP^A$ observed at pH 4.5 and $BmPBP^B$ 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 structure of $BmPBP^A$ at pH 4.5. Strikingly, a conformationally extended dodecapeptide which is on the surface in the crystal structure of the BmPBP-bombykol complex forms a regular a-helix which inserts 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 study of BmPBP under different solution conditions to provide insight into structure-function correlations, whic might be applicable to an entire class of proteins with pheromone-binding function.

Reference: Horst, R., Damberger, F., Luginbühl, P., Güntert, P., Peng, G., Nikonova, L., Leal, W. S., and Wüthrich K.
Proc. Natl. Acad. Sci. USA **98** (2001), 14374–14379

Title: Structural studies of the calreticulin P-domain.

Researchers: Lars Ellgaard**
Roland Riek*
Daniel Braun*
Torsten Herrmann*
Pascal Bettendorff*
Peter Güntert*
Francesco Fiorito*
Ari Helenius**
Kurt Wüthrich*

Institute/Group: * Institut für Molekularbiologie und Biophysik, ETH Zürich
** Institut für Biochemie, ETH Zürich

Description:
Calreticulin (CRT) is a molecular chaperone of the endoplasmic reticulum. In a previous collaboration with the group of Prof. A. Helenius we solved the solution structure of the central proline-rich P-domain, which is involved in interactions with the co-chaperone ERp57. Further studies aim at gaining more knowledge about the folding, stability and sequence-structure-relationship of the unusual single-hairpin fold of the P-domain. To this end, smaller constructs were engineered and their solution structures solved, using NMR. The central 36-residue fragment proved to be an autonomous folding unit, making it one of the smallest known natural sequences to form a stable fold in the absence of disulfide bonds or tightly bound metal ions. Additional studies are in progress to investigate the interactions between the calreticulin P-domain (or fragments thereof) and ERp57.

Reference: Ellgaard, L., Riek, R., Braun, D., Herrmann, T., Helenius, A. and Wüthrich K.
FEBS Lett. **488** (2001), 69–73

Ellgaard, L., Riek, R., Herrmann, T., Güntert, P., Braun, D., Helenius, A. and Wüthrich K.
Proc. Natl. Acad. Sci. USA **98** (2001), 3133–3138

Ellgaard, L., Bettendorff, P., Braun, D., Herrmann, T., Fiorito, F., Güntert, P., Helenius, A. and Wüthrich K.
J. Mol. Biol. (2002), in press

6
High-Performance Hardware

6.1 Competence Center for Computational Chemistry

The following resources are available:

- a cluster of 40 dual-processor PC's;
- two Compaq AlphaServers with 6 and 8 EV6/525 processors.

The research activities of the Competence Center for Computational Chemistry C^4, its members and the operation of the C^4 hardware are described in the C^4 Annual Report 2001/2002, which is published in November 2002.

6.2 HPCN Technology at CSCS Manno

In the frame of its national service mission, CSCS provides its academic, governmental and industrial user community with High Performance Computing and Networking resources and support competencies. The CSCS HPCN technology division staff offers expertise and support in the following fields of computational sciences and engineering:

- high performnace systems and networks
- applications support and performance optimization
- benchmarking and software engineering
- data mining and visualization.

Computing Resources

Massive Parallel Processing Platform

MPP (IBM Regattas):

The CSCS IBM MPP consists of 8 Regatta SMP (Power-4) nodes, and 2 Nighthawk SMP (Power-3) nodes, for a theoretical peak performance of 1379.2 TFLOPS.

The IBM Regatta "SP4" consists of eight nodes (Regatta p-690 Server with 32 CPUs Power4 @ 1.3 GHz each) for a total of 256 CPUs and 768 GB of main memory, and with 4 TB usable SSA disk space.

The SP frame is switched by a Double Colony IBM-switch providing a Parallel Environment with a peak performance of 1.3 Tflops and a Global Parallel File System of 4 TB.

The IBM Nighthawks "SP3" consists of two High Nodes (Nighthawks with 16 CPUs - Power3+ @ 375 MHz each) for a total of 32 CPUs and 32 GB of main memory, and with 1 TB usable SSA disk space.

The SP frame is switched by a Colony IBM-switch providing a Parallel Environment with a peak performance of 48 GFlops and a Global Parallel File System of 1 TB.

The overall system runs on AIX 5.1, with standard XL fortran, C/C++ compilers available.

Compilers, Libraries and Tools

XL Fortran Fortran compiler
VisualAge C/C++ C/C++ compiler
ESSL Engineering and Scientific Subroutine Library
FFTW Discrete Fourier Transform (DFT)

LAPACK Linear Algebra PACKage
MASS Mathematical Acceleration Subsystem
NAG FORTRAN, F90 and C collection of callable routines
NETCDF Network Common Data Form
P-ESSL Parallel ESSL
ScaLAPACK Scalable LAPACK
WSMP Watson Symmetric Sparse Matrix Package,
GA Toolkit Shared memory style programming environment
Loadleveler Job management system
AIX PE Developing/Executing parallel F/C/C++ codes
iDebug Distributed Debugger
xldb Source and Machine Level Debugger
hpmcount Hardware Performance Monitor

Chemistry Applications

ADF Amsterdam Density Functional, Kohn-Sham approach to the Density-Functional Theory (DFT) Amber Suite of programs to carry out Molecular Dynamics simulations (particularly on biomolecules).
CPMD Plane wave/pseudopotential implementation of Density Functional Theory.
Dalton Quantum chemistry program with SCF, MP2, MCSCF or CC wave functions.
Gamess/US Package for Hartree-Fock and semiempirical methods (RHF, ROHF, UHF, GVB, MCSCF, with CI and MP2) Gaussian General computational chemistry package for Hartree-Fock, CI and DFT methods.
GROMACS Molecular dynamics simulations for biochemical and non-biological systems.

Parallel Vector Processing Platform

NEC SX-5

The CSCS SX-5 system consists of a single node with 16 CPUs (8 Gigaflops each) and 64 Gbytes of shared main memory (expandable up to 128 GB memory max.) having a peak performance of 128 gigaflops. The network connection to the SX-5 is provided via FastEthernet and HiPPI.

The operating system is SUPER-UX R11.1 and the following SW tools and packages are available on this platform:

Compilers, Libraries and Tools

C: ANSI C Compiler
C/C++: ANSI C and C++ Compiler
FORTRAN-90: F90 and F77 Compiler with F95 extensions
HPF: High Performance Fortran Compiler
MPI/SX: MPI library for Fortran, C and C++
OpenMP/SX: OpenMP extensions for the Fortran language

NQS: (Batch) Queue system
pdbx: Parallel debugger
Psuite: Program development environment
Vampir: MPI tracer/profiler/analyzer
MathKeisan: Highly tuned and well-tested collection of Math libraries for the SX series
ASL: Scientific library for the SX Series
GPFA: Fast Fourier Transform library
NAG: NAG FORTRAN 77 and FORTRAN 90 Library
NetCDF: Network Common Data Form library
FISHPACK: Subroutines for solving separable partial differential equations in various coordinate systems.
Zufall: Random Numbers Generator

Chemistry Applications

ADF: Density functional program
Currently installed version: 2000.02
CPMD: Plane wave/pseudopotential implementation of Density Functional Theory.
Gamess-US: Package for Hartree-Fock and semiempirical methods
Currently installed version: Jun. 25 2001 R2
Gaussian: General computational chemistry package for Hartree-Fock, CI and DFT methods. Currently installed version: G98 Rev. A9
MolPro: Multiconfiguration SCF and CI, MCSCF, DFT
Currently installed version: 2000.1

Engineering Applications

STAR-CD: Engineering
CFX: Fluid Dynamics

Scalar Processing Platform

HP N-Class Cluster

CSCS provides its users community also with a HP-based compute serving environment composed of 4 Hewlett Packard N-Class servers model N4000 (9000/800) based on 360MHz PA-8500 64 bit processors.

Three N400 server systems are configured with 8 CPUs and one with 6 CPUs, 2 GB main memory and 100 GB local temporary disk space each. Home directories are centralized on the file server.

All systems run under HP-UX 11.0 and therefore allow the access to a wide applications portfolio, especially engineering and chemistry applications. The N-Class cluster integration, job scheduling and load balancing is done via Load Sharing Facility (LSF).

The following packages are available on this platform:

Compilers, Libraries and Tools

HP ANSI C: Compiler
HP FORTRAN-90: Compiler
HP FORTRAN-77: Compiler
HP C++: Compiler
LSF: (Batch) Queue system
MLIB: Scientific library
VECLIB: Scientific library
LAPACK: Scientific library
Maple: Symbolic Calculus
Mathematica: Integrated technical computing system
Matlab: Language for technical computing

Chemistry Applications

ADF: Density functional program
Currently installed version: 2000.02
Gamess-US: Package for Hartree-Fock and semiempirical methods
Currently installed version: Jun. 25 2001 R2
Gaussian: General computational chemistry package for Hartree-Fock,
CI and DFT methods. Currently installed version: G98 Rev. A9
MolPro: Multiconfiguration SCF and CI, MCSCF, DFT
Currently installed version: 2000.1
Meldf-x: Single-/multi-reference CI
Molcas: Multiconfiguration SCF and CI, MCSCF, CASSCF
Currently installed versions: 4.1 / 5.0
Prddo/M: Approximative Hartree-Fock for very large molecules
Currently installed version: 5.1
Turbomole: Program Package for ab initio Electronic Structure Calculations
Currently installed version: 4.0

Engineering Applications

STAR-CD: Engineering
FLUENT: Fluid Dynamics
CFX: Fluid Dynamics

List of current Large Users Projects (reviewed by the CSCS Research Committee)

Free Surface Prediction in Pelton Turbine
Prof. F. Avellan (Laboratoire de Machines Hydrauliques, EPFL)

First-Principles Computations of Growth-Related Defects and Molecular Nanostructures

Prof. A. Baratoff (Inst. für Physik, Uni-Basel)

Global and Regional Climate Modelling
Prof. M. Beniston (Inst. of Geography, Uni-Fribourg)

Coupling between tropospheric chemistry and aerosol in the circulation model ECHAM
Dr. I. Bey (LMCA, EPFL-ENAC)

Enantioselective Hydrogenation of Activated Carbonyl Compounds over Chirally Modified Platinum
Dr. T. Bürgi (Laboratorium für Technische Chemie, ETHZ)

Protein folding, misfolding and stability
Prof. A. Caflish (Biochemistry, Uni-Zürich)

Modelling of incommensurate Structures
Prof. G. Chapuis (Inst. de Cristallographie, Uni-Lausanne)

Computation of Stellarator Coils, Equilibrium and Stability
Dr. A. Cooper (CRPP-PPB, EPFL)

Computational Chemistry of Molecules and Solids Containing Metal Atoms
Prof. C. Daul (Department für Chemie, Uni-Fribourg)

ERA40 for NCCR-Climate
Prof. H.C. Davies (Institut für Atmosphäre und Klima, ETHZ)

Chiral Symmetric Dirac Operator in Lattice QCD
Prof. P. Hasenfratz (Inst. für Theoretische Physik, Uni-Basel)

CO2 trimers
Prof. H.P. Huber (Inst. of Physical Chemistry, Uni-Basel)

Ab initio Molecular Dynamics in Electronically Excited States
Prof. J. Hutter (Inst. of Organic Chemistry, Uni-Zürich)

Transition Metal Catalyzed Reactions and Car-Parrinello Molecular Dynamics
Prof. J. Hutter (Inst. of Organic Chemistry, Uni-Zürich)

Ab initio MD Study of Methionyl Aminopeptidases
Prof. C. Klein (Dept. Applied Biosciences, ETHZ)

Numerical Simulation of Transitional, Turbulent and Multiphase Flows
Prof. L. Kleiser (Inst. of Fluid Dynamics, ETHZ)

Simulations using Particle Methods
Prof. P. Koumoutsakos (Inst. for Computational Sciences, ETHZ)

Machine Learning Algorithms for Flow Modeling and Control
Prof. P. Koumoutsakos (Inst. for Computational Sciences, ETHZ)

Direct Numerical Simulation of the Buoyancy-Driven Turbulence in a Cavity
Mr. E. Leriche (Laboratoire d'Ingenerie Numerique, EPFL)

Proton Transfer and Hydrogen Bonding in Microsolvent Clusters and Nucleic Acid Base Pairs: Theory and Dynamics
Prof. S. Leutwyler (Dept. für Chemie und Biochemie, Uni-Bern)

Compressible Simulations
Dr. P. Leyland (Fluid Mechanics Laboratory, EPFL)

Large eddy simulation of turbolence for interface tracking-based simulation of multi-phase flows
Dr. P. Liovic (Lab. für Kerntechnik, ETHZ)

Computational Quantum Chemistry of Large Molecules
Dr. H.P. Lüthi (Laboratory for Physical Chemistry, ETHZ)

Quantum Chemical Investigations of Cyclization Reactions Involving Cationic Species
Dr. J. Mareda (Department of Organic Chemistry, Uni-Geneva)

Computational Solid State Physics
Prof. P.F. Meier (Physik Institut, Uni-Zürich)

Dark Matter in the formation of the universe
Prof. B. Moore (Inst. for Theoretical Physics, Uni-Zürich)

Global Climate Change: Modelling Atmosphere/Ocean Variability on Decadal Time Scales
Prof. A. Ohmura (Inst. for Atmospheric and Climate Science, ETHZ)

Formation and Evolution of the Milky Way
Prof. G. Ortwin (Astronomisches Institut, Uni-Basel)

Disordered Network-Forming Materials
Prof. A. Pasquarello (Dept. ITP/IRRMA, EPFL)

Structural and Electronic Properties of Solids and Surfaces
Prof. M. Posternak (Laboratoire de Théorie du Solide, EPFL)

Quantum Mechanical Simulation of Molecules and Molecular Clusters
Prof. M. Quack (Laboratorium für Physikalische Chemie, ETHZ)

First-Principles Characterization and Design of Radiopharmaceuticals
Prof. U. Rötlisberger (Inorganic Chemistry-HCI, EPFL)

QM/MM - Car Parrinello Study of Catalytic Mechanisms of DNA Repari Enzymes
Prof. U. Rötlisberger (Inorganic Chemistry-HCI, EPFL)

Rational Design of Biomimetics via Mixed Quantum/Classical Car-Parrinello Simulations
Prof. U. Rötlisberger (Inorganic Chemistry-HCI, EPFL)

Ab initio Hybrid Simulations of Electron Transfer Reactions
Prof. U. Rötlisberger (Inorganic Chemistry-HCI, EPFL)

Modelling Weather and Climate on European and Alpine scales
Prof. C. Schär (Inst. for Atmospheric and Climate Science, ETHZ)

Variability of the Sun and Global Climate
Dr. W. Schmutz (Physikalisch-Meteorolgisches Observatorium, WRC)

MONALISA: Modelling and Reconstruction of North Atlantic Climate System Variability
Prof. T. Stocker (Physics Inst., Uni-Bern)

Modelling of nanostructured materials
Prof. H. Van Swygenhoven (GPA/ASQ, PSI)

New Organic Chemistry based on Sulfur Dioxide
Prof. P. Vogel (Inst. for Physical Chemistry, EPFL)

Computational Quantum Chemistry of Increasingly Complex Systems
Prof. J. Weber (Department of Physical Chemistry, Uni-Geneva)

Modelling Complex Molecular Systems using Embedded Cluster Approach
Dr. T. Wesolowski (Department of Physical Chemistry, Uni-Geneva)

Direct numerical simulation of condensation
Prof. G. Yadigaroglu (Lab. für Kerntechnik, ETHZ)

6.3 The Beowulf Cluster "Asgard"

Beowulf clusters are massively parallel supercomputers built from commodity components, standard PCs running Linux and Ethernet networks. They profit from the low cost of the building blocks and offer the best price/performance ratio for many applications that are not limited by network bandwidth or latency. Most applications in physics are perfectly parallelizable and run with optimal speedup on a cluster – no fast network is needed except for access to the file server. These applications include embarrassingly parallel applications such as parameter studies, where a single program has to be run thousands of times with different input parameters. Other methods that are well suited to a cluster are Monte Carlo simulations, where independent samples can be created on different CPUs with minimal communication needs. Since the majority of applications in physics are of these types, the cluster provides an ideal platform, complementary to the traditional supercomputers at ETH.

The Asgard Beowulf cluster, which was installed early in the year 2000 still works very well. Software upgrades, including the change to a new kernel version have improved the stability of the machine. An additional file server with 2 Terabyte capacity, purchased with startup funds of M. Troyer will provide sufficient storage space for the next years.

The users were very satisfied with the performance of the machine, which was to be expected for the majority of CPU-intense but not network-demanding applications. Surprisingly, besides these perfectly parallelizing applications the network bandwidth and latency turned out to be good enough not only for the development and testing of nontrivial parallel applications, but also for many production runs of problems such as beam dynamics, relativistic stellar plasmas and strongly correlated quantum systems.

As regards the operating mode, the cluster us split into two main queues, one for parallel jobs with up to 256 CPUs, and one for a large number of serial applications. In addition, processes with low memory demands are run as low-priority background jobs, using up the remaining idle time. We can thus achieve near-optimal usage of more than 95% - a very high number compared to traditional supercomputers.

An upgrade/replacement of the Beowulf cluster is planned for 2003 and the procurement has been initiated.

For further details about the hardware, software, operating mode, account applications and user projects we refer to the Asgard web page at http://www.asgard.ethz.ch.

Asgard research projects

Since not all of the projects on Asgard are included in this annual report we list the main user projects here. For details we refer to the description of these projects on the Asgard web page at http://www.asgard.ethz.ch.

Theoretical Physics

- *Soliton's Dissipation Through Emission Of Radiation*
  by G. Interlandi,W. Aschbacher, J.Fröhlich and M.Troyer
- *Vortex Collisions: Crossing or Recombination?*
  by M.Bou-Diab andG.Blatter
- *Quantum Phase Transitions in the 2D Hardcore Bosonic Hubbard Model*
  by G. Schmid and M.Troyer
- *Quantum critical behavior in antiferromagnets and superconductors*
  by M. Troyer
- *Quantitative modeling of strongly correlated materials*
  by M. Troyer
- *High Temperature Series Expansion for Quantum Lattice Models*
  by M. Körner and M. Troyer
- *N-Patch Renormalization Group Study of the Two-Dimensional t-t' Hubbard Model*
  by C. Honerkamp, M. Salmhofer and T.M. Rice
- *Multiparticle Exchange Processes in the Two-Dimensional Wigner Glass*
  by K. Völker
- *Exact Diagonalization Studies of Strongly Correlated Electron Systems*
  by A. Läuchli, M. Troyer and T.M. Rice
- *Simulation of the vortex texture in a superconductor*
  by F. Mohamed, G. Blatter and M. Troyer
- *Topologically protected quantum bits*
  by D. Ivanov, M. Troyer and G. Blatter

Particle Physics

- *Monte Carlo Simulation of the L3+C Experiment at CERN*
  by Renzo Ramelli and Pierre Le Coultre
- *Monte Carlo Simulations of the AMS Detector*
  by Adrian Biland
- *Backtracing of Cosmic Ray Particles*
  by Adrian Biland

- *Simulation of Csmic Ray Showers*
  by Haitao Liu
- *Magnetic Shielding for Synchrotron Radiation Detector (SRD)*
  by Hans Anderhub
- *Atlas Event Filter Studies*

Astrophysics

- *Kinetic Simulation of Solar Plasmas*
  by Peter Messmer and Arnold O. Benz
- *Dynamics of Free-floating Planets in Stellar Clusters*
  by Kester Smith

Mathematics

- *Parallelization of Low-Communication Processes*
  by Jörg Waldvogel and Peter Leikauf
- *Solving of Boundary Integral Equations*
  by Gregor Schmidlin and C. Schwab
- *Numerical procedures for PDEs using the Feynman-Kac Formula by*
  Wesley P. Petersen and Rolf Jeltsch
- *Multi-dimensional FFT algorithms on Asgard*
  by W. Petersen
- *Accuracy comparison of N-body codes*
  by Luzi Schucan, and M. Troyer
- *Parallel Smoothing for Multigrid via Sparse Approximate Inverses*
  by Oliver Bröker and Marcus J. Grote
- *A new Field Solver for Space Charge dominated Beams*
  by Andreas Adelmann, Stefan Adam, Rolf Jeltsch and Ralph Eichler

Polymer Science

by the group of Hans Christian Öttinger

- *Rheology and Thermodynamics (GENERIC)*
- *New Models in Polymer Kinetic Theory*
- *Dynamic Models Describing the Glass Transition*
- *Crystallization in Polymer Melts under Elongational Flow*
- *Nonequilibrium dynamics computer simulation of polymer fluids*

Computer Science

- *Development and Application of Biologically Inspired Optimization Algorithms*
  by Sibylle Müller and Petros Koumoutsakos
- *Traffic simulations*
  by Kai Nagel and Res Voellmy
- *Macro-economic modeling, computational economics and statistics*
  by E.J. Kontoghiorges and P. Arbenz

6.4 Information Technology Services

The following resources are available:

- Cray SV1 Cluster consisting of
    - 1 Cray SV1-B/16-8 (Athos): 16 Vector CPUs (300 MHz), 8 MB Memory
    - 1 Cray SV1-B/8-4 (Porthos): 8 Vector CPUs (300MHz), 4 GB Memory
    - 320 Gigabyte Disk, shared through Gigaring among the cluster
    - Unicos Operating System

  The clusters major usage is highly vectorized, moderately (up to 8 processors) parallel code in the fields of climate modeling, theoretical physics and astronomy.

  The following compilers, libraries and applications are installed on the cluster:
  ANSI II C: Compiler
  C++: Compiler
  FORTRAN-90: Compiler
  MPGS: graphical library and viewer
  GROMOS: biomolecular simulation
  UniChem 5.0 (Cadpac, DGauss, MNDO): chemistry
  MOPAC, DISCO, ACES2: chemistry
  AMBER 5: chemistry
  Gaussian-94 (for educational purposes only): chemistry
  PAM: finite elements
  CFX-F3D: fluid dynamics
  NAG Mk 19, IMSL 10: numerical libraries
  Maple 4.3: symbolic calculus
  ranq, zufall: random number libraries
  mfft: multitasked fast forier transforms
  egm: graphical library
  The Cray SV1 service will be terminated by the end of 2003.

- Hewlett Packard Superdome Cluster consisting of
    - 1 HP Superdome (Stardust): 64 PA8600 CPUs (550 MHz), 64 GB Memory, 400 GB Disk, HP/UX Operating System
    - 1 HP Superdome (Pegasus): 32 PA8600 CPUs (550 MHz), 32 GB Memory, 400 GB 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

7
Outlook

This report documents the strength, scope and dynamics of CSE at the ETH. The fact that CSE is defined to be a "Strategische Erfolgs-Position", SEP, guarantees that the board of the ETH is fostering the field of CSE and of Computing in general, in almost all departments.

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. The Computational Laboratory in CSE, CoLab, should become a place of interdiciplinary research according to its mission:
"The CoLab represents an instrument that enhances research in Computational Science by creating bridges across disciplines. The CoLab provides the scientific and physical infrastructure that allows to coordinate and strengthen such interactions. It serves as an academic forum for the exchange of interdisciplinary computational ideas among researchers, educators and students.
The CoLab is open to all members of the ETH and its academic partners. Through sustained collaboration the CoLab's mission is to:
- strengthen research and educational links among ETH members in the context of CSE.
- create active collaborations with Swiss research and academic institutions in CSE.
- maintain active international collaborations with world-leading institutions in CSE.
- develop links between Industry and Academia."

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. Unfortunately, the current financial problems of the ETH slow down this process.

We do hope that the two remaining professorships in CSE will be filled in the near future.

In the coming year, we hope to finalize the Bachelor and Master program in CSE, so that students may enroll in the former in the fall of 2003. Moreover, it is hoped that more researchers in computational sciences can be seduced to contribute to the CSE education.

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, October 24, 2002
Rolf Jeltsch

8
Publications* in 2001/2002

*only CSE-related articles
in refereed journals

Group of G. Blatter

M. Bou-Diab, H. Nordborg and G. Blatter
Vortex collisions: crossing or recombination?
Phys. Rev. Lett. **86**, 5132 (2001).

L. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter
Topologically protected quantum bits from Josephson junction arrays
Nature **415**, 507 (2002).

F. Mohamed, Matthias Troyer, Gianni Blatter and I. Luk'yanchuk
Interaction of vortices in superconductors with κ close to $1/\sqrt{2}$
Phys. Rev. B **65**, 224504 (2002)

Group of H.C. Davies

List of publications:

Benoit,R., C. Schär, P. Binder, S. Chamberland, H.C. Davies, M. Desgagné, C. Girard, C. Keil, N. Kouwen, D. Lüthi, D. Maric, E. Müller, P. Pellerin, J. Schmidli, F. Schubiger, C. Schwierz, M. Sprenger, A. Walser, S. Willemse, W. Yu and E. Zala, 2002. The real-time ultrafinescale forecast support during the Special Observing Period of the MAP. *Bull. Amer. Meteor. Soc.*, **83**, 85-109

Calisesi, Y., H. Wernli and N. Kämpfer, 2001. Midstratospheric ozone variability over Bern related to planetary wave activity during the winters 1994-95 to 1998-99. *J. Geophys. Res.*, **106**, 7903-7916.

Fueglistaler, S., B.P. Luo, S. Buss, H. Wernli, C. Voigt, M. Müller, R. Neuber, C. Hostetler, L. Poole, H. Flentje, D.W. Fahey, M.J. Northway and Th.~Peter, 2002. Large NAT-particle formation by mother clouds: Analysis of SOLVE/THESEO-2000 observations. *Geophys. Res. Lett.*, **29**(12), 1610, doi:10.1029/2001GL014548.

Heck, P., D. Lüthi, H. Wernli and C. Schär, 2001. Climate impacts of European-scale anthropogenic vegetation changes: A study with a regional climate model. *J. Geophys. Res. - Atmos.*, **106** (D8): 7817-7835

Massacand, A.C., H. Wernli and H.C. Davies, 2001.Influence of upstream diabatic heating upon an Alpine event of heavy precipitation. *Mon. Wea. Rev.*, **129**, 2822-2828.

Shapiro, M.A., H. Wernli, N.A. Bond and R. Langland, 2001. The influence of the 1997-99 El Nino Southern Oscillation on extratropical baroclinic life cycles over the eastern North Pacific. *Quart. J. Roy. Meteor. Soc.*, **127**, 331-342.

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