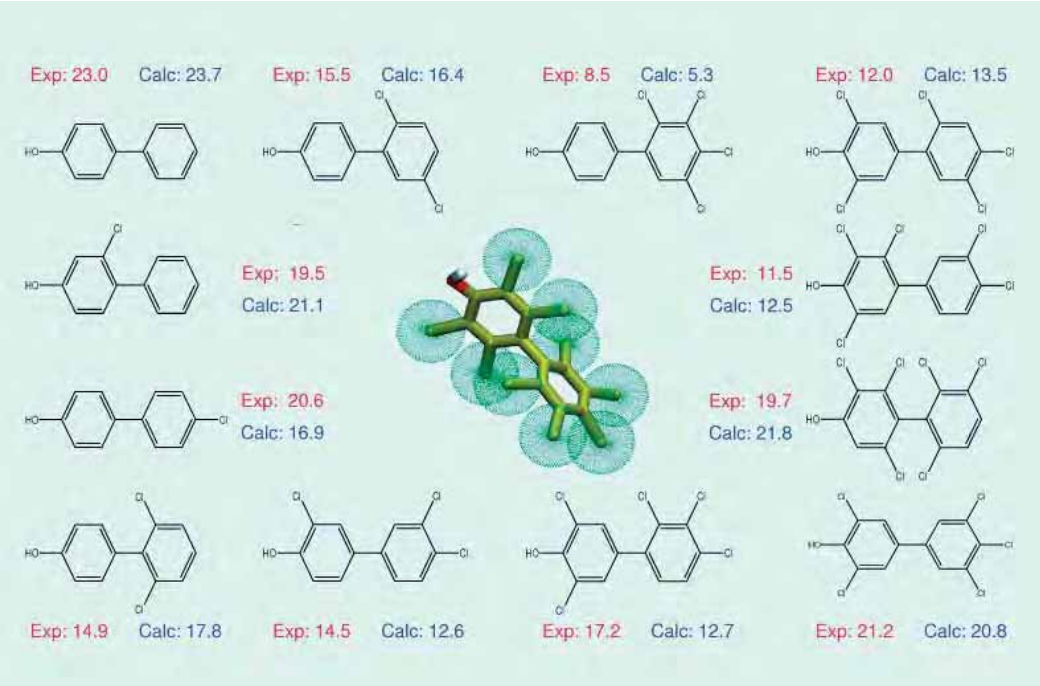
CSE

Computational Science and Engineering

Annual Report
2004 / 2005



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSE

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2004 / 2005

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Cover:
Free energies of ligand binding to the estrogen receptor: Experimental values and values from single-step free energy perturbation calculations (in kJ/mol) for a series of polychlorinated biphenyls. The reference state used for the single MD simulation is given in the center, with soft-core sites indicated as spheres.

Groups having contributed to this report:

Research Group	Institute	Projects	Publs.
J. Blatter	Theoretical Physics	125	190
K. Boulouchos	Engines and Combustion Laboratory	46	192
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Introduction

This is the fifth CSE Annual Report at ETH. Last year we moved to electronic edition only and clearly this is the way for the future. It turned out that most people found it more convenient to have it accessible on the web. We can reach more persons with the electronic version than with a report on paper. This becomes particularly important with the start of the Master Program in CSE, where we hope to attract students not only from within ETH but from all over the world. More and more persons are interested in research and education in CSE, students and colleagues, visitors and people form other universities. They all want to know what is going on at ETH in this exciting field. This new edition documents the changes that happened in the last year and gives a glimpse of the developments immediately ahead of us.

This fall the first students finished the newly established Bachelor program. They had started two years ago after a one year study in a subject closely related to CSE and having passed the basic exam at ETH, or a similar education in another institution. Most of these new bachelors have now entered the Master program and will finish it after two semesters of study and their Master thesis. By that time the first students will have passed the whole new Bachelor/Master cycle. This is the moment to review the program as a whole and therefore we plan for a workshop on CSE, Research and Education, in 2007. As it happens, 2007 will be the 10th anniversary of the CSE curriculum at ETH.

On the research side we have seen again new professors being hired who use computing as one of their important tools to do science and/or engineering. In this year our colleague Wilfred Van Gunsteren will show in the featured report (Computational Highlight, Chap. 4) some new results from Computational Chemistry and Biology.

Work on the preparation for the International Congress on Industrial and Applied Mathematics, ICIAM 2007, is now in full swing. We are looking forward to this event which will be held at the University of Zürich and at ETH, July 16-20. A large portion of the congress will cover CSE.

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

Zürich, December 5, 2005
Rolf Jeltsch, Studiendelegierter und Mitglied des Ausschusses Rechnergestützte Wissenschaften

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Education

The second year of the new Bachelor Program in CSE has started in October 2004 with 17 students. The students had done their first year's studies in another curriculum at ETH in the following fields: Mathematics 2 students, Computer Science 5, Mechanical Engineering 1, Electrical Engineering 2, Chemistry 1, Biology 4; and at the EPF Lausanne in Mathematics 1 and at the University of Zurich in Mathematics 1.

In October 2005 the first students will earn their Bachelor degree in CSE and will thus be able to continue their studies in the CSE Master Program starting this October. The Master studies will take one and a half years including the five months of the Master thesis and will lead to the degree of a Master of Science ETH in CSE.

The students in the two and a half years Diploma curriculum in CSE existing since October 1997 and started for the last turn in October 2003 are entering the diploma semester and most of them will finish their studies in 2006.

The total number of CSE students enrolled in the academic year 2004/2005 was 47.

The presentation of the CSE Bachelor/Master curriculum for ETH students of the second semester of May 19, 2005 was attended by around 50 students. It is hoped that a fair number of them will start with the CSE Bachelor studies this fall.

In the past academic year 8 students have successfully finished their CSE studies and have received a CSE diploma with very good scores. They chose the following fields of specialization: Chemistry, Fluid Dynamics, Robotics and Physics of the Atmosphere. In the following list we give the name of the student, the title of the diploma thesis and, in parentheses, the name and the department/institute of the advisor.

Diploma Theses

T. Aka	Entwicklung einer Mustererkennumgsmethode zur Niederschlags-verifikation (H. Davies, Atmospheric and Climate Science)
U. Battaglia	1-D-Strömungs- und Klimasimulation für ein variables Tunnel-Netzwerk (P. Jenny, Fluid Dynamics)
A. Dobler	A 2-D fimite volume nonhydrostatic atmospheric model implementation of cut-cells and further experiments (C. Schär, Atmospheric and Climate Science)
M. Jörg	Numerical investigations of wall boundary conditions for two-fluid flows (A. Prohl, Applied Mathematics)
T. Kühne	Parallel visualization for astrophysics (B. Moore, Astrophysics, University of Zurich)

I. Oppermann	A boundary integral solver for the parallel particle mesh library (P. Koumotsakos, Computer Science)
R. Veprek	Refined FE modelling of indentation experiments on hard coatings (M. Farshad, EMPA Dübendorf)
S. Wunderlich	A 2-D finite volume nonhydrostatic atmospheric model implementation and experiments (C. Schär, Atmospheric and Climate Science)

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

Term Papers

G.-M. Baschera	Numerical simulation of harmonic map heat flow: parallelization (R. Hiptmair, Applied Mathematics)
C. Bosshard	Hash Based Data Structures for Tetrahedral Meshes (R. Hiptmair, Applied Mathematics)
D. Caviezel	Finite-Volumen-Methode für kompressible Strömung mit mehreren Spezies (P. Jenny, Fluid Dynamics)
J. Eller	Modellierung thermodynamischer Parameter im Na2O-SiO2 System (W. Halter, Isotopengeologie)
J. Eller	Automatische Verschiebungsanalyse auf Gletschern (M. Funk, Glaciology)
A. Elsener	Sortimentsoptimierung in der Forstwirtschaft (H.-J. Lüthi, Operations Research)
M. Guidon	Worm algorithm for classical statistical models (M. Troyer, Theoretical Physics)
M. Hack	Visualisierung von Wirbelstrukturen in kompressiblen Strömungen (L. Kleiser, Fluid Dynamics)
M. Hack	Angle conditions for face and edge elements (R. Hiptmair, Applied Mathematics)
N. Hodler	Numerical simulation of harmonic map heat flow: discretization (R. Hiptmair, Applied Mathematics)

E. Huber	Constrained Optimization Using Stochastic Ranking in Evolution Strategies (P. Koumoutsakos, Computer Science)
M. Jörg	Hardware-accelerated normal fairing (M. Gross, Computer Science)
R. Mooser	Transpositions and communications strategies for multidimensional FFT on distributed memory computers (W. Petersen, Applied Mathematics)
J. Nart	Local features for image categorization (J. Buhmann, Computer Science)
Th. Oesch	Cluster algorithms for Ising models in magnetic fields (M. Troyer, Theoretical Physics)
P. Rousselot	Simulation of 2D selfpropelled anguilliform swimming (P. Koumoutsakos, Computer Science)
J. Renggli	Performance evaluation and optimization of a parallel n-body code (J. Stadel, Astrophysics, University of Zurich)
D. Sydler	Entwicklung einer High-Level-Architektur für Simulationen im Umweltbereich (W. Schaufelberger, Automatic Control)
D. Sydler	Inpainting of geometric details for point-sampled surfaces (M. Gross, Computer Science)
M. Uhr	Local features for image categorization (J. Buhmann, Computer Science)
M. Wittberger	Integrationsmethoden fuer die Dynamik polarisierbarer Moleküle" (J. Hutter, Physical Chemistry, University of Zurich)

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 12, 2005
Kaspar Nipp,
Fachberater RW und Mitglied des Ausschusses Rechnergestützte Wissenschaften

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

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 WS04/05

4. 11. 04	A. Torda, Uni Hamburg Protein Structure Prediction Force Fields: 25 Years of Disaster and Defeat
18. 11. 04	M. Sick, VA Tech Hydro, Zürich Numerische Simulation der Teillastinstabilität im Saugrohr von Pumpturbinen und Francisturbinen
16. 12. 04	D. Lakehal, Institut für Energietechnik Computational Multi-Fluid Dynamics: State-Of-The-Art
23. 12. 04	S. Trebst, Theoretische Physik und CoLab Overcoming Entropic Barriers in Monte Carlo Simulations: Optimal Ensembles and their Applications
13. 1. 05	C. Karch, DaimlerChrysler Research and Technology, Friedrichshafen Elektromagnetisches Umformen
20. 1. 05	M. Fey, Bruker Schweiz AG NMR-Spektroskopie: Numerik von Fourier bis Maxwell

Case Studies Seminar SS05

14. 4. 05	G. Blatter, Theoretische Physik Quantum Computing
21. 4. 05	M. Müller, Computer-Graphik Echtzeit-Simulationen und ihre Anwendungen
28. 4. 05	L. Bonaventura, Politecnico di Milano The ICON Global Weather and Climate Modeling Project
26. 5. 05	R. Walder, Astrophysik Simulationen von Supernovae - Das Zusammenwirken von Fluiddynamik, Strahlungstransport und Gravitation
2. 6. 05	D. Landau, Center for Simulational Physics, University of Georgia A New Kind of Monte Carlo Sampling in Statistical Physics
16. 6. 05	S. Rjasanow, Universität des Saarlandes, Saarbrücken Die Boltzmann-Gleichung: Theorie und Numerik

4

Computational Highlight

Biomolecular simulation: some achievements and challenges

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Abstract

Computation based on molecular models is playing an increasingly important role in biology, biological chemistry and biophysics. Since only a very limited number of properties of biomolecular systems is actually accessible to measurement by experimental means, computer simulation can complement experiment by providing not only averages, but also distributions and time series of any definable quantity, e.g. conformational distributions or interactions between parts of systems.

Present day biomolecular simulation is limited in its application by four main problems: (i) the force field problem, (ii) the search (sampling) problem, (iii) the ensemble (sampling) problem, and (iv) the experimental problem. Some of these problems are illustrated by examples. Challenges to more accurate biomolecular simulation are sketched.

1. Introduction

The role of computation in biology, biological chemistry and biophysics has shown a steady increase over the past decades. Due to the continuing growth of computing power, in particular in the context of personal computers, it has become possible to analyse, compare and characterise large and complex data sets that are obtained from experiments on biomolecular systems. This has in turn led to the formulation of models for biomolecular processes that are amenable to simulation or analysis on a computer. When undertaking a biomolecular modelling study of a particular system of interest, the level of modelling, *i.e.* the spatial resolution, time scale and degrees of freedom of interest, must be considered [1]. Which level of modelling is chosen to describe a particular biomolecular process depends on the type of process. Here we briefly illustrate two of the four biomolecular processes illustrated in Fig. 1, (i) polypeptide folding, (ii) molecular (*e.g.* protein-ligand, DNA-ligand, protein-DNA, etc.) complexation, (iii) partitioning of molecules among different environments, such as lipid membranes, water, mixtures (*e.g.* water-urea, ionic solutions) and apolar solvents, and (iv) the formation of lipid membranes or micelles out of mixtures of their components. These four processes play a fundamental role in the behaviour of biomolecular systems. They have in common that they are driven by weak, non-bonded interatomic interactions. Such interactions govern the thermodynamic properties of the condensed phase in which the four processes occur. Therefore these processes are most promisingly modelled at the atomic or molecular level. Since the temperature range of interest basically lies between room and physiological temperatures, and energies involved in these processes are on the order of $1 - 10k_BT$ (tens of kJmol^{-1}, k_B is Boltzmann's constant), the processes are largely

determined by the laws of classical statistical mechanics. Although quantum mechanics governs the interactions between the electrons of the atoms and molecules and the motions of light particles such as protons, the non-bonded interactions can be very well described by a classical potential energy function or force field as part of a classical Hamiltonian of the system of interest [2].

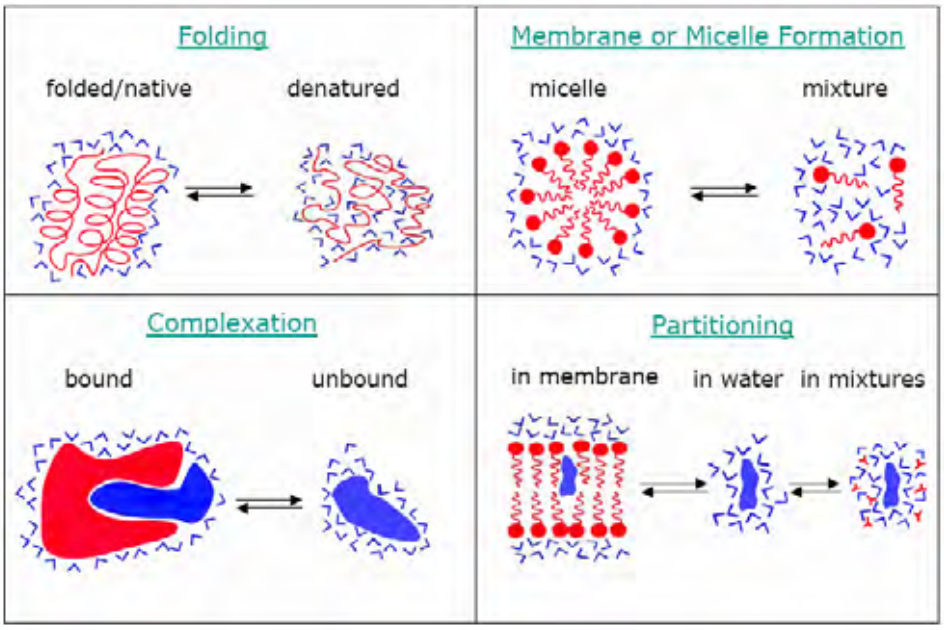

Fig. 1: Four biomolecular processes that are governed by thermodynamic equilibria.

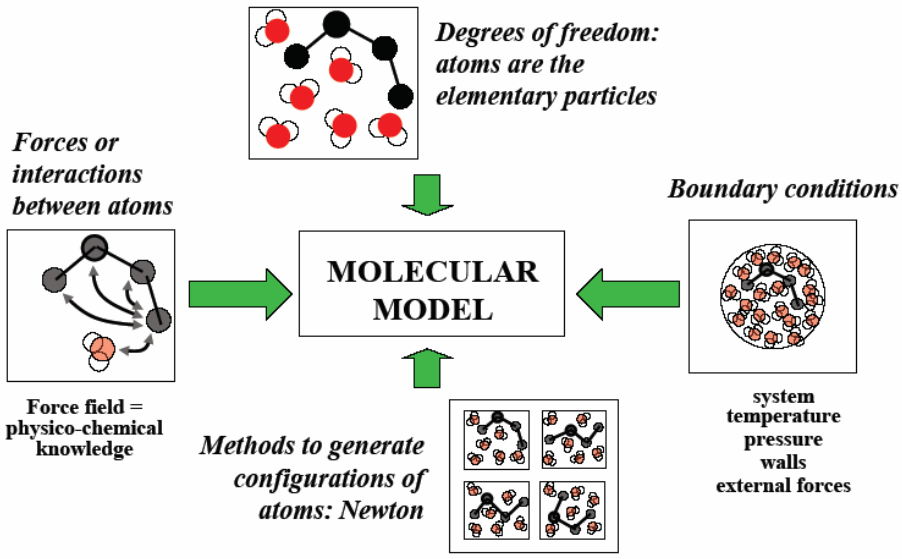

Fig. 2 Four basic choices in the definition of a model for molecular simulation.

Fig. 2 shows the four choices to be made when modelling a biomolecular system: (i) which atomic or molecular degrees of freedom are explicitly considered in the model, (ii) which interaction function or force field is used to describe the energy of the system as function of the chosen degrees of freedom, (iii) how these, generally many, degrees of freedom are to be sampled, and (iv) how the spatial boundaries and external forces are modelled. As already mentioned, we mainly consider atomic and molecular degrees of freedom with the corresponding classical force fields and classical Newtonian dynamics to sample the degrees of freedom. System sizes that can be considered range up to 10^5 or 10^6 atoms or particles, which is still very small compared to Avogadro's number, *i.e.* macroscopic sizes. For such small systems, the modelling of the boundary or surface will have a large effect on the calculated properties. Such surface effects can be minimised by using periodic boundary conditions, where the box that contains the molecular system is surrounded by an infinite number of copies of itself. This avoids surface effects at the expense of introducing periodicity artefacts [3-5].

Biomolecular Modelling: Goals, Problems, Perspectives

Four Problems

1. the force field problem

- *A* very small (free) energy differences, many interactions
- *B* entropic effects
- *C* variety of atoms, molecules

2. the search (sampling) problem

- *A* convergence
- *B* the search problem alleviated
- *C* the search problem aggravated

3. the ensemble (sampling) problem

- *A* entropy
- *B* averaging
- *C* non-linear averaging

4. the experimental problem

- *A* averaging
- *B* insufficient number of data
- *C* insufficient accuracy of data

Perspectives

A.	Polarisable force fields:	solutions, liquid mixtures
B.	Quantum-dynamical simulation:	reactions
C.	Coarse-grained models:	membranes, mixtures

Fig. 3 Four basic problems of biomolecular modelling.

Present day biomolecular modelling is limited in its application by the four problems mentioned in Fig. 3: (i) the force field problem, (ii) the search (sampling) problem, (iii) the ensemble (sampling) problem, and (iv) the experimental problem. Two of these four problems will be illustrated using examples from our own work.

Simulation can *replace* or *complement* an experiment:

1. Experiment is impossible	*Collision of stars or galaxies* *Weather forecast*
2. Experiment is dangerous	*Flight simulation* *Explosion simulation*
3. Experiment is expensive	*High pressure simulation* *Windchannel simulation*
4. Experiment is blind	*Many properties cannot be observed on very short time-scales and very small space-scales*

Fig. 4 Four reasons why computer simulation is used in science.

The key reason why computer simulation is used in the study of biomolecular systems in spite of the above mentioned limitations to its accuracy resides in the fourth of the four reasons listed in Fig. 4. Only a very limited number of properties of a biomolecular system is actually accessible to experimental measurement, whereas in a computer simulation not only averages, but also distributions and time series of any definable quantity can be determined. Thus computer simulation represents a complement to experiment by providing the detailed conformational and other distributions that determine the space and time averages obtained experimentally. As such it is an indispensable tool to interpret experimental data. Moreover, it can be used to predict properties under environmental conditions that are difficult or expensive to realise.

2. The force field problem

A biomolecular force field generally consists of potential energy terms representing covalent interactions between atoms, such as bond-stretching, bond-angle bending, improper and proper dihedral-angle torsional terms on the one hand and non-bonded interactions on the other hand between atoms in different molecules and between atoms in a molecule that are separated by more than two or three covalent bonds [6-7].

Since non-bonded interactions govern the thermodynamic equilibria and processes of interest depicted in Fig. 1, we focus on the formulation and parametrisation of these potential energy terms. Three problems dominate the topic of force-field development (Fig. 3, points A-C).

A first problem is that the (free) energy differences driving the processes of Fig. 1 are of the order of $1 - 10k_BT$ (tens of kJmol^{-1}). These relatively small energies result from a summation over very many ($10^6 - 10^8$) atom-atom energies: a system of $N = 1000$ atoms has about $\frac{1}{2}N(N-1) = 500'000$ pairs of atoms contributing to the non-bonded interaction. In order to reach the requested accuracy for the total non-bonded energy, the accuracy of the individual terms in the summation, the atom pair energies, must be much higher. This difficulty becomes increasingly severe when trying to derive a force field of high accuracy for larger systems, *i.e.* for larger N.

A second problem is to appropriately account for entropic effects. Since we are not interested in biomolecular systems at a temperature of -273.15°C (0K), we have to consider the contribution of entropy, S, to the free energy $F = U - TS$ of the system of interest. It is well known that entropy plays an essential role in all four processes of Fig. 1. Free energy changes that drive processes may result from changes in energy (U) or in entropy (S), which may co-act or counter-act depending on the relative strengths of the non-bonded interactions between the various components (atoms, molecules) of the system [8-9]. Fig. 5 illustrates the energy-entropy compensation phenomenon: two conformations x_1 and x_2 of a molecule may have $U(x_1) << U(x_2)$, whereas $F(x_1) > F(x_2)$ due to $S(x_1) << S(x_2)$ at a given temperature. The entropy is a measure of the extent of conformational space (x) accessible to the molecular system at a given temperature T. Fig. 5 also illustrates that searching for and finding the global energy minimum for a biomolecular system is meaningless when its entropy accounts for a sizeable fraction of its free energy. For example, for liquid water at room temperature and pressure one has F = -24kJmol^{-1}, U = -41kJmol^{-1} and TS = -17kJmol^{-1}. The properties of water in the condensed phase can therefore only be described through a conformational distribution, which in turn can be generated by computer simulation. Similar considerations apply to biomolecular systems: an energy-minimised structure of a protein corresponds to a possible conformation at 0K, and lacks information on the conformational distribution of the protein at physiological temperatures. This state of affairs has consequences for force-field development: if a force field is to be used in computer simulations at non-zero temperature, its parameters should be derived or calibrated taking into account entropic effects in order to be consistent. In other words, calibration of force-field parameters involves computer simulations to generate configurational ensembles, which makes it a more costly task than when only single minimum-energy conformations or measured average structures are used.

A third problem in biomolecular force-field development is the enormous variety of chemical compounds for which adequate force-field parameters should be derived. If the force-field parameters are (to some extent) transferable between atoms or groups of atoms in different molecules, this problem may be (at least partially) alleviated. In general, putting the force-field terms on a physical (in contrast to a pure statistical) basis and keeping them simple and local will enhance the transferability of parameters from one compound to another. In addition, by keeping them computationally simple, the efficiency of biomolecular simulation can be enhanced, which facilitates the sampling of configurational space.

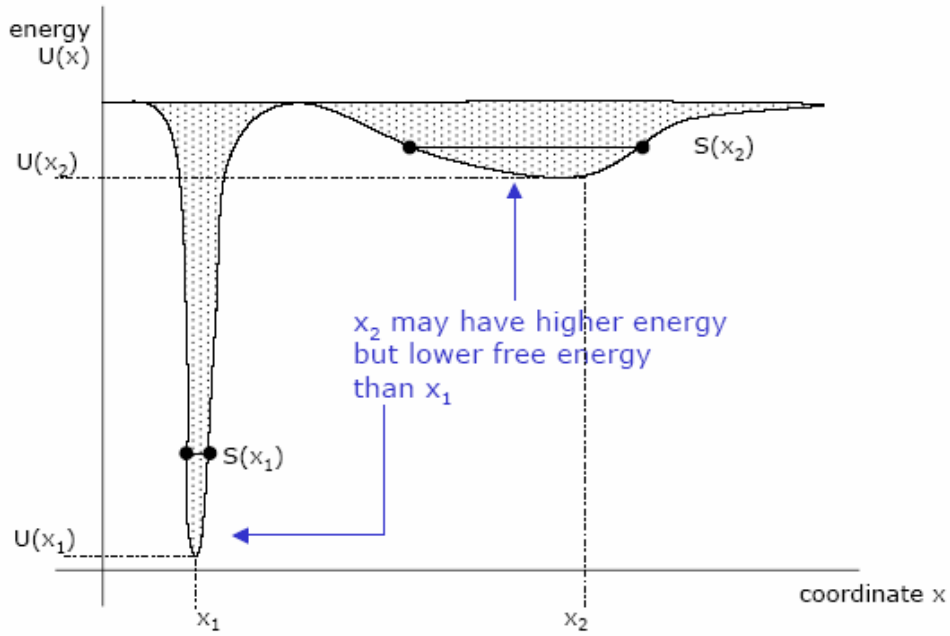

Fig. 5 Energy-entropy compensation at finite temperatures.

In order to be able to simulate peptide or protein folding (Fig. 1), the relative free energies of solvation of the 20 amino acid residues in polar solution (water) versus non-polar solution (cyclohexane) as obtained from simulation should compare well with the corresponding experimental data, since these differences are likely to largely determine the driving force for folding. Gibbs free energies of solvation obtained with the GROMOS 53A6 force field [7] are shown in Fig. 6. The average absolute deviations from experiment for the 18 amino acid side chains (no Gly and Pro) are 1.0kJmol^{-1} in water and 2.0kJmol^{-1} in cyclohexane. Both values are below k_BT, which makes the 53A6 GROMOS force field suitable for protein folding studies.

A particular challenge to biomolecular force fields is the prediction of the fold of a polypeptide in solution as function of its amino acid residue composition and of the type of solvent. How well this challenge is met by the GROMOS force field [10] is illustrated in Fig. 7. Using the GROMOS force-field parameter sets 43A1 and 45A3 left-handed or right-handed helices of different types as well as beta-turns were found as dominant conformations in MD simulations of beta- and alpha-peptides in methanol or water, see Fig. 7, in agreement with the dominant conformations derived from NMR NOE data [11-16].

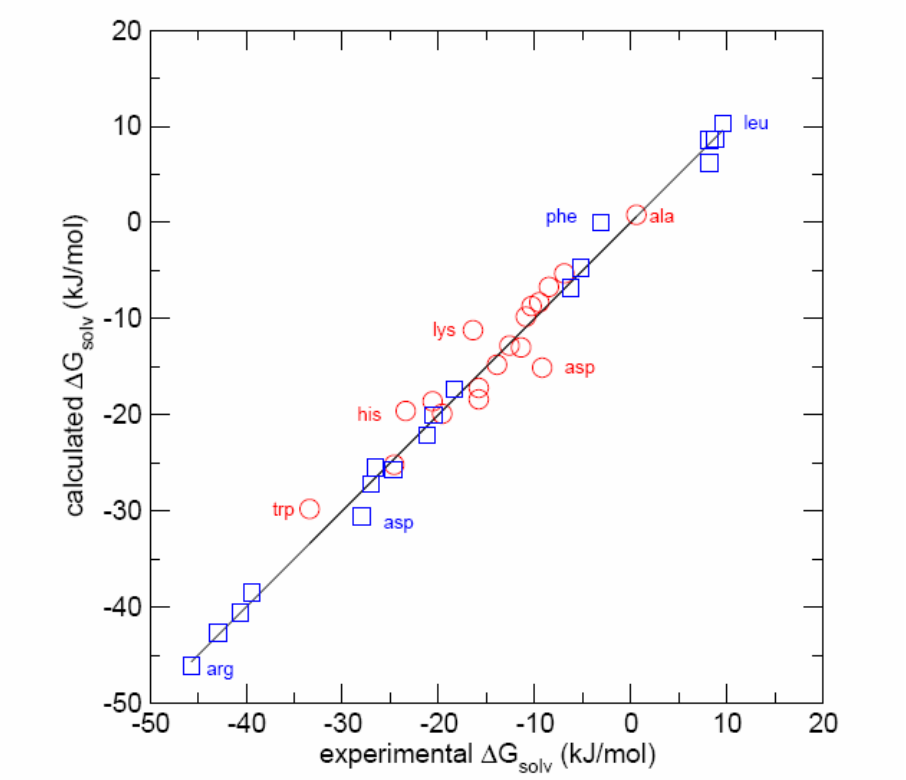

Fig. 6 Gibbs free energies of solvation in cyclohexane (circles) and in water (squares) of 18 amino-acid analogs (no Gly and Pro) as calculated from MD simulation using the GROMOS 53A6 force field in comparison with experimental values [7].

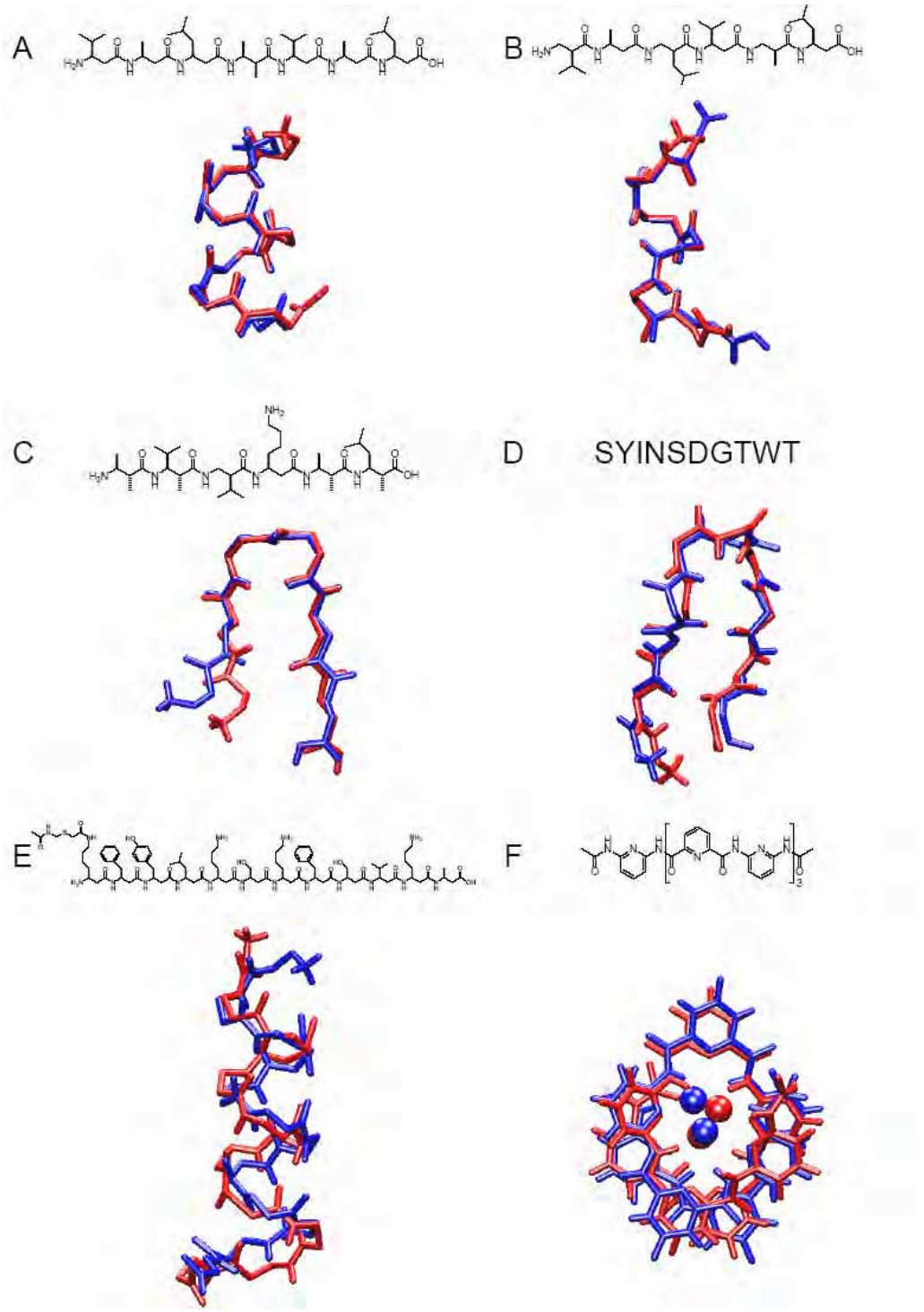

Fig. 7 Folding of different polypeptides and peptoides into different folds in different solvents by MD simulation. The following is shown: the chemical formula, a folded structure (red) modelled from the available NMR or X-ray experimental data, and, superimposed on the latter, a folded structure (blue) representing the most populated conformation from the MD simulations of the folding/unfolding equilibrium [11-16]. The solvents are water (D), methanol (A-C, E) and water or chloroform (F). The versions of the GROMOS force field used are: 43A1 (A-D), 45A3 (F) and 53A6 (E).

3. The search problem

A biomolecular system is generally characterised by a very large number of degrees of freedom, of the order of 10^4-10^6 or more. The motions along these degrees of freedom show a variety of characteristics, from highly harmonic to anharmonic, chaotic and diffusive. Moreover, correlations are present that cover a wide range of time- and spatial scales, from femtoseconds and tenths of nanometers to milliseconds and micrometers. The energy hypersurface of such a system, which is defined by the potential energy function, is therefore a very rugged surface, with energy basins and mountains of a wide range of depths or heights and spatial extent. This makes the search for the global energy minimum of such a high-dimensional function, or rather the search for those regions of the surface that contribute most to the free energy of the system, a daunting if not impossible task.

As mentioned before, the state of a biomolecular system cannot be described by a single global minimum-energy configuration or structure, but only by a statistical-mechanical ensemble of configurations, in which the weight of a configuration x is given by the Boltzmann factor,

$$P(x) \sim exp\ [-V(x) / k_B T], \qquad (1)$$

with k_B being Boltzmann's constant and T the (absolute) temperature. The exponential weighting in (1) implies that high-energy regions of the energy hypersurface will not contribute configurations that are relevant to the state of the system, unless they are very many in number (entropy). The equilibrium properties of the system are dominated by those parts of configuration space, for which $V(x)$ is low. Therefore, one of the fundamental challenges to biomolecular modelling is to develop methodology to efficiently search the vast biomolecular energy surface for regions of low energy.

Below, we only mention and classify the major techniques that are currently used to search and sample configuration space [17-19]. There are also search and sampling techniques in which not only the molecular coordinates x serve as variables, but also their (Boltzmann) probabilities $P(x)$. For a discussion and examples of these so-called probability search techniques we refer to [17,20,21].

A variety of search methods is available, each with its particular strengths and weaknesses, depending on (i) the form of the function $V(x)$, and (ii) the number and types of degrees of freedom in the system. Two basic types of search methods can be distinguished.

Systematic or exhaustive search methods scan the complete or a significant fraction of the configuration space of the biomolecular system. Particular subspaces can be excluded from the search without loss in the quality of the solution found, thanks to rigorous arguments that these subspaces cannot contain the desired solution [22]. Such arguments are based on a priori knowledge, often of physical or chemical nature, about the structure of the space or energy hypersurface to be searched. Systematic search techniques can only be applied to small molecules involving only a few degrees of freedom [23-26], because of the exponential growth of the required computing effort as function of the number of degrees of freedom included in the search.

Heuristic search methods, although visiting only a tiny fraction of the configuration space, aim at generating a representative (in the Boltzmann weighted sense) set of system configurations. These methods may generally be divided into three types, see Fig. 8.

I. Non-step methods
- distance geometry methods

II. Step methods: build up of a configuration from fragments
- combinatorial chain growing
- configurational bias Monte Carlo (CBMC)

III. Step methods: change of a complete configuration

change based on	method				
	EM	MC	MD	SD	PEACS
energy	y	y	n	n	y
energy gradient	y	n	y	y	y
2nd derivative of the energy	y	n	n	n	n
memory	n	n	y	y	y
randomness	y	y	n	y	n

Fig. 8 Heuristic methods to search configuration space for configurations x with low energy V(x). EM: energy minimisation, MC: Monte Carlo, MD: molecular dynamics, SD: stochastic dynamics, PEACS: potential energy annealing conformational search [37].

I. Non-step methods, in which a series of system configurations is generated, which are independent of each other. An example is the so-called distance-geometry metric-matrix method [27,28], which, for a search problem that can be cast into a distance based form, generates, at least in principle, an uncorrelated series of random configurations.

II. Step methods that build a complete molecular or system configuration from configurations of fragments of the molecule or system in a step-wise manner. Examples are the build-up procedure of Scheraga [29,30], combinatorial build-up methods that make use of dynamic programming techniques [31], and Monte Carlo (MC) chain growing methods [32,33], such as the so-called configurational bias Monte Carlo (CBMC) technique [34].

III. Step methods, such as energy minimisation (EM), Metropolis Monte Carlo (MC), molecular dynamics and stochastic dynamics (SD) [35], that generate a new configuration of the complete system from the previous configuration. These methods can be further classified according to the way in which the step direction and step size are chosen, see Fig. 8. Energy minimisation can be based on only energy values and random steps (simplex methods), or on energy and energy gradient values (steepest-descent and conjugate-gradient methods), or on second-order derivatives of the energy

(Hessean matrix methods). In MC methods the step direction is taken at random, and the step size is limited by the Boltzmann acceptance criterion: when the energy of the system changes by $\Delta V<0$, the step in configuration space is accepted, while for $\Delta V>0$, the step is accepted with probability $exp(-\Delta V/k_BT)$. In MD simulation the step is determined by the force, the negative of the local gradient $\partial V/\partial x$, and the inertia of the degrees of freedom, which serves as a short-time memory of the path followed so far. In SD simulation a random component is added to the force, the size of which is determined by the temperature of the system and the atomic masses and friction coefficients. In the potential-energy contour tracing (PECT) algorithm [36] and in the potential–energy annealing conformational search (PEACS) algorithm [37] the energy values are monitored and kept constant (PECT) or annealed (PEACS) in order to locate saddle points and pass over these. There exists a large variety of search procedures based on stepping through configuration space using a combination of the five mentioned basic elements, energy, gradient, Hessean, memory, and randomness, combined in one way or another [17].

I. *Deformation or smoothening of the potential energy surface*
- a. omission of high-resolution structure factor data in structure refinement based on X-ray diffraction data
- b. gradual introduction of longer-range distance restraints in variable target structure refinements based on NMR NOE data
- c. softening of the hard core of atoms in the non-bonded interaction (soft-core atoms)
- d. reduction of the ruggedness of the energy surface through a diffusion-equation type of scaling
- e. avoiding the repeated sampling of an energy well through local potential energy elevation or conformational flooding
- f. softening of geometric restraints derived from experimental (NMR, X-ray) data through time-averaging of these
- g. circumvention of energy barriers through an extension of the dimensionality of the cartesian space (4D-MD)
- h. freezing of high-frequency degrees of freedom through the use of constraints
- i. coarse-graining the model by reduction of the number of interaction sites

II. *Scaling of system parameters*
- a. temperature annealing
- b. mass scaling
- c. mean-field approaches

III. *Multi-copy searching and sampling*
- a. genetic algorithms
- b. replica-exchange and multi-canonical algorithms
- c. cooperative search: SWARM

Fig. 9 Techniques to enhance the searching and sampling power of simulation methods. For details see [17-19] and references therein.

The efficacy of search methods for biomolecular systems is severely restricted by the nature of the energy hypersurface $V(x)$ that is to be explored to find low energy regions. Due to the occurrence of a multitude of high-energy barriers between local minima, the radius of convergence of the step methods is generally very small. Therefore, a variety of techniques has been developed to enhance the search and sampling power of searching methods. In Fig. 9, three general types of search and sampling enhancement techniques are distinguished [17].

I. Deformation or smoothening of the potential energy hypersurface in order to reduce barriers.

a) Generally, a smoothening of the potential energy function *V(x)* allows for a faster search for its minima. This technique has been applied to different problems, such as structure determination based on X-ray diffraction or NMR spectroscopic data, conformational search and protein structure prediction. In method *Ia* of Fig. 9, the electron density of a biomolecular crystal is smoothened by the omission of high-resolution diffraction intensities when back calculating the electron density from these through Fourier transforms. This smoothening enhances the radius of convergence of the structure refinement.

b) When building a protein structure from atom-atom distance data obtained from NMR, the convergence of the configurational search process is enhanced by gradually introducing distance restraints that connect atoms at longer distances along the polypeptide chain in the potential energy function. This is called a variable-target function method [38].

c) The hard core of atoms, *i.e.* the strong repulsive interaction between atoms overlapping with each other, is responsible for many barriers on the energy hypersurface of a molecular system. These barriers can be removed by making the repulsive short-range interactions between atoms soft [39-42]. Soft-core atoms smoothen the energy surface and lead to strongly enhanced sampling [43].

d) In the diffusion-equation based deformation methods [43,44] the deformation of the energy surface during a simulation is made proportional to the local curvature (second derivative) of the surface, which leads to a preferential smoothening of the sharpest peaks and valleys in the surface and a very efficient search.

e) Incorporation of information on the energy hypersurface obtained during the search into the potential energy function is another possibility to enhance sampling. Once a local energy minimum is found, it is removed from the energy surface by a suitable local deformation of the potential energy function. This idea is the basis of the deflation method [45], the local-elevation search method [46], recently also called meta-dynamics [47].

f) Another way to introduce a memory into the search is the use of a potential energy term, which uses a running average of a coordinate over the trajectory or ensemble generated so far rather than its instantaneous value [48]. Application of this type of time-dependent or ensemble dependent restraints in protein structure determination based on NMR or X-ray data leads to much enhanced sampling of the molecular configuration space [49,50].

g) Barriers in the energy hypersurface can be circumvented by an extension of the dimensionality of the configuration space beyond the three Cartesian ones. The technique of energy embedding locates a low energy conformation in a high-dimensional Cartesian space and gradually projects this conformation to 3-dimensional Cartesian space while perturbing its energy and configuration as little as possible [103]. Dynamic search methods can also be used in conjunction with an extension of the dimensionality. By performing MD in 4-dimensional Cartesian

space, energy barriers in 3-dimensional space can be circumvented [52], and free energy changes calculated [53].

h) A long used standard technique to smoothen the energy surface is to freeze the highest-frequency degrees of freedom of a system through the application of constraints [54,55]. Bond-length constraints are standardly applied in biomolecular simulation and allow for a four times longer time step size [56]. High-frequency motion elimination can also be eliminated using soft constraints [57]: the (bond-)constraint lengths change adiabatically due to the forces.

II. Scaling of system parameters can also be used to enhance sampling.

a) The technique of simulated temperature annealing [58] involves simulation or search at a high temperature *T,* followed by gradual cooling. By raising the temperature, the system may more easily surmount energy barriers, so a larger part of configurational space can be searched. The technique of simulated temperature annealing has been widely used in combination with MC, MD and SD simulation. An example of potential energy annealing can be found in [37].

b) Scaling of atomic masses can be used to enhance sampling. In the classical partition function and in case no constraints are applied, the integration over the atomic momenta can be carried out analytically, separately from the integration over the coordinates. Thus, the atomic masses do not appear in the configurational integral, which means that the equilibrium (excess) properties of the system are independent of the atomic masses. This freedom can be exploited in different ways to enhance the sampling. By increasing the mass of specific parts of a molecule, its relative inertia is enhanced, which eases the surmounting of energy barriers [59], and may allow for larger time steps.

c) Enhanced sampling by a mean-field approximation is obtained by separating the biomolecular system into two parts, *A* and *B*, each of which moves in the average field of the other. The initial configuration of the system consists of N_A identical copies of part *A* and N_B identical copies of part *B*, where the positions of corresponding atoms in the identical copies may be chosen to be identical. The force on atoms of each copy of part *A* exerted by the atoms in all copies of part *B* is scaled by a factor N_B^{-1}, in order to obtain the mean force exerted by part *B* on the individual atoms of part *A*. Likewise, the force on atoms of each copy of part *B* exerted by the atoms in all copies of part *A* is scaled by a factor N_A^{-1}. The forces between different copies of part *A* are zero, and so are the forces between different copies of part *B*. The MD simulation involves the integration of Newton's equation of motion, $\boldsymbol{f} = m\boldsymbol{a}$, for all copies of parts *A* and *B* simultaneously. Thus one obtains N_A individual trajectories of part *A* in the mean field of part *B* and vice versa. This comes at the loss of correct dynamics: Netwon's third law, $\boldsymbol{f}_{AB} = -\boldsymbol{f}_{BA}$ is violated. The technique only enhances efficiency when the system is partitioned into parts of very different sizes, *e.g.* size *(A)* << size *(B)* and the bigger part is represented by one copy: $N_B = 1$. Enhanced searching and sampling procedures based on a mean-field approximation have been proposed in different forms [60].

III. Multi-copy simulation with a given relation between the copies can also be used to enhance searching and sampling.

In the mean-field approach sketched above, multiple copies of a part of the system were simulated. This idea has also been used in other ways to enhance searching and sampling, see Fig. 9.

a) In genetic algorithms [61] a pool of copies of the biomolecular system in different configurations is considered, and new configurations are created and existing ones deleted by mutating and combining (parts of) configurations according to a given set of rules.

b) In the so-called replica-exchange algorithm multiple copies of the system are simulated by MC, MD or SD, each at a distinct temperature. From time to time copies from simulations close in temperature are exchanged using an exchange probability based on the Boltzmann factor (1). This leads, in the limit of infinite sampling, to Boltzmann-distributed (canonical) ensembles for each temperature [62]. So-called multi-canonical algorithms are a generalisation of this procedure [18].

c) The so-called SWARM type of MD [63] is based on the idea of combining a collection or swarm of copies of the system each with its own trajectory into a cooperative multi-copy system that searches configurational space. To build such a cooperative multi-copy system, each copy is, in addition to physical forces due to $V(x)$, subject to (artificial) forces that drive the trajectory of each copy toward an average of the trajectories of the swarm of copies, in analogy to the fact that intelligent and efficient behaviour of a whole swarm of insects can be achieved even in the absence of any particular intelligence or forethought of the individuals. SWARM-MD is less attracted by local minima and is more likely to follow an overall energy gradient toward the global energy minimum.

This overview of methods to search and sample configurational space is rather limited. More extensive reviews can be found in [17-19]. Since biomolecular configurational space is too large to be exhaustively sampled, one generally has to use heuristic search methods in biomolecular modelling. The overview (Figs. 8 and 9) of types of methods and tricks that can be used and combined to obtain a powerful search method, may offer the practical modeller a hand when choosing a combination of methods and tricks that will be particularly suited to the specific problem or energy hypersurface of interest.

There is certainly still room to enhance the search and sampling efficiency of biomolecular simulation techniques, but the past ten years have already shown encouraging progress that we expect to be of benefit also for the study of larger, more interesting and relevant biomolecular systems. In particular the technique of smoothening the potential energy surface can enhance sampling through the use of soft-core atoms, local-elevation and diffusion-equation types of deformation of the energy surface, and on another level through the formulation of coarse-grained models. The so-called single-step perturbation methodology to obtain ligand-binding free energies or solvation free energies for a great many compounds from only a few simulations involving non-physical reference states involving soft-core atoms chosen to widen the configurational ensemble offers orders of magnitude gains in efficiency compared to standard (thermodynamic integration or perturbation) free energy calculations

[64-69]. This is illustrated in Fig. 10, where binding (Gibbs) free energies of 16 hydroxylated polychlorinated biphenyls to the estrogen receptor as calculated using the single-step perturbation technique from only two MD simulations are compared to the corresponding experimental values [67]. The average deviation of the simulated values from the experimental ones is with 2.5kJmol^{-1} smaller than the variation of 4.2kJmol^{-1} in the experimental values themselves, which implies that the force field used and the sampling te
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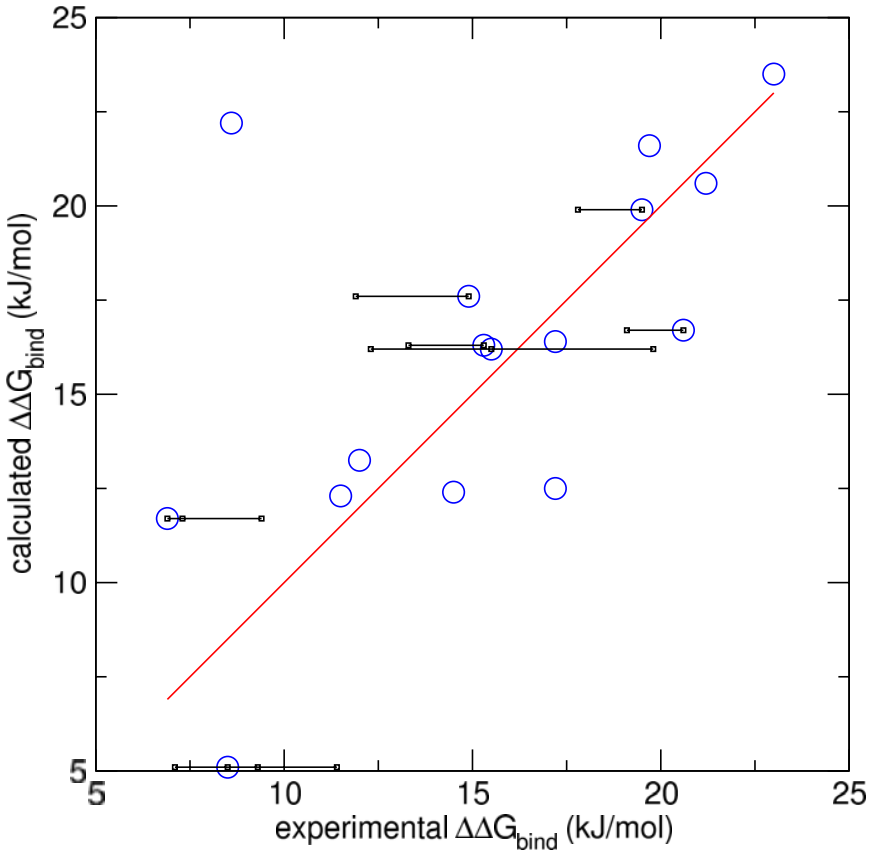

Fig. 10 Experimental versus calculated relative Gibbs free energies of binding for 16 hydroxylated polychlorinated biphenyls to the estrogen receptor binding domain in solution [67]. The horizontal lines connect different experimental values for one compound. The calculated values were obtained from only two simulations and the one-step perturbation method. The GROMOS 43A1 force field was used.

4. Perspectives in biomolecular simulation

The essential driving force behind the growth and development of the field of biomolecular modelling was, is and still will be the steady and rapid increase of computing power. Fig. 11 shows an average increase by a factor of 10 about every 5 years over the past decades. This trend will probably continue in the near future, based on the on-going application of parallel computing. The possibilities of parallel computing can be exploited in biomolecular simulation, since the most time-consuming part is the force or interaction calculation, which can be carried out in parallel for all atoms in the system. Especially, the advent of new hardware designed to solve the protein-folding problem through classical dynamical simulation opens perspectives on more accurate simulations and new applications [70].

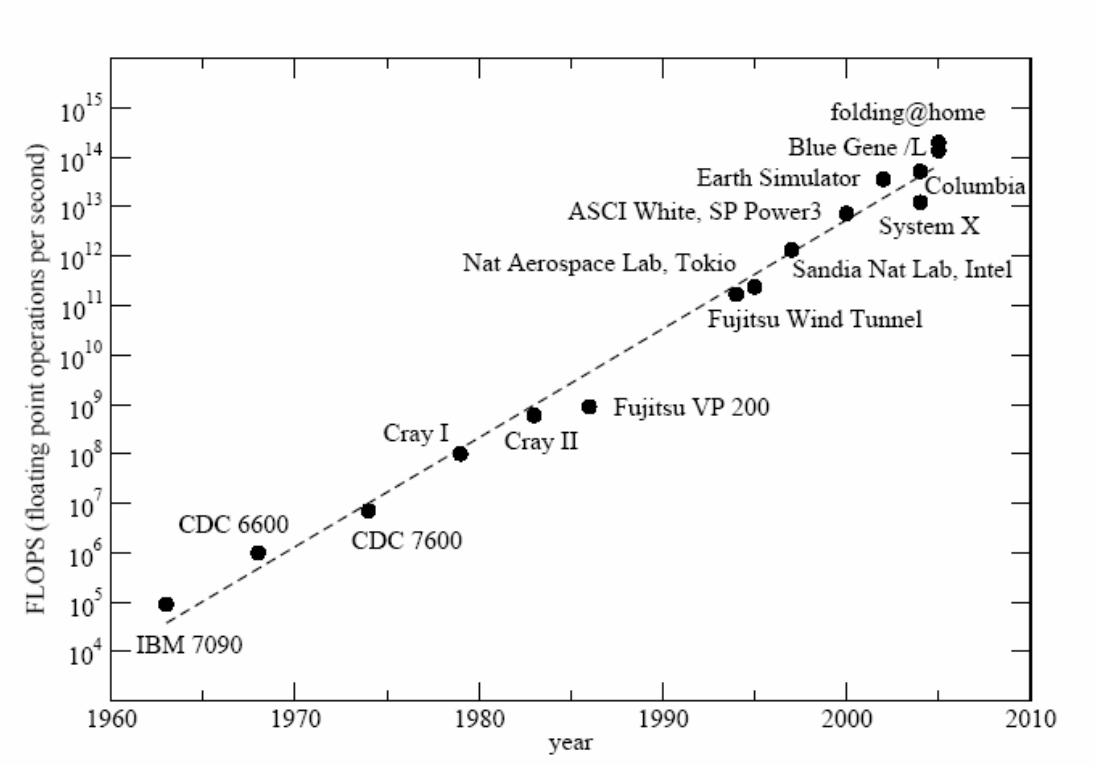

Fig. 11 Development of computing power of the most powerful computers.

A second driving force behind biomolecular modelling is the advancement of modelling techniques. Efficient algorithms to compute long-range electrostatic forces have become available. Methodology to extend and enhance sampling has been developed, and biomolecular force fields have been refined.

These driving forces led to simulations of ever larger systems or over ever longer time periods. Practical applications of simulation address a variety of systems, processes and applications: molecular complexation, ligand-binding, polypeptide folding, transport across membranes, membrane formation, crystallisation. The efficiency increase of simulation is

unlikely to continue indefinitely. First, computing power is unlikely to continue to grow for ever as fast as observed up till now. Second, when simulating ever-larger systems in atomic detail, more and more pair interactions need to be added to obtain the system energy. To obtain the same overall accuracy for a large system as for a small one, the accuracy of the pair interactions must be much higher for the large system. However, this accuracy is limited by the approximations on which a force-field description of the system rests. Third, one may question the value of a detailed atomic description of macroscopic systems. In other words, it still remains mandatory to formulate simple and approximate models that contain just the necessary degrees of freedom to adequately represent the phenomenon of interest.

Along which lines should current biomolecular models be extended, improved or simplified? First, an appropriate description of enzyme reactions requires the inclusion of electronic degrees of freedom. Hybrid quantum-classical (QM/MM) modelling will be further developed to this end. In order to simulate proton transfer reactions it may be necessary to employ quantum-dynamical methodology, which requires even more computing power than QM/MM calculations. Second, at the classical level of modelling, improvements will come from the introduction of polarisability in biomolecular force fields, from the incorporation of co-solvent effects through explicit simulation, and from techniques to extend the sampling power of simulations. Third, simplification of models by averaging over atomic degrees of freedom, coarse-graining, will open up longer time scales and processes, such as membrane formation, to simulation.

The reason to use simulation and modelling was indicated in Fig. 4: to provide a microscopic picture of unrivalled resolution in time, space and energy that complements the limited set of properties obtainable from experiment. Second, in modelling, system parameters can be changed at will to study particular cause-effect relationships, leading to enhanced understanding of biomolecular systems.

When modelling a biomolecular system the challenge lies in a proper balance between the choices to be made regarding degrees of freedom, force field, sampling and boundary conditions (Fig. 2). These choices will depend on the three factors shown in Fig. 12.

1. The properties of the biomolecular system one is interested in should be listed and the size of the configuration space (or time scale) to be searched for relevant configurations and sampled should be estimated.

2. The required accuracy of the properties should be specified.

3. The available computing power should be estimated.

If the model selected is too simple, the phenomena of interest may be lost or the accuracy may be insufficient. If the model is too elaborate, sampling of the required extent of configuration space may be impossible. It is the art of biomolecular modelling to sail safely between these *Scylla* and *Charybdis*.

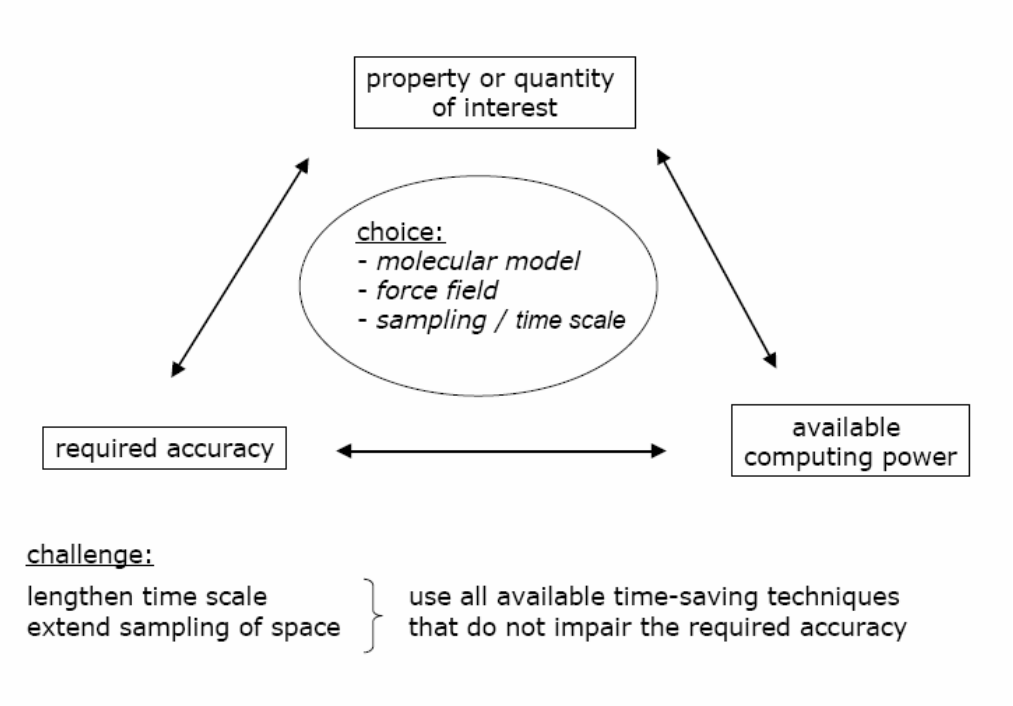

Fig. 12 Choice of molecular model (degrees of freedom), force field and extent of sampling depends on the property of interest, the required accuracy of the result, and the available computing power to generate the Boltzmann ensemble.

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5

CSE Research Projects

Title: Pulsating jet diffusion flames

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[4]Laboratory of Marine Engineering, National Technical University of Athens, Greece

Description:

Flame oscillations near extinction have been observed for a variety of non-premixed configurations, including jet flames and candle flames in microgravity, and flames spreading over liquid pools, or condensed-phase fuels In the EPFL diluted propane-oxygen jet diffusion flame experiments (M. Füri, P. Papas, P. A. Monkewitz *Proc. Combust. Inst.* 28:831–838, 2000), the anchoring flame base oscillated in the streamwise direction. The flame tip also oscillated at a comparable amplitude but with a phase shift of 180^o relative to the flame edge, resulting in a periodic extension and contraction of the flame length. This motion, or limit cycle, was quite regular and axisymmetry was maintained throughout the cycle.

Despite the different geometries mentioned above, several characteristics of the oscillations are similar: they occur near extinction, their characteristic frequencies are a few Hz, and the reactant Lewis numbers (the ration of thermal to species diffusivities) are typically larger than unity. These different instabilities may be driven by several different factors, and/or their onset may be related to a common mechanism. Despite recent work, the interrelationship between the different instabilities mechanisms is still unclear. To help elucidate the instability mechanism, numerical simulations of the jet experiments of Füri *et al* were performed, using our MPI-based parallel, spectral element code to solve the conservation equations of mass, momentum, species and energy in the low Mach number limit.

The simulations reproduce all the experimental observations: the appearance of pulsating flames in a small range of oxygen mass fraction in the oxidizer stream, Y_{O_2}, close to extinction, the growth of the pulsation amplitude as Y_{O_2} is decreased, and the eventual *dynamic* extinction of the flame when the pulsation amplitude becomes too large.

References: Manuscript in preparation.

Title: Large Eddy Simulation of a turbulent jet using the Approximate Deconvolution Model

Researchers: Marco Küng[1], Ananias G. Tomboulides[2], Christos E. Frouzakis[1], Steffen Stolz[3], Konstantinos Boulouchos[1]

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

Description:

A parallel spectral element code was used for the large eddy simulation (LES) of a turbulent jet. The LES model is based on the Approximate Deconvolution Model (ADM), which approximates the inverse of the filtering operator to obtain information about subgrid scales. The decay of the mean axial velocity and the spreading rate are in fair agreement with experimental and DNS data. The self similarity of the mean velocity profiles and the Reynolds stresses is recovered. This is the first step in coupling ADM with spectral elements towards the LES of turbulent non-premixed jet flames.

References: European Combustion Meeting ECM05, Louvain-la-Neuve, Belgium, April 3-6, 2005

Title: Consistent lattice Boltzmann method

Researchers: S. Ansumali, I. V. Karlin

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

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

References: Phys. Rev. Letters, in press (2005)

Title:	Thermodynamic theory of incompressible hydrodynamics
Researchers:	S. Ansumali, I. V. Karlin, H. C. Öttinger (D-MATL)
Institute/ Group:	Aerothermochemistry and Combustion Systems Laboratory

Description:

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

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

Title: Entropic lattice Boltzmann method for microflows

Researchers: S. Ansumali, I. V. Karlin, Ch. E. Frouzakis, K. B. Boulouchos

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

Description:

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

References: Physica A **359**, 289305 (2006).

Title: Quasi-equilibrium closure hierarchies for the Boltzmann equation

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

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

Description:

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

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

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

Researchers: S. Ansumali, S. S. Chikatamarla, I. V. Karlin

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

Description:

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

References: Europhys. Letters, submitted, (2005).

Title: Entropic Lattice Boltzmann Models for Hydrodynamics in Three Dimensions

Researchers: S. Ansumali, S. S. Chikatamarla, I. V. Karlin

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

Description:

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

References: Phys. Rev. Letters, submitted, (2005).

Title: Invariant manifolds for physical and chemical kinetics

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

Institute/ Group: Aerothermochemistry and Combustion Systems Laboratory

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

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

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

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

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

Title: Computational Solid State Electronics

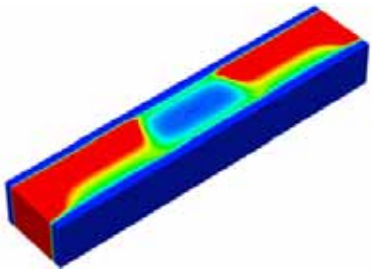
Researchers: Wolfgang Fichtner
Andreas Schenk
Bernhard Schmithüsen
Stefan Röllin
Beat Sahli
Dölf Aemmer

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

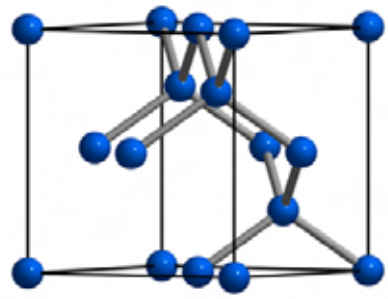
Description:

For the development of novel micro- and nano-electronic processes and devices, the use of advanced numerical simulation tools has become indispensable. With the continuing advances in semiconductor technology, and the trend to further scaling of the active device dimensions, computational solid state electronics has reached an extremely high level of physical and numerical sophistication. As we are rapidly approaching nanoscale dimensions, effects at the atomistic or quantum-mechanical level are becoming dominant.

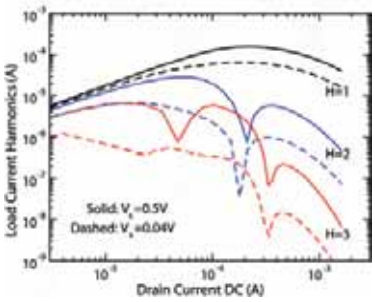
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulation tools for molecular dynamics studies in material diffusion, novel devices such as single-electron transistors, and quantum devices. 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 including parallelization on shared memory architectures. These simulations were carried out on compute-servers of our laboratory and we also use the IBM SP4 system at CSCS Manno in a *Large User Project*. The following pictures illustrate some of our activities:



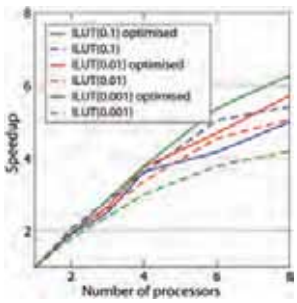
Quantum-ballistic simulation of silicon-based nanodevices: electron density distribution in a 25nm DGSOI nMOSFET.



Atomistic simulation in nano-electronics: ab initio study of vacancy diffusion in silicon.



Harmonic Balance in semiconductor device simulation: distortion of a MOSFET at low frequency (1 kHz) for two signal amplitudes.



Parallel iterative solver for semiconductor device simulation: speed-up of the ILU-factorization.

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

Researchers: Oscar Chinellato
Peter Arbenz

Institute/ Group: Institute of Computational Science

Description:

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

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

References:

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

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

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

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

Title: CSE-SEP project TH-1/02-4: Large Scale Eigenvalue Problems in Opto-Electronic Semiconductor Lasers and Accelerator Cavities

Researchers: Peter Arbenz[⋆]
Wolfgang Fichtner[†]
Hansruedi Fitze[‡]
Olaf Schenk[§]

Institute/ Group: [⋆]Institute of Computational Science
[†]Integrated Systems Laboratory
[‡]Paul Scherrer Institute
[§]Department of Informatics, University of Basel

Description:

For the development and optimization of both modern and future optoelectronic semiconductor lasers, such as vertically-cavity surface-emitting lasers (VCSELs), and of particle accelerator cavities, computer aided design became an indispensible tool building a tremendous challenge for researchers in physics, computational science, and engineering. Though both problems differ in their technical background and their dimensions by several orders of magnitude (a few micrometers versus a few meters) they both require the solution of the three- dimensional homogeneous Maxwell equations describing the optical and electromagnetic field, respectively. Their numerical discretization by finite element methods lead to large sparse generalized eigenvalue problems which are hard to solve on contemporary computer architectures with respect to memory constraints and simulation time. In laser simulation these eigenvalue problems describe only a part of the physical description, i.e. they are naturally imbedded into a much more complex nonlinearly coupled optoelectronic model.

The aim of this project is the extension of an existing Maxwell equation eigensolver to very lare scale problems and its integration into an semiconductor laser simulator bringing research and development of computational science and engineering together.

References:

P. Arbenz, M. Bečka, R. Geus, and U. Hetmaniuk: *Towards a Parallel Eigensolver for Electromagnetic Fields in Cavities*. Proceedings of the PARA'04 Workshop on the State-of-the-Art in Scientific Computing. Lyngby, DK, June 20-23, 2004. (Springer Notes in Computer Science)

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

P. Arbenz and R. Geus: *Multilevel preconditioned iterative eigensolvers for Maxwell eigenvalue problems.* Appl. Numer. Math. 54 (2): 107-121 (2005).

R. Geus and P. Arbenz: *PySparse and PyFemax: A Python framework for large scale sparse linear algebra.* Contributed paper at PyCon03, Washington DC, USA, 26-28 March, 2003. `http://www.python.org/pycon/papers/pysparse.html`

S. Röllin: *Parallel Iterative Solvers in Computational Electronics.* PhD thesis ETH Zürich, 2005

S. Röllin and O. Schenk: *Maximum-weighted matching strategies and the application to symmetric indefinite systems.* Proceedings of the PARA'04 Workshop on the State-of-the-Art in Scientific Computing. Lyngby, DK, June 20-23, 2004. (Springer Notes in Computer Science)

O. Schenk, M. Hagemann and S. Röllin: *Recent Advances in Sparse Linear Solver Technology for Semiconductor Device Simulation Matrices.* Invited Paper, Proceedings of the 2003 IEEE International Conference on Simulation of Semiconductor Processes and Devices, pp. 103–108, Boston MA, USA.

O. Schenk, S. Röllin, and A. Gupta: *The Effects of Unsymmetric Matrix Permutations and Scalings in Semiconductor Device Simulation.* IEEE Trans. on Computer-Aided Design of Integrated Circuits and Systems, 23 (3) 2004, pp. 400–411.

L. Stingelin: *Beam-cavity interactions in high power cyclotrons.* PhD thesis EPF Lausanne No. 3169, 2004.

M. Streiff: *Opto-Electro-Thermal VCSEL Device Simulation.* PhD thesis ETH Zürich No. 15464, 2004.

Title: The influence of platelet disorientation on the barrier properties of composites: a numerical study

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

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory for Corrosion and Materials Integrity, EMPA, Dübendorf

Description:

Direct finite element calculations are carried out to study the relationship between the platelet orientational distribution and the overall effective barrier properties (gas permeability) of mineral filled composites. We consider multi-inclusion computer models with microstructures representative of the dilute, semi-dilute and concentration regimes. In the dilute regime, our numerical predictions validate the results of multiple scattering expansion theory. For the semi-dilute and concentration regimes representative of most real composites, we present numerical estimates quantifying the difference between the barrier properties of composites with fully aligned and randomly oriented platelets. Our numerical results can also be used to quantify the effect of the geometric factor on the gas barrier properties of polymer-mineral hybrid nanocomposites.

References: H.R. Lusti, A.A. Gusev, O. Guseva, *Model. Simul. Mater. Sci. Eng*. **2004,** *12,* 1201-1207.

Title: A new domain-model approach to theoretically predict the stress relaxation of thermoplastic elastomers

Researchers: Stephan A. Baeurle[*,**]
Atsushi Hotta[*]
Andrei A. Gusev[**]

Institute/Group: [*]Department of Chemical Engineering & Materials, University of California, Santa Barbara
[**]Institute of Polymers, Department of Materials, ETH

Description:

In this paper we report on a new theoretical approach to predict the long-time stress relaxation behavior of thermoplastic elastomers. This approach relies on the method of Gurtovenko and Gotlib [J. Chem. Phys. 115 (2001), pp. 6785-6793], which has originally been conceived to describe the relaxation dynamics of inhomogeneously crosslinked polymers forming agglomerations of crosslinks. In this work we demonstrate that the method can be extended to describe the stress relaxation behavior of homogeneously crosslinked thermoplastic elastomers, which are subjected to an extensional strain pertaining to the nonlinear regime of mechanical properties. In our approach thermal fluctuations induce fluctuations in size of domains of crosslinks via a chain-pullout mechanism. We compare our theoretical predictions to the experimental measurements of Hotta et al. [Macromolecules 35 (2002), pp. 271-277] performed on poly-(styrene-isoprene-styrene) triblock copolymers, which are composed of hard domains of polystyrene embedded in a rubbery polyisoprene matrix. Our study confirm the importance of the chain-pullout mechanism in the stress relaxation process and demonstrates the involvement of multiple time- and structural-length-scales.

References: S.A. Baeurle, A. Hotta, A.A. Gusev, *Polymer* **2005**, *46*, 4344-4354.

Title: Approaching representative volume element size in interpenetrating phase composites

Researchers: Martin Heggli[*]
Thomas Etter[**]
Peter Wyss[***]
Peter J. Uggowitzer[**]
Andrei A. Gusev[*]

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory of Metal Physics and Technology, Department of Materials, ETH
[***]Electronics / Metrology Section, Centre for NDT&E, EMPA, Dübendorf

Description:

Numerical estimation of the effective properties of complex microstructure materials is becoming increasingly popular today. For particulate composites comprised of isolated, particulate inclusions, such as spheres, fibres, platelets, it has been shown, both theoretically and numerically, that the representative volume element (RVE) is surprisingly small. However, for composites with multiple continuous phases, such as the interpenetrating graphite-aluminium (C/Al) composites studied in this work, it is still unclear how large the uniform RVE size is. Here, based on the results of 3-D X-ray microtomography measurements, we build realistic computer models of C/Al interpenetrating composites and use them to investigate, for the first time to the best of our knowledge, the approach to the uniform RVE size for the effective electrical conductivity of such composites. Our results indicate that the uniform RVE size in such composites is very large, and that one in fact cannot rely on commonly employed in practice single estimate numerical results obtainable using currently accessible computer models. Nonetheless, we show that by averaging the numerical estimates obtained with computer models of relatively small size, one can obtain remarkably accurate estimates for the effective properties, thus, in practice, enabling rational computer aided studies of the property-microstructure relationships of such complex microstructure composites.

References: M. Heggli, T. Etter, P. Wyss, P.J. Uggowitzer, A.A. Gusev, *Adv. Eng. Mater.* **2005**, *7*, 225-229.

Title: Aging of electrical conductivity in C/Al interpenetrating composites: An X-ray microtomography and numerical study

Researchers: Martin Heggli[*]
Thomas Etter[**]
Peter Wyss[***]
Peter J. Uggowitzer[**]
Andrei A. Gusev[*]

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory of Metal Physics and Technology, Department of Materials, ETH
[***]Electronics / Metrology Section, Centre for NDT&E, EMPA, Dübendorf

Description:

Three different graphite-aluminium (C/Al) composites have been investigated. Experimentally, it was observed that the electrical conductivity significantly decreases after a cyclic thermal treatment. Based on the results of 3-D X-ray microtomography measurements, we built realistic computer models of the different C/Al interpenetrating composites. The numerical calculation was able to reproduce the observed drop in the electrical conductivity. Moreover, it could be demonstrated that by filling the pores in the aluminium phase the initial conductivity could be recovered. This proved that the development of pores in the aluminium phase is responsible for the observed decrease of the conductivity.

References:

M. Heggli, T. Etter, P. Wyss, P.J. Uggowitzer, A.A. Gusev, *in preparation*.

Title: Numerical prediction of gas barrier properties of polymer/phosphate glass hybrids

Researchers: Martin Heggli[*]
Kevin Urman[**]
Joshua U. Otaigbe[**]
Andrei A. Gusev[*]

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]School of Polymers and High Performance Materials, The University of Southern Mississippi, Hattiesburg, Mississippi

Description:

Polymer/phosphate glass hybrids are candidates as gas barrier materials because of the very low gas permeability of the inorganic phosphate glass. Potential fields of application are for example food or beverage packaging. The microstructure of such a hybrid has been measured by X-ray microtomography. From the resulting data realistic 3-D computer models have been built. The barrier properties of such a hybrid have been predicted numerically by a finite element method. The relative permeability depending on the phosphate glass content has been calculated. It was found that a significant reduction in the gas permeability can be expected.

References:

M. Heggli, K. Urman, J.U. Otaigbe, A.A. Gusev, *in preparation*.

Title: Phase continuity and elastic properties of a polymer/phosphate glass hybrid

Researchers: Martin Heggli[*]
Kevin Urman[**]
Joshua U. Otaigbe[**]
Andrei A. Gusev[*]

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]School of Polymers and High Performance Materials, The University of Southern Mississippi, Hattiesburg, Mississippi

Description:

The microstructure of a polymer/phosphate glass hybrid was measured by X-ray microtomography. With this method true 3-D microstructural information is available. The microtomography data was used to directly build realistic 3-D finite element models. The continuity of the two phases was tested by calculating the conductivity of the composites while assuming the conductivity of one phase equal to zero. It could be shown that the composite has a truly interpenetrating microstructure. The numerical prediciton of the elastica properties showed that a stiffness close to the upper Hashin-Shtrikman bound can be expected. The measured stiffness, however is far lower. A potential explanation for this was found by calculating the local stresses which seem to cause damage in the high stiffness glass phase.

References:

M. Heggli, K. Urman, J.U. Otaigbe, A.A. Gusev, *in preparation*.

Title: Finite Element Mapping for Spring Network Representations of the Mechanics of Solids

Researchers: Andrei A. Gusev

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

Description:

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

References:

A.A. Gusev, *Phys. Rev. Let*. **2004**, *93*, 034302.

Title: Prediction of Elastic Properties of a Poly(styrene-butadiene-styrene) Copolymer Using a Mixed Finite Element Approach

Researchers: Stephan A. Baeurle[*,**]
Glenn H. Fredrickson[*]
Andrei A. Gusev[**]

Institute/Group: [*]Department of Chemical Engineering & Materials, University of California, Santa Barbara
[**]Institute of Polymers, Department of Materials, ETH

Description:

Despite several decades of research, the nature of linear elasticity in microphase-separated copolymers with chemically connected glass-rubber phases is still not fully understood. In this paper we investigate the linear elastic properties of a poly(styrene-butadiene-styrene) triblock copolymer using a mixed finite element approach. The technique permits phases of full incompressibility as well as phases of near incompressibility as they occur in this two-component system to be dealt with. Strikingly and contrary to the common belief, we find that the continuum description is accurate and that no additional detailed molecular information is needed to reproduce the available linear elastic experimental data. Our investigation indicates that the anomalous Poisson ratio of the polybutadiene phase of 0.37, determined by previous authors and attributed to molecular characteristics of the polybutadiene phase, might be related to sample end effects arising in their tensile and torsional experiments. We also test the suitability of several semiphenomenological models in reproducing the experimental measurements. We find that some of the methods provide reliable results of accuracy comparable to results from our mixed finite element approach.

References: S.A. Baeurle, G.H. Fredrickson, A.A. Gusev, *Macromolecules* **2004**, *37*, 5784-5791.

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

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

Institute/Group: [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory for Corrosion and Materials Integrity, EMPA, Dübendorf

Description:

Finite element numerical simulations have been carried out to demonstrate that by the dispersing of a small amount of exfoliated muscovite mica platelets in a solid polymer one can considerably reduce and even match the thermal expansion coefficients of metal and polymer components of hybrid polymer-metal structures. In practice, such mismatch reduction may lead to the extension of the service life of hybrid polymer-metal structures. Computer models comprised of a random dispersion of fully aligned round muscovite mica platelets have been studied. It was found that the decrease of the thermal expansion for such nanocomposites is controlled by the product of the aspect ratio and the volume fraction of the mineral platelets, and that the dependence can be accurately described by a stretched exponential master curve, thus considerably facilitating the task of designing mica-polymer nanocomposites with tailored thermal expansion.

References: O. Guseva, H.R. Lusti, A.A. Gusev, *Model. Simul. Mater. Sci. Eng*. **2004,** *12*, S101–S105.

Title: Finite element predictions for the thermoelastic properties of nanotube reinforced polymers

Researchers: Hans Rudolf Lusti
Andrei A. Gusev

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

Description:

The overall effective thermoelastic properties of nanotube reinforced polymers (NRP) were estimated numerically by using a finite element based procedure. Three-dimensional multi-inclusion periodic computer models were built for three different nanotube orientation states, namely, fully aligned, two-dimensional random in-plane and three-dimensional random states. The enhancement of the Young's modulus as well as the decrease of the thermal expansion coefficient were calculated numerically, assuming technologically relevant combinations of the nanotube aspect ratio and volume fraction. Maximal changes of the thermoelastic properties can be achieved in the longitudinal direction of NRPs with fully aligned carbon nanotubes whereas two-dimensional random in-plane and three-dimensional random composite morphologies exhibit more moderate enhancements but in more than one direction. Numerical predictions for the enhancements of the thermoelastic properties confirmed that carbon nanotubes can be considerably more effective for the reinforcement of polymers than conventional glass or carbon fibres.

References: H.R. Lusti, A.A. Gusev, *Model. Simul. Mater. Sci. Eng*. **2004,** *12,* S107-S119.

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, Department of Materials, ETH

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 nonoverlapping identical spheres, whereas the second type were 10 slightly fused spheres. Numerical results reveal that by using agglomerates with fused spheres, one can significantly increase the composite stiffness, whereas the use of nonfused agglomerates does not allow one to achieve any additional stiffness increase compared to a composite with evenly dispersed nonagglomerating spheres.

References: H.R. Lusti, I.A. Karmilov, A.A. Gusev, *Soft Mater*. **2003**, *1*, 115-120.

Title: On the possibility of reduced variable predictions for the thermoelastic properties of short fibre composites

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

Institute/Group: [*]IRC in Polymer Science and Technology, University of Leeds, UK
[**]Institute of Polymers, Department of Materials, ETH

Description:

Computer aided design offers the potential for the rapid development of new advanced structures from short fibre reinforced composites. The advantage of a validated numerical simulation is clear, as it allows a large number of the potential structure's solutions to be studied before proceeding to a manufacturing stage, reducing cost and risk accordingly. In our recent work we have demonstrated that the direct finite-element-based procedure of Gusev could be reliably employed for the prediction of thermoelastic properties of laboratory injection moulded samples, on the basis of Monte Carlo multi-fibre computer models built based on the measured fibre orientation distribution functions. Most injection moulded or extruded structures however, exhibit non-uniform fibre orientation states across the final parts, with a diverging variety of different local fibre orientation states. It Would be impractical to characterize all the possible orientation states by their full distribution functions, and it would be equally impractical to attempt direct numerical property predictions for all the various orientation states. Here we show that real injection moulded and extruded materials show fibre orientation states close to a maximum entropy prediction (i.e. most random) and that local thermomechanical properties can be excellently predicted based on the second order orientation moments and a constant strain assumption between the phases. Our results landmark a practical possibility of computer aided design of advanced structural parts from short fibre reinforced composites.

References: P.J. Hine, H.R. Lusti, A.A. Gusev, *Compos. Sci. Technol.* **2004**, *64*, 1081-1088.

Title: Stable FEM-BEM coupling for Helmholtz transmission problems

Researchers: R. Hiptmair
P. Meury

Institute/ Group Seminar for Applied Mathemtaics
ETH Zurich

Description:

When solving Helmholtz transmission problems we have to tackle a problem which is posed on an unbound domain. By coupling finite element and boundary element methods the transmission problem can be reduced to a variational saddle-point problem which is posed on a bounded domain.
However, classical symmetric FEM - BEM coupling suffers from spurious resonances although the underlying transmission problem is initially well posed. By combining a suitable regularization operator and the Calderon projector we obtain a resonance-free variational formulation which is amenable to finite element discretizations. Figure 1 shows the behaviour of the condition number of the matrices underlying the symmetric and the regularized FEM - BEM coupling in the neighbourhood of a resonant frequency.

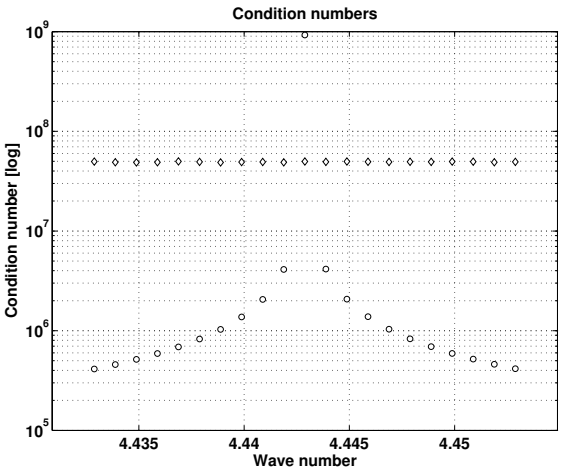


Figure 1: symmetric (○) and regularized (◇) FEM - BEM coupling.

References:

R. Hiptmair and P. Meury, Stable FEM-BEM Coupling for Helmholtz Transmission Problems, SAM Report, June 2005.

Title: Radiative heat transport for plasma arc simulations

Researchers: Gisela Widmer
Ralf Hiptmair

Institute/ Group: Seminar for Applied Mathematics,
in collaboration with ABB Corporate Research

Description:

When simulating a dense gas at very high temperatures, energy transport by means of radiation has to be taken into account. However, as even the stationary monochromatic radiation equation is stated in five dimensions, with the intensity depending on space and direction, it is a bottleneck of such computations. This project aims at reducing the number of degrees of freedom by applying sparse grid and a-posteriori adaptive methods. Sparse grid methods have been used to overcome the 'curse of dimension' of multidimensional problems. Applied to the radiation equation, the complexity of the problem is reduced from five to three dimensions up to logarithmic terms.

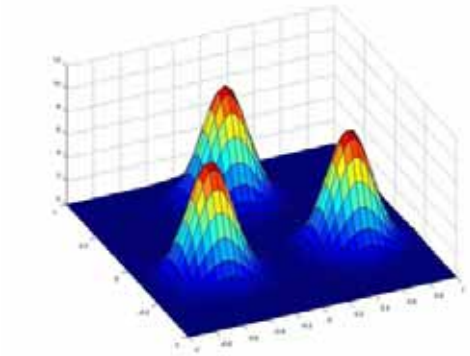


Figure 1: Emission f(x)

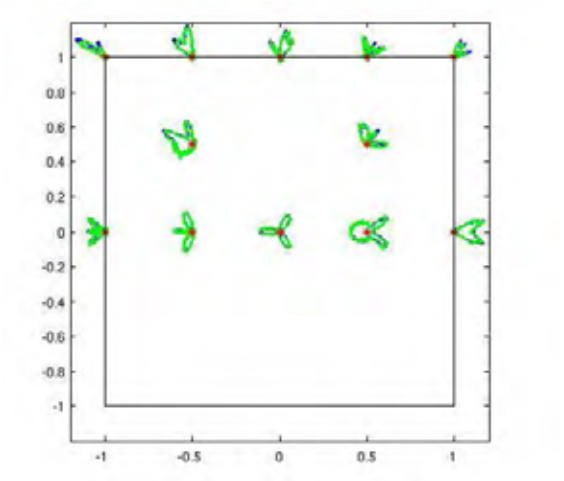


Figure 2: Radiation intensiy in two dimensions. Comparison of sparse grid (green) and full grid (blue) for emission in fig. 1 for absorption $\kappa = 1$.

References:

Title: Conservative Discretization of Einstein-Dirac Equations in Spherical Symmetry

Researchers: Benedikt Zeller
Ralf Hiptmair

Institute/ Group: D-MATH,
Seminar for Applied Mathematics

Description:

We consider the gravitational field of a 2-fermion system in the spherical symmetric case. The fermions are modeled by two wave functions in singlett state. We derived the Einstein-Dirac equations in Schwarzschild coordinates and ended up with a first order system of five partial differential equations for two components $A = A(t,r) \geq 0$, $B = B(t,r) \geq 0$ of the metric tensor and the two complex valued functions $\alpha = \alpha(t,r)$, $\beta = \beta(t,r)$ in the spherical symmetric ansatz for the spinor fields.

Four of the equations define the time evolution of the system and two of them impose constraints on the initial values. These constraints are propagated. Two conserved the quantities can be identified, the total electric charge

$$Q := 2q \int_0^\infty |\alpha|^2 + |\beta|^2 \, \mathrm{d}r \,,$$

and the ADM-mass

$$M_{\mathrm{ADM}} := \frac{c^2}{2G_N} \lim_{r\to\infty} r \left(1 - \frac{1}{B}\right) = \frac{4\hbar}{c^2} \int_0^\infty \mathrm{Im}(\alpha\dot{\bar{\alpha}} + \beta\dot{\bar{\beta}}) \frac{1}{\sqrt{AB}} \mathrm{d}r \,.$$

We aim to develop a stable reliable numerical scheme for the approximate numerical solution of the 2-fermion Einstein-Diract equations. To do so we introduce new variables by $A = e^a$, $B = e^b$ and employ a finite element Galerkin discretization in conjunction with an implicit Runge-Kutta-Gauss timestepping. The resulting discrete evolution will conserve a discrete analogue of the charge Q. This will hold for all admissible finite element spaces so that the scheme is amenable to hp-adaptivity.

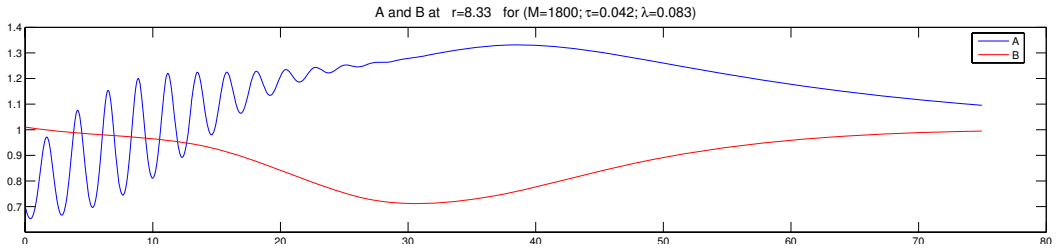


Figure 1: Temporal evolution of metric coefficients A and B at (scaled) radius $r = 8.33$

Title: *hp*-adaptive FEM for time-harmonic Eddy current problems

Researcher: Kersten Schmidt

Institute/ Group: Seminar for Applied Mathematics
Department of Mathematics

Description:

We are interested in the electromagnetic field generated by an alternating current density in the computational domain Ω with dielectric media. In many situations the quasi-static eddy current model is reliable. Unlike for the full Maxwell's equations the electric field E is determined only up to gradients of potential functions ϕ inside the non-conducting regions. However, by introducing additional constraints a uniquely solvable mixed formulation for E and ϕ results.

In this project an existing C++ class library is extended to incorporate coordinated, fully *hp*-adaptive edge and nodal element spaces on a quadrilateral mesh. Coordinated spaces means that the implementation of both spaces ensure the discrete analogon of properties given in the deRham complex. Fully *hp*-adaptive spaces include adaptive refinement in polynomial degree in each direction (anisotropically) and in mesh size. The code allows independent refinement of elements since conforming as well as non-conforming meshes can be dealt with.

Boundary and interface effects can be resolved accurately at low computational cost.

Title: Virtual Forming Tools for Extrusion Processes

Researchers: Pavel Hora
Longchang Tong

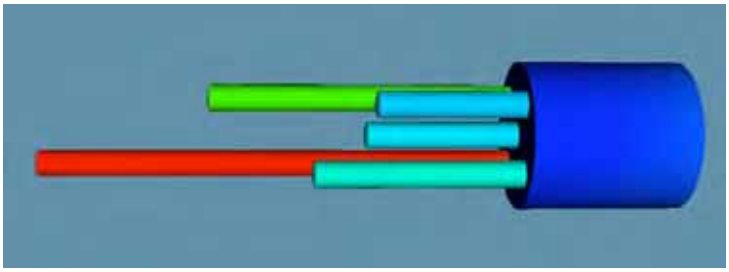
Institute: Institute of Virtual Manufacturing

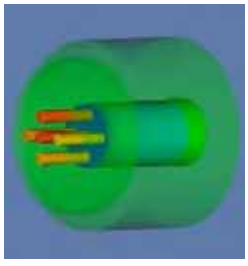
Description: The results from most commercial FE programs showed unacceptable deviation from the experimental of bench mark test at the conference Extrusion'05 in Zurich. That means, the model to realize virtual extrusion has to be improved. The most important characters of extrusion process are the long contact time, large contact area and high friction stress between the workpiece and forming tools. In order to describe these boundary conditions reasonably, a new friction model is developed and implemented. Experiments are also necessary to verify the model and to determine the parameters for the friction and the heat flux. The goal of the project is to achieve a simulation package to realize the virtual extrusion process and get systematic knowledge about the process.

References:

C. Karadogan et al., "State of the art and potential development of digital extrusion modeling", Light Metal Age, vol. 63, No. 3, 2005

P. Hora at al.: Benchmark of Extrusion Zurich 05, Conference proceedings, IVP, ETH-Zurich, 2005





ALE-Method for simulation of extrusion process with a new formulation of friction contact based on a Bingham material model.

Title: Virtual modeling of fine blanking processes

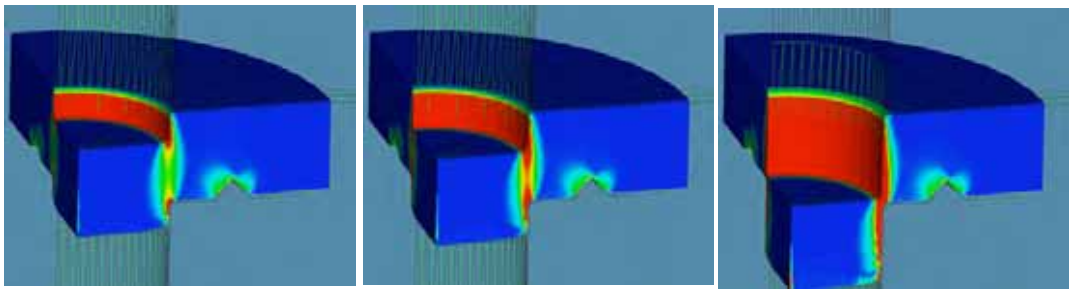
Researchers: Pavel Hora
Longchang Tong

Institute: Institute of Virtual Manufacturing

Description:

Fine blanking is a kind of competitive net shape process and has been getting more and more applications. However, failure on the blanking surfaces by thick sheet limits the expanding of the usage. To save the cost of trail and error method, the virtual experiment can be used. Because of the extreme deformation in the shear zones, most commercial programs are not suitable for the numerical simulation. In order to realize the 3D simulation of the fine blanking process, a FE package is being developed at Institute of Virtual Manufacturing, ETH-Zurich. The program is able to perform the re-meshing process and deliver reliable results in reasonable time in spite of the great magnitude of computation. The results are compared with the experiment conducted by the industrial project partner. The goal of the project is to achieve a FE-Package which allows the optimization of fine blanking processes for industrial relevant cases.

References: "Umformen und Feinschneiden", Handbuch für Verfahren Werkstoffe Tielegestaltung, 1997



Numerical simulation of fine blanking processes with a special ALE-rezoning method

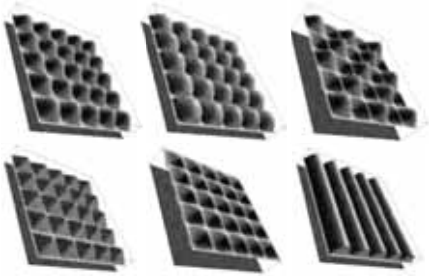
Title: Simulation of the Tribological System in Sheet Metal processes on the Micro Scale

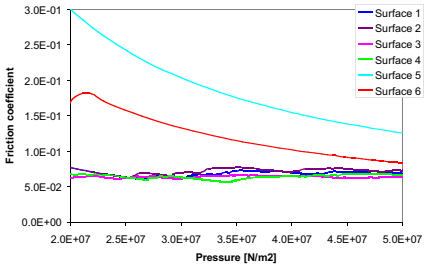
Researchers: Reto Grueebler

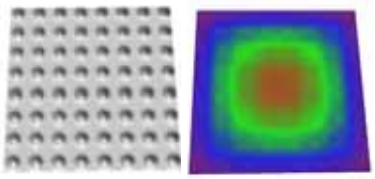
Institute/ Group: Institute of Virtual Manufacturing

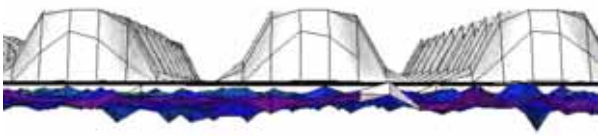
Description:

The topography of the sheet metal and tool surface influences the contact behavior between the tool and the sheet metal. With a simulation on the micrometer scale the topographical deformation of the sheet metal is elasto-plastically modeled using an explicit finite element method. The model of the lubricant in between is based on a simplified method calculating the pressure and velocity of the liquid with Darcy's law. A flat rigid tool is pressed on the sheet metal surface simultaneously with a constant lateral motion. Simulations were performed with real and modeled surfaces. The topographies show different tribological behavior depending on their texture.
The simulation was used to perform calculations with different surface topographies. The tribological behavior of mathematical modeled sheet metal surfaces was compared. Real textured surfaces with similar properties like the modeled ones were analyzed also. In addition to the textured sheet metal surfaces simulations with textured tool surfaces were performed to see the behavior of the tool surface.









References:

R. Grüebler, P. Hora
Simulation of the Tribological System in Sheet Metal processes on the Micro Scale, WTC (2005)

Title: Molecular dynamics simulations of phospholipid bilayers: influence of artificial periodicity, system size, and simulation time.

Researchers: Alex H. de Vries*
Indira Chandrasekhar*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

The convergence of structural and dynamical properties with system size and with time are investigated in molecular dynamic simulations of solvaled phospholipid bilayers, performed at constant colume under periodic boundary conditions using lattice-sum electrostatics. The electron density profile across the bilayer, the carbon-deuterium order parameters, and the surface tension are shown to be converged for a bilayer containing 36 lipids per leaflet and simulated over a period of 3-4 ns. Reasonable estimates for these properties can already be obtained from a system containing 16 lipids per leaflet. The convergence limit of 36 lipids per leaflet and the investigation of the correlation between lipid headgroup dipoles suggest a correlation length of about 3-5 nm in the lateral directions for a hydrated DPPC bilayer in the liquid-crystalline phase. Although these (relatively small) system sizes and (relatively short) time scales appear sufficient to obtain converged collective structural properties at constant volume, two restrictions should be kept in mind: (*i*) the relaxation times associated with the motion of individual lipids may be much longer and (*ii*) simulated properties converge significantly faster under constant volume conditions as compared to constant pressure conditions. Therefore, an accurate assessment of the dynamical properties of the system or of the relaxation of the bilayer under constant pressure conditions may require longer simulation time scales.

References: de Vries, A.H., Chandrasekhar, I., van Gunsteren, W.F. & Hünenberger, P.H.
J. Phys. Chem. B **109** (2005) 11643-11652.

Title: Combining the lattice-sum and reaction-field approaches for computing electrostatic interactions in molecular simulations.

Researchers: Tim N. Heinz*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

A new scheme, the lattice–sum emulated reaction–field (LSERF) method, is presented that combines the lattice–sum (LS) and reaction–field (RF) approaches for evaluating electrostatic interactions in molecular simulations. More precisely, the LSERF scheme emulates a RF calculation (based on an atomic cutoff) via the LS machinery. This is achieved by changing the form of the electrostatic interactions in a standard LS calculation (Coulombic) to the form corresponding to RF electrostatics (Coulombic plus quadratic reaction–field correction term, truncated at the cutoff distance). It is shown (both analytically and numerically) that in the limit of infinite reciprocal–space accuracy: (*i*) the LSERF scheme with a finite reaction–field cutoff and a given reaction–field permittivity is identical to the RF scheme with the same parameters; (*ii*) the LSERF scheme is identical to the LS scheme in the limit of an infinite reaction–field cutoff, irrespective of the reaction–field permittivity. This new scheme offers two key advantages: (*i*) from a conceptional point of view, it shows that there is a continuity between the RF and LS schemes and unifies them into a common framework; (*ii*) from a practical point of view, it allows to perform RF calculations with arbitrarily–large reaction–field cutoff distances for the same computational costs as a corresponding LS calculation. The optimal choice for the cutoff will be the one that achieves the best compromise between artifacts arising from the dielectric heterogeneity of the system (short cutoff) and its artificial periodicity (long cutoff). The implementation of the LSERF method is extremely easy, requiring only very limited modifications of any standard LS code. For practical applications to biomolecular systems, the use of the LSERF scheme with large reaction–field cutoff distances is expected to represent a significant improvement over the current RF simulations involving comparatively much shorter cutoffs.

References: Heinz, T.N. & Hünenberger, P.H.
J. Chem. Phys. **123** (2005) 034107(1)-034107(19)

Title: A new GROMOS parameter set for hexopyranose-based carbohydrates.

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

Institute/ Group: * Laboratory of Physical Chemistry

Description :

A new parameter set (referred to as 45A4) is developed for the explicit-solvent simulation of hexopyranose-based carbohydrates. This set is compatible with the most recent version of the GROMOS force field for proteins, nucleic acids and lipids, and the SPC water model. The parametrization procedure relies on : (*i*) reassigning the atomic partial charges based on a fit to the quantum-mechanical electrostatic potential around a trisaccharide ; (*ii*) refining the torsional potential parameters associated with the rotations of the hydroxymethyl, hydroxyl and anomeric alkoxy groups by fitting to corresponding quantum-mechanical profiles for hexopyranosides ; (*iii*) adapting the torsional potential parameters determining the ring conformation so as to stabilize the (experimentally predominant) $^4C_1$ chair conformation. The other (van der Waals and non-torsional covalent) parameters and the rules for third- and excluded neighbors are taken directly from the most recent version of the GROMOS force field (except for one additional exclusion). The new set is general enough to define parameters for any (unbranched) hexopyranose-based mono-, di-, oligo- or polysaccharide. This force field has currently been validated for a limited set of monosaccharides (α- and β-D-glucose, α- and β-D-galactose) and disaccharides (trehalose, maltose and cellobiose) in solution, by comparing the results of simulations to available experimental data. More extensive validation will be the scope of a forthcoming report.

References: Lins, R.D. & Hünenberger, P.H.
J. Comput. Chem. **26** (2005) 1400-1412.

Title: A multiple-timestep algorithm compatible with a large number of distance classes and an arbitrary distance dependence of the timestep size for the fast evaluation of non-bonded interactions in molecular simulations.

Researchers: Vincent Kräutler*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

A new algorithm is introduced for performing the multiple-timestep integration of the equations of motion for a molecular system, based on the splitting of the non-bonded interactions into a series of distance classes. The interactions between particle pairs in successive classes are updated at a progressively decreasing frequency. Unlike previous multiple-timestepping schemes relying on distance classes, the present algorithm sorts interacting particle pairs by their next update times rather than by their update frequencies. For this reason, the proposed scheme is extremely flexible with respect to the number of classes that can be employed (up to hundred or more) and the distance dependence of the relative timestep size (arbitrary integer function of the distance). Different variants of the algorithm are tested in terms of accuracy and efficiency for simulations of a pure water system (6167 molecules) under truncated-octahedral periodic boundary conditions, and compared to the twin-range method standardly used with GROMOS96 (short- and long-range cutoff distances of 0.8 and 1.4 nm, pairlist and intermediate-range interaction updated every five steps). In particular, multiple-timestepping schemes with an accuracy comparable to that of the twin-range method can be designed, that permit to increase the effective (long-range) cutoff distance from 1.4 to 3.0 nm with a performance loss of only about a factor two. This result is quite encouraging, considering the benefits of doubling the cutoff radius in the context of (bio-)molecular simulations.

References: Kräutler, V. & Hünenberger, P.H.
J. Comput. Chem., submitted (2005).

Title: Computation of methodology-independent ionic solvation free energies from molecular simulations: I. The electrostatic potential in molecular liquids

Researchers: Mika A. Kastenholz*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

The computation of ionic solvation free energies from atomistic simulations is a surprisingly difficult problem, that has found no satisfactory solution for more than fifteen years. The reason is that charging free-energies evaluated through such simulations are affected by very large errors. One of these is related to the choice of a specific convention for summing up the contributions of solvent charges to the electrostatic potential in the ionic cavity, namely on the basis of point charges within entire solvent molecules (M-scheme) or on the basis of individual point charges (P-scheme). The use of an inappropriate convention may lead to a charge-independent offset in the calculated potential, which depends on the details of the summation scheme applied to evaluate this potential, on the quadrupole-moment trace of the solvent molecule, and on the approximate form used to represent electrostatic interactions in the system. However, whether the M- or P-scheme (if any) represents the appropriate convention is still a matter of an on-going debate. In an attempt to settle this long-standing controversy, the properties of the electrostatic potential in molecular liquids (and inside cavities within them) are carefully analyzed (both analytically and numerically) Restricting the discussion to real liquids of 'spherical' solvent molecules (represented by a classical solvent model with a single van der Waals site), it is concluded that (*i*) for Coulombic (or straight-cutoff truncated) electrostatic interactions, the M-scheme is the appropriate way of analyzing electrostatic potentials (while the P-scheme introduces a spurious model-dependent offset in the estimated values) ; (*ii*) for non-Coulombic interactions deriving from a continuously-differentiable function, both M- and P-schemes generally deliver an incorrect result (for which an analytical correction term must be applied) ; (*iii*) finite-temperature effects, including intermolecular orientational correlations and preferential orientational structure of the solvent in the neighborhood of a liquid-vacuum interface, must be taken into account. Applications of these results to the computation methodology-independent ionic solvation free energies from molecular simulations will be the scope of a forthcoming report.

References: Kastenholz, M.A. & Hünenberger, P.H.
J. Chem. Phys., submitted (2005).

Title: Efficient Finite-Volume Schemes for Atmospheric Modeling

Researchers: William Sawyer*,**
Rolf Jeltsch*
Atsumu Ohmura**
Arthur A. Mirin***

Institute/ Group: * Seminar for Applied Mathematics, ETHZ
** Institute for Atmospheric and Climate Science, ETHZ
*** Lawrence Livermore National Laboratory, USA

We investigate the use of pentagonal/hexagonal grids for the solution of the advection and shallow water equations on the sphere. Such grids avoid problems due to converging points near the pole. In the numerical scheme used to solve the shallow water equations, we ensure that key physical quantities, such as mass and vorticity are conserved in the discrete sense. This makes the scheme useful as a building block for atmospheric dynamics on time scales of months to years, where conservation properties are crucial.

The resulting algorithm has shown to be viable for long term simulations. Moreover, the data dependencies of the finite volumes are limited to immediate neighbors, thus limiting communication and allowing scalability on massively parallel computers.

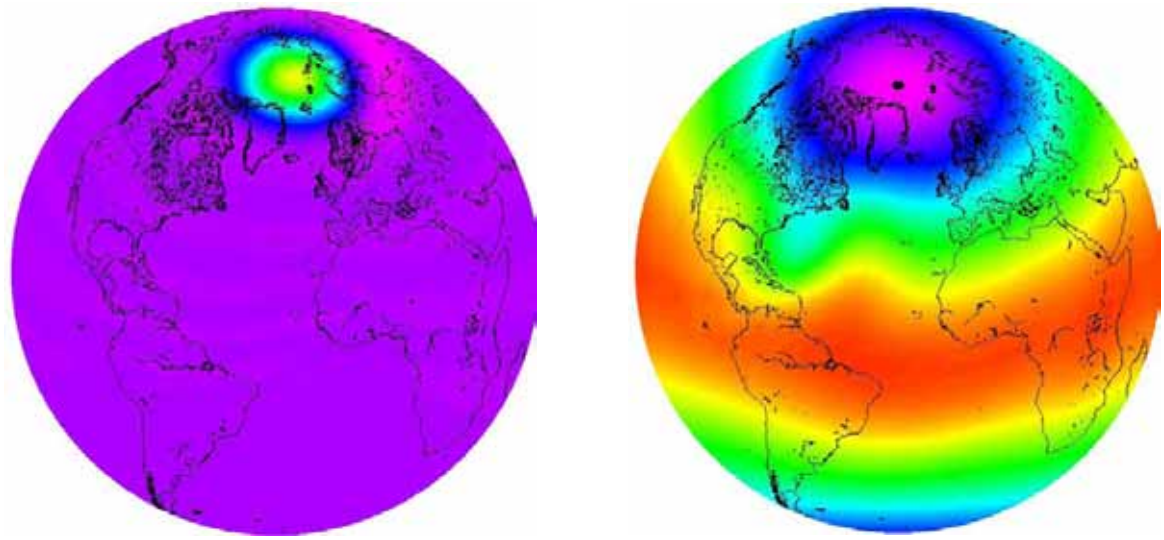


Figure 1: *On the left, a 3-day (1/4 rotation) advection simulation illustrates that a conic concentration of a constituent can be advected without distortion over the north pole. On the right, a 3-day simulation of mass in an initially west-to-east flow builds eddies in the lee of a large, fictitous mountain centered on New Orleans, USA.*

References:

1. Arthur A. Mirin and William Sawyer. A scalable implementation of a finite-volume dynamical core in the Community Atmosphere Model. *International Journal for High Performance Computer Applications*, 19(3):203–212, August 2005.

Title: Multidimensional Numerical Methods for the Regularized 13–Moment Equations

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

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Thermodynamics of gases provides a field theory with the main objective of determing fields of the basic variables, density, velocity and temperature. In order to obtain the fields one needs balance equations, namely the conservation of mass, momentum and energy and additional constitutive relations. The Euler-equations of gas dynamics are a classical choice. However these equations do not consider dissipative effects.

The moment equations, derived from extended thermodynamics in the context of kinetic gas theory, are dissipative, hyperbolic field equations for monatomic gases. In recent work a new closure for the 13–moment equations has been presented ([1], [2]). The regularized 13–moment equations are based on 13 moments (figure (1)) which correspond to the density, velocity and temperature, as well as stress tensor and heat flux. Beside the conservation laws the system provides two additional equations for the stress tensor and the heat flux. In a first part Grad's 13 moment equations have been solved using a second order FVM with limiters applied to every wave (see figure (1)). Furthermore convergence analysis have been made to show the convergence– rate and velocity. So far all calculations have been done for one dimensional shock-tube test experiments.

References:

[1] H. Struchtrup, M. Torrilhon *Regularization of Grad's 13 moment equations: Derivation and linear analysis*, Phys. Fluid 15/9, (2003), 26689–2680

[2] M. Torrilhon, H. Struchtrup *Regularized 13–Moment–Equations: Shock Struckture Calculations and Comparison to Burnett Models*, J. Fluid Mech. 513, (2004), pp.171-198

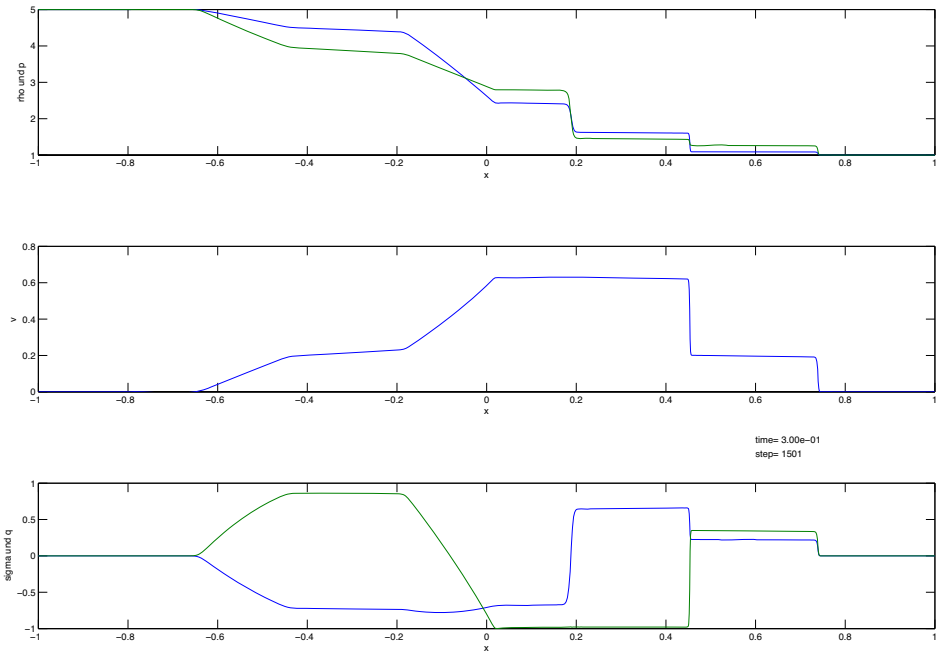


Figure 1: Solution of Grad's 13 moment equations at t=0.3s

Title: An exit probability approach to solve high dimensional Dirichlet problems

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

Institute: *Seminar for Applied Mathematics

Description:

In a previous work [1], *Solving Dirichlet Problems Numerically Using the Feynman-Kac Representation*, we studied a numerical procedure for elliptic problems which uses bounded increments for the driving Brownian motion in stochastic differential equations. There, the bounded increments are not isotropic and may introduce small errors in finding the boundary of the domain. A method for generating random rotation matrices (from G.W. Stewart) in $n-$space uses Householder transformations makes the increments isotropic. Another approach [2,3] which relies on statistical estimations is less computationally expensive and is globally order $O(h)$ in the stepsize h.

Two situations are evident:

- At time t_k, the process $X(t_k) \in D$ and also at the end of the timestep, $X(t_{k+1}) \in D$. The probability of an excursion must be estimated and a standard weak test is made. If the test shows an excursion, the exit time is sampled and a bridge process is used to estimate the exit postion.
- While at time t_k, the process $X(t_k) \in D$ but at the end of the step, $X(t_{k+1}) \notin D$. In this case, the process clearly exited, so what remains is to estimate when during this timestep. Once the exit time is estimated, a bridge can be used to sample the exit position.

We find extremely good results with this procedure and have simulated model problems in hypercubic and hypersherical domains up to 128 dimensions on the ETH Beowulf machine Hraidar.

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

References:

[1] F.M. Buchmann and W.P. Petersen, *An Exit Probability Approach to Solve High Dimensional Dirichlet Problems*, SIAM J. on Scientific and Statistical Computing, accepted Sept. 2005.

[2] *Weak approximation of stopped diffusions*, refereed paper in the proceedings of MC2QMC, Juan-les-Pins, 2004. Published by Springer-Verlag, 2005.

[3] F.M. Buchmann, *Simulation of Stopped Diffusions*, J. Computational Physics, **202**, (2005), pp. 446-462.

Title: Repetition test for pseudo-random number generators

Researchers: G.H. Gonnet†
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Description:

For a uniform random number generator with integer range, say $0 < RNG < 2^w$, the expectated step k at which some number in the sequence repeats can be shown to be approximately

$$\mathbb{E}[k] = \sqrt{\frac{\pi}{2}} 2^{w/2} + O(1)$$

steps. Linear congruential (LC) methods, $u_n = a \cdot u_{n-1}$ **mod** 2^w, cannot repeat any number u_k before $k = 2^w$. Otherwise, the entire sequence repeats since the recurrence is a one-step whose period is 2^w. Lagged Fibonacci (LF) sequences, or their generalizations, have vastly longer periods. For example, the simple recurrence $u_n = u_{n-p} + u_{n-q}$ **mod** 2^w has a period of approximately $2^w \cdot 2^{p \vee q}$ for suitably chosen p, q. If $\max(p, q) = p \vee q$ is large enough, the period of the sequence is astronomically large. However, numbers in LF sequences do re-appear at the above expected rate $\mathbb{E}[k]$. For pattern matching algorithms, satisfying the expected repetition time is very important.

With this in mind, a RNG test called the **repetition test** was implemented and tested using several random number generators. A repetition is expected to occur at approximately $O(2^{w/2})$ steps, not 2^w. Thus, keeping a history of which values have already been generated becomes possible. A hashing procedure which requires storage of only $O(2^{w/2})$ numbers serves this purpose. We tested various popular RNGs: James' version of `RANLUX`, Mersenne Twister of Matsumoto et al, and the `WELLRNG` from Panneton and L'Ecuyer [3].

References:

[1] G. H. Gonnet, *Repeating time test for $U(0, 1)$ random number generators*, Technical Report, Dept. Informatik, ETH, Zürich, May, 2003.
`http://www2.inf.ethz.ch/~gonnet/RepetitionTest`.

[2] G. H. Gonnet, M. Gil, and W. P. Petersen, submitted to Monte Carlo Methods and Applications, 2005.

[3] F. Panneton and P. L'Ecuyer, *Improved Long-Period Generators Based on Linear Recurrences Modulo 2*, TOMS, 2005, in print.

Title: A Model for the Light Arc Simulations

Researcher: Harish Kumar
Dr. Manuel Torrilhon
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

A light arc phenomenon occurs when a sudden change in the electric field takes place which in turn charge the fluid particles around it so that the fluid start behaving like plasma. Hence current start flowing in the fluid and a large amount of energy generates. Also due to the current flow a magnetic field also develop. This phenomena is of high interest for the switching industry due to its application in the circuit breakers.

In this project we try to model this phenomenon. We consider Magnetohydrodynamics (MHD) equations (which govern the plasma flow in the magnetic field) in a 3D box. The box is filled with some fluid. Than we apply the electric field in a cylinder in the box joining two faces. When we change the electric field suddenly, the temperature in the box rise due to generation of the energy and increases the conductivity of the fluid and a strong current start flowing in the domain. Also a magnetic field develop. We observe that the temperature first rise very fast due to fast change in electric field and than slowly decrease and attains a stable state as the electric field attain a stable state. Also a strong current generated initially also attain a stable state.

References:

[1] M. Torrilhon *Zur Numerik der Idealen Magnetohydrodynamics*, Shaker Verlag, Anchen(2004)

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

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

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

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

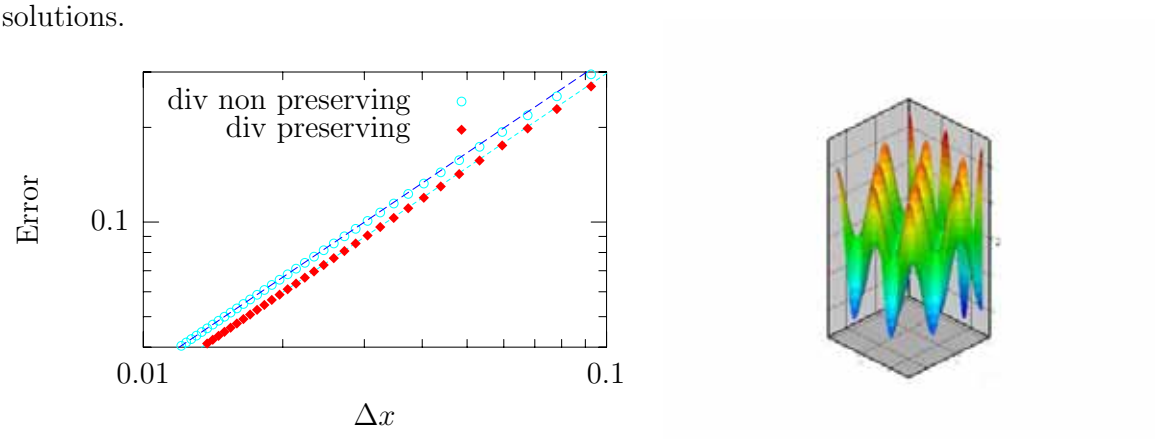

Figure 1: Two 2D simulations for TE wave are illustrated. On the left an l_2 error comparison between a standard 1st order FV method and a divergence-preserving version of the same method. Both are of 1st order convergence, but the divergence-preserving one is slightly better. The initial data for B_z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

References:

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

Title: Turbulent reactive flow

Researchers: Benjamin Rembold
Daniel W. Meyer
Michael Hegetschweiler
Gaurav Anand
Patrick Jenny

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

Description:

Joint probability density function (PDF) methods are extremely attractive for turbulent reactive flow simulations, since turbulence-reaction interaction and convection appear in closed form and do not have to be modeled. The main reason why joint PDF methods are not more widely used in industry is the high computational cost of the solution algorithms compared with Reynolds-averaged Navier-Stokes (RANS) models.

Motivated by this fact, we developed a new hybrid particle/finite-volume PDF solver, which proved to be faster by orders of magnitude than previous solution algorithms. Currently, we are generalizing this algorithm for problems with complex 3D geometries with the objective to apply PDF methods in industry on a regular basis. The structure of our code is highly modular, such that the new models which we develop can easily be integrated. Moreover, the block structure of the grid provides a natural framework for parallel computing. We will employ a domain decomposition approach with message passing (MPI).

In terms of modeling we focus on four topics: multi-scalar mixing, non-premixed turbulent combustion with local extinction and re-ignition, premixed turbulent combustion, and wall turbulence. A further project is concerned with LES of heat transfer, where a PDF method is used as a sub-grid scale model for turbulent and molecular mixing.

References:

D. W. Meyer and P. Jenny. A mixing model for turbulent flows based on parametrized scalar profiles. Submitted to Physics of Fluids

B. Rembold and P. Jenny. A hybrid joint PDF multiblock algorithm for complex turbulent flow applications. 17th AIAA Computational Fluid Dynamics Conference, Toronto, Canada, 2005

Title: Multi-phase flow in porous media

Researchers: Ivan Lunati
Manav Tyagi
Patrick Jenny

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

Description:

Flow and transport in porous media has many applications in energy science, e.g. for catalytic processes, oil and gas recovery, and CO_2 sequestration in sub-surface formations. One of the major challenges in macroscopic simulations is the correct treatment of complex permeability distributions with strong variations and many length scales. To deal with this issue, various upscaling and multi-scale methods have been developed.

We devised a new method, i.e. the multi-scale finite-volume (MSFV) algorithm, which has several advantageous properties compared with the other multi-scale approaches. With the MSFV method it could be demonstrated for the first time that it is possible to run large and difficult test cases in a small fraction of the time required by conventional simulators. At the same time the accuracy of the solution is hardly compromised. Currently the MSFV method is further being developed, i.e. more physical processes are incorporated, with the objective to integrate it into a commercial simulator. Note that the MSFV is an ideal target for massive parallel computing, since virtually all CPU time is consumed by solving many small, independent, elliptic problems.

A topic with high relevance is the sequestration and storage of CO_2. Currently, this seems to be one of the most promising feasible technologies to stabilize the CO_2 concentration in the atmosphere. Together with the Petroleum Engineering Department of Stanford University, we conduct a project with the objective to improve our understanding of the relevant processes and dynamics which are involved when CO_2 is injected and transported in geological formations. To study the relevant mechanisms and time scales we devised a stochastic particle approach which will allow us to model the physical processes in a Lagrangean framework. Since this particle method is significantly more expensive than standard finite-volume schemes, parallel computing will be of great importance at a later time.

A problem which is intrinsic to flow and transport in porous media is the uncertainty of the input data like property distributions of the medium and initial conditions. Together with Professor Hamdi Tchelepi (Petroleum Engineering Department at Stanford University) we addressed this issue and developed a joint PDF method for uncertainty assessment in transport, e.g. of a radioactive contaminant. Conceptually, our approach has a number of crucial advantages above established methods and we intend to generalize it for multi-phase flow. The solution algorithm is a particle method and for realistic, big problems, a parallel version has to be developed.

References:

P. Jenny and I. Lunati. Treating Highly Anisotropic Subsurface Flow with the Multi-Scale Finite-Volume Method. Submitted to SIAM Journal of Multiscale Modeling and Simulation

I. Lunati and P. Jenny. Multiscale Finite-Volume Method for Compressible Multiphase Flow in Porous Media. Submitted to Journal of Computational Physics

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

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

P. Jenny, S. H. Lee and H. Tchelepi. Adaptive multiscale finite-volume method for multi-phase flow and transport in porous media. SIAM Journal for Multiscale Modeling and Simulation, 3(1), pp. 50—64, 2004

Title: Radiation and light scattering in turbid media

Researchers: Lalit Kumar
Patrick Jenny

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

Description:

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

Based on the transport theory, we developed a modeled evolution equation for the photon number density and the PDF of photon propagation direction. Compared with other models, which simply assume diffusion of the scattered photon concentration in the medium, the level of closure is much higher and the solutions contain more relevant statistical information. It is possible to account for anisotropic media and spatially varying coefficients, and later we will extend the method by a model for re-emission and intend to couple it with combustion simulations. Since the solution algorithm is a particle method, we have to deal with statistical errors. These can be reduced by employing a large number of particles and therefore parallel computing will be an important issue in the future.

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

Researchers: Andreas Jocksch, Felix Keiderling, Leonhard Kleiser, Sebastian Müller, Philipp Schlatter, Steffen Stolz, Jörg Ziefle

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

Description:

Most engineering and geophysical flows occur at high Reynolds numbers and are thus turbulent. Due to their wide range of length and time scales such flows are not amenable to Direct Numerical Simulations (DNS) in which all relevant scales need to be resolved. In Large-Eddy Simulations (LES) one only resolves the large scales, while their interaction with the non-resolved subgrid scales is modeled. 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. Moreover, LES can be expected to yield much more reliable results for the mean flow and turbulence statistics than RANS for a number of complex flow cases.
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. Another approach involves the use of high-pass filtered eddy-viscosity subgrid models. LES using these novel models have been demonstrated to give excellent results for a range of flows, all at a fraction (order one percent) of the cost that would be needed for a DNS of the same flows. These include laminar-turbulent transition, isotropic turbulence, incompressible channel flow, supersonic channel, boundary-layer, compression-ramp flows, turbulent spot propagation in compressible boundary layers and compressible rectangular jet flow. DNS and LES data for rectangular subsonic jet flow have been evaluated successfully with respect to computation of noise radiation.
A DNS/LES code for cylindrical geometries was developed and is being applied for simulations of swirling mixing layers and circular jet flows with direct computation of noise radiation into the near field. The ADM approach was also implemented in an industrial-type finite volume code, including an extension to flexible multiblock geometries. Excellent results were obtained for compressible turbulent channel flow, turbulent shock-boundary-layer interaction and massively separated flow in a channel with periodic constrictions.

References: See separate list.

Title: Simulation of Particle-laden Flows

Researchers: Thorsten Bosse, Leonhard Kleiser, Anna Kubik, Eckart Meiburg*

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

Description:

This project is concerned with the simulation of disperse two–phase flows, in which a large number of small particles are suspended in a carrier fluid. We consider dilute suspensions, i. e. flows with small particle concentrations where the particle–fluid interaction is the predominant process while direct particle–particle interactions may be neglected (two–way coupling). The particles are assumed to be much smaller than the smallest relevant scales of the fluid motion. This allows us to model the particles as point–forces without resolving their finite size. Each particle is tracked along its trajectory (Lagrangian tracking), while the fluid equations are solved in an Eulerian framework.
In order to study fundamental aspects of particle suspensions, the settling of suspension drops under the influence of gravity was investigated. Here, the fluid motion remains laminar providing a test case for low and moderate Reynolds number flows. An initially spherical suspension drop usually deforms into a torus that eventually becomes unstable and breaks up into a number of secondary blobs. With increasing Reynolds number a growing number of sub-structures is formed. At fixed Reynolds number the instability depends primarily on the number of particles and their distribution inside the torus.
Furthermore, settling of an initially random particle suspension in homogeneous turbulence was studied. In the case of one-way coupling, the mean particle settling velocity is increased by the preferential sweeping effect. Under gravity they accumulate preferably in regions of downward fluid motion. In the case of two-way coupling an additional enhancement of the settling velocity is observed. Here, the particles exert a collective downward drag force on the fluid in regions of increased particle concentration, such that the downward fluid velocity increases there leading to an enhanced settling velocity.
Turbulent, wall-bounded particulate flows with separation were investigated using the setup of a particle-laden flow over a backward-facing step (BFS). To account for the wall–particle interaction models of this process were extended and refined. Two-way coupling for the particulate flow was implemented allowing for studies of turbulence attenuation. The examination of the various forces acting on solid particles in laminar and turbulent BFS flow has shown that generally, a simplified particle force model is sufficient for larger calculations. Developed particle-laden channel flow was found to be the most favorable inflow condition for the BFS flow. The first studies of channel and BFS configurations yielded promising results for mean, instantaneous, and statistical quantities.

References: See separate list.

Title: Melting and nucleation in hexagonal ice

Researchers: Davide Donadio
Paolo Raiteri
Michele Parrinello

Institute/ Group: Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

We use classical molecular dynamics combined with the recently developed metadynamics method [A. Laio and M. Parrinello, Procs. Natl. Acad. Sci. USA 99, 20 (2002)] to study the process of bulk melting in hexagonal ice. Our simulations show that bulk melting is mediated by the formation of topological defects which preserve the coordination of the tetrahedral network. Such defects cluster to form a defective region involving about 50 molecules with a surprisingly long life-time. The subsequent formation of coordination defects triggers the transition to the liquid state. The process of nucleation and freezing is currently under investigation.

References: J. Phys. Chem. B, 109, 5421 (2005)

Title: Melting and crystallization of thin films of ice on a hydrophilic surface

Researchers: Oliviero Andreussi*
Davide Donadio**
Michele Parrinello**

Institute/ Group: *Scuola Normale Superiore, P.zza dei Cavalieri 7, 56100 Pisa, Italy
**Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

We study by Molecular Dynamics the melting and recrystallization processes of interfacial water. The system is characterized by a hydrophilic substrate, which consists of a chlorine terminated Si(111) surface, and three/nine bilayers of cubic ice (111). For this system, experimental data on the structure and the melting process, obtained with ultrafast electron crys- tallography (UEC), have recently been reported by Zewail and co-workers [Science 304, 81-84]. In our simulations, water is modelled by the classical non-polarizable TIP4P potential, which is known to reproduce correctly the phase diagram of H2O [Sanz et al., Phys. Rev. Lett. 92, 255701 (2004)], while the paraemters that mimic the interaction with the substrate have been tted to density functional theory (DFT) calculations. In order to accellerate the transitions and to comupte the thermodynamics of the system, metadynamics runs have been performed adopting various sets of collective variables, such as the Steinhardt order parameter Q6 [Steinhardt et al., Phys. Rev. B 28, 784 (1983)] and the structure factor. The dynamical aspects of the melting process reported by Zewail have also been investigated. Simulations of the whole process, from the ultra-fast temperature jump to the complete thermal relaxation of the system, have been performed and the results have been compared to the experi- mental data.

Title: Nucleation of a Lennard-Jones Fluid

Researchers: Federica Trudu
Davide Donadio
Alessandro Laio
Michele Parrinello

Institute/ Group: Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

We investigate the crystallization of a Lennard-Jones fluid at moderate undercooling by classical molecular dynamics (MD) simulations combined with state of the art techniques, developed to study rare events. By path sampling MD everal unbiased trajectories, where nucleation and crystallization occurs, have been obtained. The analysis of such trajectories provides an accurate description of the structural evolution of pre-critical and critical nuclei toward crystallization. The relative stability of the critical nuclei (about 200 ps) allowed to investigate their termodynamics properties, namely the internal pressure and the surface tension. We then compute the free energy barrier for the nucleation by metadynamics, adopting a set of local order parameters, devised from the study of the trajectories obtained by path sampling. We show that, by this choice of reaction coordinates, it would be possible to avoid the artifacts in the estimation of the free energy and of the reaction path which arise from the use of global order parameters.

Title: Evolution of the structure of amorphous ice from low density to very high density

Researchers: Roman Martonak
Davide Donadio
Michele Parrinello

Institute/ Group: Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

We report results of molecular dynamics simulations of amorphous ice for pressures up to 22.5 kbar. The high-density amorphous ice (HDA) as prepared by pressure-induced amorphization of Ih ice at T=80 K is annealed to T=170 K at various pressures to allow for relaxation. Upon increase of pressure, relaxed amorphous ice undergoes a pronounced change of structure, ranging from the low-density amorphous ice (LDA) at p=0, through a continuum of HDA states to the limiting very high-density amorphous ice (VHDA) regime above 10 kbar. The main part of the overall structural change takes part within the HDA megabasin which includes a variety of structures with quite different local and medium-range order as well as network topology and spans a broad range of densities. The VHDA represents the limit to densification by adapting the hydrogen-bonded network topology, without creating interpenetrating networks. The connection between structure and metastability of various forms upon decompression and heating is studied and discussed.

References: Phys. Rev. Lett. 92, 225702 (2004)
J. Chem. Phys. 122, 134501 (2005)

Title: Dehydroxylation and Rehydroxylation of pyrophyllite

Researchers: Esther Molina-Montes*
Davide Donadio**
A. Hernandez-Laguna*
C. I. Sainz-Diaz*
Michele Parrinello**

Institute/ Group: *Instituto Andaluz de Ciencias de la Tierra (CSIC/Universidad de Granada), Av. Fuentenueva s/n, 18002 Granada, Spain
**Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

Pyrophyllite is a 2:1 phyllosilicate of great interest for material design. Industrial applications of this mineral require thermal treatment, dehydration, dehydroxylation, and transformation processes, in which the hydroxyl groups of this mineral are lost. If this thermal process is not fully completed, the presence of water can produce a rehydroxylation process and lead to recover the initial pyrophyllite structures with a memory effect. The mechanisms of dehydroxylation and rehydroxylation are not well known although an unidentified intermediate has been spectroscopically detected. Molecular Dynamics calculations are perfomed at the density functional theory level with the CPMD code. To explore to an accurate extent the reaction path way and the free energy surface we apply the metadynamics algorithm at different temperatures.Different competitive reaction paths and transition states are found for both processes. We have observed that the apical tetrahedral oxygens play an unexspected role both in the dehydrixolitation and in the rehydroxylation of pyrophyllite.

Title: Ab-initio simulation of photoinduced transformation of small rings in amorphous silica

Researchers: Davide Donadio*
Marco Bernasconi**

Institute/ Group: *Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland
**Dipartimento di Scienza dei Materiali and INFM, Universita' di Milano-Bicocca, via Cozzi 53, I-20125, Milano, Italy

Description:

We have studied the photoinduced transformation of small rings (3-membered) in amorphous silica by Car-Parrinello simulations. The process of ring opening leading to the formation of a couple of paramagnetic centers, namely an E' and a non-bridging-oxygen hole center (NBOHC), has been proposed experimentally to occur in silica exposed to F2 laser irradiation (at 7.9 eV). By metadynamics, we have identified a transformation path for the opening of a 3-membered ring induced by a self-trapped triplet exciton, the migration of NBOHC and formation of a couple of stable E' and NBOHC paramagnetic defects.

References: Phys. Rev. B, 71, 073307 (2005)

Title: 'Site Binding' of Ca^{2+} Ions to Polyacrylates in Water: A Metadynamics Study of Coiling and Aggregation

Researchers: Davide Donadio*
Rosa Bulo*
Alessandro Laio*
Ferenc Molnar**
Jens Rieger**
Michele Parrinello*

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**BASF Aktiengesellschaft, Polymer Physics, Carl-Bosch Str. 38, 67056 Ludwigshafen, Germany.

Description:

The remarkably strong interaction of Ca^{2+} ions with polyacrylate chains in water is investigated using molecular dynamics simulations, accelerated with the recently developed metadynamics algorithm. The much discussed 'site-binding' of calcium ions to these industrially relevant polymers is identified as the coordination of four monomers per calcium ion. The 1:4 relation, which leaves the positive charge of the calcium ion strongly overcompensated by COO^- coordination, shows an intriguing correspondence to experimental findings for the precipitation threshold. The noticeably high coordination of Ca^{2+} ions is the result of an entropy gain as water molecules are released into the solution, inducing modest coiling of the polymer chains. At higher Ca^{2+} concentrations, however, the probability for strong local coiling of PA oligomers is low. This counterintuitive result is due to the crowded nature of highly coiled configurations with many coordinated Ca^{2+} ions. Since the uncoiled state of the crowded chain obstructs formation of the desired 1:4 Ca^{2+} COO^- coordination, inter-chain interactions become probable. It is demonstrated that the charge shielding effect of Ca^{2+} coordination allows short range interactions between multiple chains at low calcium concentrations relative to the precipitation threshold. We conclude that charge shielding, combined with a preference for four-fold coordination of a Ca^{2+} ion to polyacrylates and a low tendency towards local coiling, enables interchain interactions at threshold Ca^{2+} concentrations, ultimately resulting in aggregation and precipitation.

References: submitted to J. Amer. Chem. Soc.

Title: New algorithms for flexible docking in solution

Researchers: F. L. Gervasio*
D. Branduardi*
Michele Parrinello*

Institute/ Group: *Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

Understanding the mechanism of the recognition process between a ligand and its receptor (docking) presents a fundamental theoretical challenge and has significant importance in the drug discovery process. In this project we applied our recently developed method to sample rare events to the docking of ligands on flexible receptors in water solution. This method, building on pre-existing algorithms as *local elevation method* or the *Filling Potential method*, mimics the real dynamics of a ligand exiting or entering an enzyme and in so doing reconstructs the free energy surface. We first applied it to four docking cases: β-trypsin/benzamidine, β -trypsin/ chloro-benzamidine, immunoglobulin McPC-603/phosphocholine and cyclin dependent kinase-2/ staurosporine. In every case studied the method is able to predict the docked geometry and the free energy of docking. Its added value with respect to many other available methods is that it reconstructs the complete free energy surface including all the relevant minima and the barriers between them. We then applied it to a relevant docking problem, namely the ligand recognition by the peripheral anionic site and its penetration of the human AChE gorge. The role of both the peripheral anionic sites and the formation of cation-π interactions in the ligand entrance were clearly shown. In particular, a simulation with W286A mutant has shown the fundamental role of this residue in anchoring the ligand at the peripheral anionic site of the enzyme and in positioning it prior to the gorge entrance. Once the ligand was properly oriented, the formation of specific and synchronized cation- π interactions with W86, F295, and Y341 enabled the gorge penetration. Eventually, the ligand is stabilized in a free energy basin by means of cation- π interactions with W86.

References: [1] F.. L. Gervasio, A. Laio and M. Parrinello, *J. Am. Chem. Soc*., 127(8): 2600-2607, 2005.
[2] D. Branduardi, F. L. Gervasio, A. Cavalli, M. Recanatini and M. Parrinello,
J. Am. Chem. Soc., 127(25): 9147-9155, 2005

Title: Mechanism of charge transfer and oxidation of DNA

Researchers: F. L. Gervasio*
M. Boero**
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Institute/ Group: * Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland
**Institute of Physics, Special Nanoscience Project, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan

Description:

Charge transfer in DNA is currently the subject of intense theoretical and experimental investigation. This is due both to a possible use of DNA as a component in nanoelectronic and electrochemical devices and to the fundamental role of conductivity in the oxidative damage of DNA. In this project we first studied by first-principles molecular dynamics the mechanism of electron hole (positive charge) localization in a laboratory realizable radical cation Z DNA crystal. We found that at room temperature structural deformation does not provide an efficient localization mechanism. Instead we found evidence for the importance of changes in the protonation state for stabilizing the radical defect. In the second part of our study using state-of-the-art ab-initio molecular dynamics simulations and QM/MM, we studied the mechanism that guides the first steps of the oxidative damage to DNA. In the mechanism that we proposed, guanine, which among the bases has the lowest oxidation potential, and the phosphate backbone play a crucial role. We found that the rate limiting step is the water protolysis. Moreover we illuminated the role of the local environment in considerably lowering the barrier. Of particular relevance in this respect is the role of the phosphate backbone.

References: [1] F. L. Gervasio, A. Laio, M. Iannuzzi and M. Parrinello. *Chem. Eur. J.*, 10: 4846-4852, 2004.
[2] F.. L. Gervasio, M. Boero, A. Laio and M. Parrinello. *Phys. Rev. Lett.*, 84: 158103, 2005.

Title: BIOMACH

Researchers: Paolo Raiteri*
Gabriele Petraglio*
Michele Parrinello*

Institute/ Group: *Computational Science, Department of Chemistry and Applied Biosciences
ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

BIOMACH is a European Union Project for Nanotechnology. BIOMACH is a cross-disciplinary research initiative dealing with molecular machines, in particular biological and artificial motors. A close collaboration between chemists known for their expertise in designing functional (bio)molecular motors, biophysicists experienced in dealing with molecular biomachines and physicists addressing single-molecules will advance the basic understanding in this domain. BIOMACH comprises ten partners from five countries (France, Germany, Italy, Switzerland, The Netherlands) and three different research areas (Chemistry, Biophysics and Physics). Our part in this project is to provide a better understanding of the atomic mechanisms which rule the behavior of a molecular nanomotor. We focus on a two-state rotaxane which has been well characterized by the group of Prof. Balzani. The system is composed of a dumbbell-shaped part that is encircled by a crown-ether ring which displays a shuttling movement between two charged stations. At equilibrium, both have a +2 charge but electrochemical reactions or light inputs can reduce one of them inducing the movement of the ring. Our aim is to compute the energy barriers related to this process and to understand at the atomic level how the movement occurs.

Title: Linear scaling electronic structure calculations and accurate sampling with noisy forces

Researchers: Florian R. Krajewski*
Michele Parrinello*

Institute/ Group: *Computational Science, Department of Chemistry and Applied Biosciences ETH Zurich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

Description:

Numerical simulations based on electronic structure calculations are finding ever growing applications in many areas of physics. A major limiting factor is however the cubic scaling of the algorithms used. By using the localization property of the high temperature density matrix we developed an exact deterministic algorithm that scales linearly in one dimension and quadratically in all others. This algorithm was tested successfully for carbon nanotubes. In addition we have introduced a novel statistical method for evaluating the inter-atomic forces which scales linearly with system size in all dimensions and is applicable also to metals. The method is based on exact decomposition of the fermionic determinant and on a mapping onto a field theoretical expression. We have solved exactly the problem of sampling the Boltzmann distribution with noisy forces. The novel approach which we have developed can be used in such diverse fields as quantum chromodynamics, quantum Monte Carlo or colloidal physics.

References: F. R. Krajewski and M. Parrinello, Phys.Rev. B71, 233105 (2005)
F. R. Krajewski and M. Parrinello, submitted to Phys.Rev. Lett.

Title: Automatic tests of the compatibility of 1D and 2D NMR spectra and chemical structures

Researchers: Lóránt Bódis
Ernö Pretsch

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

Description:

Today, different one- and two-dimensional NMR spectra can be automatically recorded with such a high rate that more and more, their interpretation has become a bottle-neck. In this project, we make use of our ^{1}H and ^{13}C NMR spectra prediction programs to estimate the corresponding 1D and 2D NMR spectra. Various strategies of comparing the measured and predicted spectra are being developed and tested. They are optimized for detecting both structure incompatibilities and the presence of impurities.

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

Title: Computational Micromagnetism

Researcher: Andreas Prohl

Institute/ Group: Department of Mathematics/ Seminar of Applied Mathematics

Description:

Magnetization in ferromagnetic specimen on a mesoscopic scale is described by the evolutionary Landau-Lifshitz-Gilbert equation (LLG), which is e.g. used to improve devices in harddisk industries. As is motivated from theory of related heat flow harmonic maps, existing weak solutions are supposed to develop finite-time blow-up, which in turn asks for convergent approximations of nonregular solutions. Main problems to overcome during the construction process of convergent schemes are (i) strong nonlinearities, (ii) the sphere constraint for magnetizations, and (iii) the stiffness of used finite element spaces. In a first step, explicit methods were considered, which suffer from limiting spatio-temporal mesh-constraints (studied in the context of heat flow of p-harmonic maps) to make convergence hold; then, we succeeded to construct fully discrete, implicit discretizations which are unconditionally convergent towards weak solutions of (LLG), and computationally evidenced finite-time blow-up.

Title: Theoretical Chemistry: Molecular Spectroscopy and Dynamics - 39th Symposium on Theoretical Chemistry 2003 (STC 2003) 28 September to 2 October 2003, Gwatt, LakeThun, Switzerland

Researchers: F. Mariotti*
M. Quack*
M. Willeke*
J. Stohner**

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

Description:
We provide a short review of the scientific meeting defined by the title of this article, which may at the same time serve as a compact review of the field with a substantial number of references to recent work in computational chemistry. Exciting new developments in experiments on high-resolution molecular spectra and their analysis as well as new theoretical developments in the calculations of such spectra and the related time-independent and time-dependent quantum dynamics of molecules have led to new answers but also to new questions in the fields of molecular kinetics, molecular reaction dynamics, molecular chaos and statistical mechanics as well as fundamental symmetries in molecular processes. Particular stress is placed on fundamental aspects and new directions.

References:
F. Mariotti, M. Quack, M. Willeke, J. Stohner, Chimia **58**, 263-275 (2004).

Title: Doppler-limited FTIR spectrum of the $\nu_3(a')$/ $\nu_8(a'')$ Coriolis resonance dyad of $CHClF_2$: analysis and comparison with *ab initio* calculations

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

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

Description:

The Doppler-limited FTIR spectrum of the band system in the region 1070–1170 cm^{-1} (Doppler width ≈ 0.0015 cm^{-1}, FWHM) was measured with our new Bruker IFS 120 HR Zürich prototype (ZP2001) spectrometer. This instrument allows for an unapodized resolution of 0.0007 cm^{-1} (FWHM). Up to now, this is the highest resolution realized by a commercial FTIR spectrometer system. It allows a high resolution analysis of the room temperature spectra of the strongly coupled modes $\nu_3(a')$ and $\nu_8(a'')$, corresponding to the symmetric and antisymmetric CF-stretching vibrations, including also further couplings not analyzed previously. The present analysis is based on effective rotational Hamiltonians for the $\nu_3 = 1$ and $\nu_8 = 1$ states including all terms up to sextic, and involves the full first order Coriolis interaction operator. The final analysis involves both chlorine isotopomers and includes all hybrid components wich are allowed by symmetry. It results in the band centers ν_3^0 = 1108.7274 cm^{-1}, ν_8^0 = 1127.282 cm^{-1}, $3\nu_9^0$ = 1098.5 cm^{-1} and $(\nu_6 + 2\nu_9)^0 = 1144.32$ cm^{-1}. The main Coriolis interaction parameters are $\xi_a^{3,8} = 0.385$ cm^{-1}, $\xi_c^{3,8} = -0.095$ cm^{-1}. In addition, smaller interactions could be determined quantitatively as well [1,2]. Our results are in essential agreement with the original analysis by Luckhaus and Quack [3], which was, however, much less complete and precise.
We report *ab initio* calculations for this molecule on the MP2 level of theory with an aug-cc-pVDZ or a aug-cc-pVTZ basis set. Various subspaces of the potential energy and electric dipole moment hypersurfaces have been calculated in reduced normal coordinates including up to three dimensions. With these hypersurfaces we determined the corresponding vibrational absorption spectra, comprising transition wavenumbers and intensities. An analysis of the vibrational levels with an effective Hamiltonian was used to derive anharmonic constants.

References:

[1] S. Albert, H. Hollenstein, M. Quack, M. Willeke, Mol. Phys. **102**, 1671–1686 (2004)
[2] S. Albert, H. Hollenstein, M. Quack, M. Willeke, Proc. 18th Coll. High Resol. Mol. Spectroscopy, Dijon 2003, p. 87
[3] D. Luckhaus, M. Quack, Mol. Phys. 68, 745-758 (1989).

Title: Time and Time Reversal Symmetry in Quantum Chemical Kinetics

Researchers: M. Quack

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

Description:
Our work in quantum chemical kinetics has an experimental (spectroscopic) and a theoretical and computational component. The present review deals with the more theoretical aspects also in a broader context.
Irreversibility in molecular kinetics is first to be understood as a *de facto* breaking of time reversal symmetry. Some experimental results on the molecular short time quantum dynamics on the femtosecond to nanosecond time scale demonstrate the increase with time of entropy in single isolated molecules in the gas phase. Nevertheless, these processes show, in principle, time reversal symmetry. However, one finds fundamentally different dynamical behaviour for the quantum vibrational motion of molecules depending upon anharmonicity – at the same level of "quantization" – which is an important experimental result of our more recent research.
Not all forces of nature (strong nuclear force, weak nuclear force, electromagnetic force and gravitational force) show the separate discrete symmetries C, P, T.

References:

[1] M. Quack, in *Fundamental World of Quantum Chemistry. A Tribute to the Memory of Per-Olov Löwdin, Vol. 3* (Eds.: E. J. Brändas, E. S. Kryachko), Kluwer Adacemic Publishers, Dordrecht **(**2004**)**, 423-474

Title: Global Analytical Potential Energy Surface for Large Amplitude Nuclear Motions in Ammonia

Researchers: R. Marquardt*
K. Sagui*
W. Klopper**
M. Quack***

Institute/Group:
* Laboratoire de Chimie Théorique, Université de Marne-la-Vallée, 5, Bd.descartes
** Lehrstuhl für Theoretische Chemie, Institut für Physikalische Chemie ; Universität Karlsruhe (TH)
*** Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

An analytical, full-dimensional, and global representation of the potential energy surface of NH_3 in the lowest adiabatic electronic state is developed, and parameters are determined by adjustment to ab initio data and thermochemical data for several low-lying dissociation channels. The electronic structure is calculated at the CASPT2 level within an active space. The representation is compared to other recently published potential energy surfaces for this molecule. The present representation is distinguished by giving a qualitatively correct description of the potential energy for very large amplitude displacements of the nuclei from equilibrium. Other characteristic features of the present surface are the equilibrium geometries $r^{eq}(NH3) \approx 101.24$ pm, $r^{eq}(NH_2) \approx 102.60$ pm, $\alpha^{eq}(NH_3) \approx 106.67°$ and the inversion barrier at $r^{inv}(NH_3) \approx 99.80$ pm and 1781 cm^{-1} above the NH_3 minimum. The barrier to linearity in NH_2 is 11914 cm^{-1} above the $NH_2(^2B_1)$ minimum. While the quartic force field for NH_3 from the present representation is significantly different from that of the other potential energy surfaces, the vibrational structures obtained from perturbation theory are quite similar for all representations studied here.

References:

[1] R. Marquardt, K. Sagui, W. Klopper, M. Quack, Journal of Physical Chemistry B **109**, 8439-8451 (2005).

Title: Isotopic chirality and molecular parity violation

Researchers: R. Berger**
G. Laubender**
M. Quack*
A. Sieben*
J. Stohner***
M. Willeke*

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

Description:
Electroweak quantum chemistry leads to the prediction of a new isotope effect for molecules that are chiral as a result of isotopic substitution. The electron-nucleon interaction mediated by the Z-boson results in surprisingly large parity-violating energy differences $\Delta_{pv}E$ between isotopic enantiomers. For isotopic substitution of heavier atoms such as $^{35}Cl/^{37}Cl$ $\Delta_{pv}E$ is almost as large as in ordinary chiral molecules. This is important for spectroscopic experiments on parity violation. For the wider context see [2].

References:

[1] R. Berger, G. Laubender, M. Quack, A. Sieben, J. Stohner, M. Willeke, Angew. Chem. **117**, 3689-3693 (2005), Angew. Chem. Int. Edit. (Engl.) **44**, 3623-3626 (2005).
[2] M. Quack, Angew. Chem. Int. Ed. (Engl.) **114**, 4618-4630 (2002)

Title: High resolution Fourier transform spectroscopy of CH_2D_2 in the region 2350 – 2650 cm^{-1}: The bands $\nu_5 + \nu_7$, $2\nu_9$, $\nu_3 + \nu_4$, $\nu_3 + \nu_7$, and $\nu_5 + \nu_9$.

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

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

Description:
The IR spectrum of the CH_2D_2 molecule has been measured in the region of 2350 - 2650 cm^{-1} on a Bomem DA002 Fourier transform spectrometer with a resolution of 0.004 cm^{-1} (FWHM, apodized) and analyzed with a Hamiltonian model which takes into account resonance interactions between all vibrational states in that region. More than 3000 transitions have been assigned to the bands $2\nu_9$, $\nu_3 + \nu_4$, $\nu_5 + \nu_9$, $\nu_5 + \nu_7$ and $\nu_3 + \nu_7$ using ground state combination differences from the known ground state parameters. A set of 115 spectroscopic parameters for the excited vibrational states is obtained from a least squares adjustment. This reproduces the 646 initial upper ro-vibrational energies used in the fit with a d_{rms} = 0.0036 cm^{-1}. Extensive computations are carried out in the analysis.

References:

[1] O. N. Ulenikov, E. S. Bekhtereva, S. V. Grebneva, H. Hollenstein, M. Quack, Phys. Chem. Chem. Phys. **7**, 1142-1150 (2005).

Title: Isotope Selective Infrared Spectroscopy and Intramolecular Dynamics

Researchers: M. Hippler**
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Department of Chemistry, University of Sheffield, Sheffield S3 7HF

Description:
The title subject is reviewed with reference also to the theoretical and computational analysis of the spectra.

References:

[1] M. Hippler and M. Quack, "Isotope Selective Infrared Spectroscopy and Intramolecular Dynamics", Chapter 11 in "Isotope Effects in Chemistry and Biology, Part III Isotope Effects in Chemical Dynamics", pages 305 – 359, Ed. Amnon Kohen and Hans-Heinrich Limbach, Marcel Dekker Inc., New York 2005.

Title: Steps Towards Molecular Parity Violation in Axially Chiral Molecules: (I) Theory for Allene and 1,3-Difluoroallene

Researchers: M. Gottselig
M. Quack

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

Description:

In view of exploring possibilities for an experimental investigation of molecular parity violation we report quantum-chemical calculations of the parity-conserving and parity-violating potentials in the framework of electroweak quantum chemistry in allene C_3H_4 and 1,3-difluoroallene $C_3H_2F_2$, which is nonplanar and axially chiral in the electronic ground state but expected to be nearly planar and achiral in several electronically excited states. The parity-violating potentials E_{pv} for allene and 1,3-difluoroallene calculated with the multiconfiguration linear-response (MC-LR) approach of Berger and Quack [J. Chem. Phys. **112**, 3148 (2000)] show qualitatively similar behavior as a function of torsional angle τ with maximum values of about 0.5 pJ mol^{-1} for C_3H_4 and 2 pJ mol^{-1} for $C_3H_2F_2$. However, in the latter case they are asymmetrically shifted around $\tau = 90°$, with a nonzero value at the chiral equilibrium geometry resulting in a parity-violating energy difference between enantiomers $\Delta_{pv}E = E_{pv}(P) - E_{pv}(M) = 1.2\text{pJmol}^{-1}$ equivalent to about 10^{-13} cm^{-1}). The calculated barrier heights corresponding to the nonrigid (multiple, and in part chiral) transition states in 1,3-difluoroallene fall in the range of 180–200 kJ mol^{-1}. These high barriers result in hypothetical tunneling splittings much smaller than $\Delta_{pv}E$ and thus parity violation dominates over tunneling for the stereomutation dynamics in 1,3-difluoroallene. Therefore, $\Delta_{pv}E$ is predicted to be a spectroscopically measurable energy difference. Two of the lower excited electronic states of $C_3H_2F_2$ (^1A and ^3A) are calculated to be planar or quasiplanar, allowing, in principle, for spectroscopic state selection of states of well-defined parity. The results are discussed in relation to possible schemes of measuring parity violation in chiral molecules.

References:

[1] M. Gottselig, M. Quack, J. Chem. Phys. **123**, 84305-1 – 84305-11 (2005)

Title: Parity violation in chiral molecules

Researchers: M. Quack*
J. Stohner**

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

Description:
We briefly review the current status of the computational approach to electroweak quantum chemistry which includes the parity violating weak nuclear interaction. After a short introduction and discussion of current experimental efforts in measuring parity violation in chiral molecules, we outline the general theoretical background and recent approaches predicting order of magnitude increases in parity violating potentials. We then summarize current results on these increased values, the role of biomolecular chirality, calculation of properties, use of density functional theory, anharmonic vibrational and relativistic corrections, as well as a new isotope effect for isotopically chiral molecules.

References:
[1] M. Quack, J. Stohner, Chimia, **59**, 530 – 538 (2005)

Title: Modeling Weather and Climate on European and Alpine scales

Researchers: Bodo Ahrens, Andreas Dobler, Erich Fischer, Christoph Frei, Olivier Fuhrer, Joachim Gurtz, Martin Hirschi, Cathy Hohenegger, Simon Jaun, Jan Kleinn, Michael Litschi, Daniel Lüthi, Christoph Schär, Reinhard Schiemann, Jürg Schmidli, Sonia Seneviratne, Mark Verbunt, Pier Luigi Vidale, André Walser, Massimiliano Zappa

Institute/Group: Institute for Atmospheric and Climate Science, ETH Zürich
Group of Prof. Christoph Schär

Description:

Our research is directed towards continental and Alpine-scale weather and climate, with special focus on the water cycle. A broad continuum of temporal scales (from short-range weather forecasting to climate change) and horizontal resolutions (grid spacing between 1 to 50 kilometers) is considered. Regional climate processes are investigated with the help of two regional climate models (RCMs), namely the Climate LokalModell (CLM, running on the NEC SX-5 at CSCS), and the Climate High-Resolution Model (CHRM, running on the IBM system at CSCS). The dynamics of dry and moist atmospheric flow past realistic and idealized topography are investigated using a hierarchy of atmospheric models (e.g. LM and ARPS, both running on the NEC SX-5 at CSCS). Hydrological processes in intermediate and major catchments are investigated with the help of hydrological models (mostly the PREVAH model, running on local UNIX workstations).

Research on climate aspects is dedicated to the study of natural and anthropogenic climate variations on seasonal to centennial time scales. This work involves conducting comprehensive RCM numerical simulations. The main thrust of our recent work is dedicated towards better understanding and simulating the European summer climate, and towards assessing its sensitivity with respect anthropogenic greenhouse gas forcing. Previous results of our group regarding pronounced increases in interannual (year-to-year) variability have largely been confirmed by the work of several European research groups. Our research in this area is funded by the Swiss National Science Foundation (NCCR Climate) and the European Commission (project ENSEMBLES).

Research on weather aspects is motivated by the emergence of high-resolution cloud-resolving models. Such models offer promising prospects in numerical weather prediction as well as quantitative precipitation and flood forecasting. Our research uses state-of-the-art non-hydrostatic models to address predictability issues. Recent work on probabilistic precipitation forecasting is currently being extended towards the generation of probabilistic flood forecasting. We are also conducting idealized high-resolution experiments of flow past topography to study the dynamics of embedded convection, and are involved in the formulation of future atmospheric prediction models.

References: See list of publications.

Title: Efficient pricing under multiscale stochastic volatility models

Researchers: Norbert Hilber
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The Black and Scholes (BS) model, which relates derivative prices to current stock prices and quantifies risk through a constant volatility parameter, rests upon assumptions which turned out to be not longer sufficient to capture modern market phenomena. An extension of the BS model is to make the volatility a function of $d \geq 1$ stochastic processes, so-called "background driving processes" (BDP). Option pricing under such extensions leads to parabolic partial differential equations (PDE), if the BDP is a diffusion process, and to partial integro–differential equations (PIDE), if the BDP is a Lévy process. These PDEs/PIDEs are set in $d+1$ space dimensions and have to be solved numerically. Standard discretizations of such equations via Galerkin Finite Element Methods suffer from high complexity and poorly conditioned discrete equations.

The aim of the project is the development, analysis and implementation of a wavelet based sparse grid numerical scheme that breaks down the complexity of numerical asset pricing to the complexity of constant volatility. Embedded in the numerical scheme are discontinuous Galerkin time stepping as well as A-posteriori error estimators for given target functionals.

References:

[1] N. Hilber, A.M. Matache and C. Schwab, *Sparse wavelet methods for option pricing under stochastic volatility*, J. Comp. Fin. **8**(4) (2005) 1–42

Title: Modelisation of High Current Arc

Researcher: Patrick Huguenot
Prof. Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The disconnecting process in air/gas insulated generator circuit breaker (GCB) is accompanied with a highly ionsied plasma (electric arc) appearing between the arcing contacts.
The major issue of this project is to describe 3D behaviors of the burning arc during its high current phase of the switching process and calculate the pressure build up generated in the arcing chamber.
The physical model is given by the equations of magnetohydrodynamics (MHD). As full 3D simulations are very time consuming, the objective is to formulate a new mathematical model using the spectral method for the angular components. In this way, 3D results (non axisymmetric) will be achieved by resolving a set of 2D equations.
The "V&V" process (Validation and Verification) is part of the project: the mathematical model has to represent the physical events with sufficient accuracy (Validation), and the discretisation of this mathematical model has to represent the model with sufficient accuracy.
This "V&V" process will ensure that the simulation reproduces all known and observed.

Title: Generalized *hp*-FEM for Lattice Structures

Researchers: A. W. Rüegg
Ch. Schwab

Institute: Seminar for Applied Mathematics
Group: Department of Mathematics
ETH Zürich

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 [2]). 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 200020-100017/1.

References:

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

[2] A.W. Rüegg. A. Schneebeli, R. Lauper, *Generalized hp-FEM for Lattice Structures*, SAM-Research Report 2002-23

Title: FEM for Elliptic Problems with Stochastic Data

Researcher: R.A. Todor
P. Frauenfelder
Prof. Ch. Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Often the data of a PDE is either incompletely known or uncertain to some extent, which makes its description as a random field more realistic. The solution to such a PDE is, in general, a random field taking values in a suitable function space. Complete description of this random field requires knowledge of its joint probability densities, so that in applications one is often interested only in the first (expectation), second (correlation) and sometimes even higher order moments of the random solution. Deterministic PDEs for the moments of the random solution can be derived, but solving them poses serious difficulties due to their high-dimensional character. The project aims to develop efficient algorithms for the computation of various statistics of the solution to an elliptic PDE with stochastic data, and reduce thereby the apparently huge numerical complexity of such problems. More precisely,

a) for the problem with deterministic coefficients, but stochastic right hand side, we achive essentially the same scalability of the solution algorithm for the second (and higher) order moments as for the solution of the deterministic problem, using *sparse grids*.

b) for the problem with stochastic coefficients, we investigate several approaches: the Monte Carlo simulation, Perturbation algorithms and the stochastic Galerkin method. We develop strategies for complexity reduction based on *sparse interpolands* and *adaptivity*.

References:

[1] R.-A. Todor, *Sparse perturbation algorithms for elliptic PDE's with stochastic data*, ETH Dissertation (2005)

[2] P. Frauenfelder, Ch. Schwab, R.-A. Todor, *Finite elements for elliptic problems with stochastic coefficients*, Comput. Methods Appl. Mech. Engrg. **194** (2005), no. 2-5, 205–228

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
Department of Mathematics
ETH Zürich

Description:

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 and their generalization to less standard finite element approximations (edge elements, for instance) is far from being straightforward.

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. In addition it aims at developing robust DD strategies for three dimensional electromagnetic problems. 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.

Extensive numerical tests showing the performance and robustness of domain decomposition preconditioners for the solution of algebraic linear systems arising from *hp* finite element approximations of scalar elliptic problems on geometrically refined boundary layer meshes in two and three dimensions have been performed. In addition, a novel dual-primal FETI strategy has been developed for three-dimensional edge element approximations.

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

Title: First Exit Time of Diffusion: A Computational Approach

Researcher: Christoph Winter (SAM)
Dr. Pierre Patie (RiskLab)
Prof. Christoph Schwab (SAM)

Institute: Seminar for Applied Mathematics \ RiskLab
ETH Zürich

Description:

First exit time distributions are required in many phenomena in chemistry, physics, biology and neurology where systems often depend on a random variable reaching some threshold value. In quantitative finance, such questions arise in different practical issues such as the pricing of path-dependent options and credit risk. Despite the importance and wide applications, explicit analytic solutions to such problems are not known except for very few instances. Therefore, Monte-Carlo methods are mostly used. But here the error only decreases like $O(N^{-\frac{1}{2}})$ if one uses a work of N operations. We present a PDE approach where the not exit probability u is the solution of the Kolmogoroff equation for diffusions in high dimensions

$$\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} a_{i,j}\frac{\partial^2 u}{\partial x_i x_j} + \sum_{i=1}^{d} b_i \frac{\partial u}{\partial x_i}$$

over some bounded domain $A \in \mathbb{R}^d$ with zero boundary conditions. The initial conditions are $u(0,x) = 1 \quad \forall x \in A$.

Straightforward application of standard numerical schemes fails due to the so-called 'curse of dimension': the number of degrees of freedom on a tensor product Finite Element mesh of width h in dimension d grows like $O(h^{-d})$ as $h \to 0$. This can be avoided by using sparse tensor products and an *hp*-Discontinous Galerkin time stepping procedure as in [1]. The resulting algorithm requires $N = O(h^{-1}|\log h|^{2d+6})$ operations and provides an error of $O(N^{-p})$ where p is the degree of the finite elements which can be any integer ≥ 1.

References:

[1] T. von Petersdorff and C. Schwab, *Numerical Solution of Parabolic Equations in High Dimensions*, M2AN Math. Model. Numer. Anal. 38 (2004)

Title: Frustrated Quantum Spin Systems

Researchers: G. Schmid, S. Wessel, M. Troyer, M. Sigrist [*]
A. Läuchli[**]

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

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.

References:

- A. Läuchli, G. Schmid and M. Troyer, Phys. Rev. B **67**, 100409 (R) (2003)
- A. Läuchli, J.C. Domenge, C. Lhuillier, P. Sindzingre and Matthias Troyer,

Phys. Rev. Lett. **95**, 137206 (2005)

Title: Numerical investigation of strongly correlated systems

Researchers: S. Wessel, M. Sigrist, M. Troyer, T.M. Rice[*]
A. Läuchli [**],
H.-D. Chen,, S.-C. Zhang, [***]
F. Alet, S. Capponi, D. Poilblanc [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] IRRMA, EPF Lausanne
[***] Stanford University, USA
[****] Université de Toulouse

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.

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- A. Koga, N. Kawakami, T.M. Rice and M. Sigrist ,Physica B **359**, 1366 (2005).

Title: Bosonic Lattice Supersolids

Researchers: G. Schmid, M. Troyer [*]
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F. Alet [***]
P. Sengupta, L. Pryadko[****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
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[***] Université de Toulouse, France
[****] UC Riverside, USA

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 this project we study unusual phases occurring in such bosonic lattice models, where the "supersolid" phase which simultaneously shows superfluidity and crystalline order is of special interest.

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- P. Sengupta, L. Pryadko, F. Alet, G. Schmid and Matthias Troyer, Phys. Rev. Lett. **94**, 207202 (2005).
- S. Wessel and Matthias Troyer, Phys. Rev. Lett. **95**, 127205 (2005)

Title: Quantitative modeling of quantum magnets

Researchers: A. Läuchli, M. Troyer, F. Alet [*]
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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

C. Yasuda, S. Todo, K. Hukushima, F. Alet, M. Keller, Matthias Troyer, H. Takayama, Phys. Rev. Lett. **94**, 217201 (2005)

B. Pedrini, J. L. Gavilano, D. Rau, H. R. Ott, S. M. Kazakov, J. Karpinski, S. Wessel, Phys. Rev. B **70**, 024421 (2004)

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N. Fukushima, A. Honecker, S. Wessel, W. Brenig, Phys. Rev. B **69**, 174430 (2004)

N. Fukushima, A. Honecker, S. Wessel, S. Grossjohan, W. Brenig, Physica B **359-361,** 1409 (2005)

Title: Quantum criticality

Researchers: S. Wessel M. Troyer [*]
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S. Sachdev [***]
O. Nohadani, S. Haas [****]

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

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:

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- B. Normand, M. Matsumoto, O. Nohadani, S. Wessel, S. Haas, T.M. Rice, and M. Sigrist, Conference Proceedings, J. Phys. Condens. Matter, Vol. 16, No. 11, S867 (2003).

Title: Topologically protected quantum bits

Researchers: D. Ivanov, P. Dayal, M. Troyer, G. Blatter [*]
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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

Our most recent work concentrates on a more practical device which still has some of the valuable topological features preserved. We propose a design for a qubit involving four superconducting islands in the topology of a symmetric tetrahedron, uniformly frustrated with one-half flux-quantum per loop and one-half Cooper-pair per island. This structure emulates a noise-resistant spin-1/2 system in a vanishing magnetic field. The flux-frustration boosts quantum fluctuations and relieves the constraints on junction fabrication. Variability of manipulation and optimized readout through single-shot measurements are additional benefits of this design. For specific limits, the spectrum of this `3-body' quantum system can be found analytically using quasi-classical methods, but an accurate and general determination requires numerical solution. This has been implemented successfullyusing exact diagonalization techniques (Lanczos) both in the charge and phase representation of the Hamiltonian.

References:

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Title: New Quantum Monte Carlo Algorithms

Researchers: **P. Corboz, E. GUll**M. Troyer, P. Werner [*]
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S. Wessel [***]
F.F. Assaad [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Toulouse, France
[***] Universität Stuttgart, Germany
[***] 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 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. We also investigated the generalization of detailed balance equations required during the Quantum Monte Carlo simulations. We obtain accordingly improved "directed loop" algorithms, which are shown to be more efficient than conventional ones.

A new project started recently concerns the investigation of new algorithm for fermionic quantum Monte Carlo simulations.

References:

M. Troyer, S. Wessel and F. Alet, Phys. Rev. Lett. **90**, 120201 (2003).

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S. Wessel, S. Trebst, and M. Troyer, SIAM Multiscale Model. Simul. **4**, 237 (2005)

F. F. Assaad, P. Werner, P. Corboz, E. Gull and M. Troyer, Phys. Rev. B (2005) in press

Title: Flat-Histogram Algorithms

Researchers: P. Dayal, S. Trebst, M. Troyer, S. Wessel, D. Wuertz [*]
S. Sabhapandit, S. Coppersmith [**]
D. Huse [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Department of Physics, University of Madison, USA
[***] Princeton University, USA

Description:

When studying phase transitions the traditional Metropolis algorithm becomes inefficient when the temperature approaches the critical temperature of the transition. For second order phase transitions the problem of ``critical slowing down'' -- a rapid divergence of the number of Monte Carlo steps needed to obtain a subsequent uncorrelated configuration -- was solved more than a decade ago by cluster update algorithms. At first order transitions and in systems with many local minima of the free energy, such as frustrated magnets or spin glasses, there exists the similar problem of long tunneling times between local minima. Recently proposed flat histogram methods produced promising results to effectively study first order phase transitions in these systems as well.

By studying the optimal scaling of flat-histogram methods with system size for classical 2D and 3D Ising models we determined a lower algorithmic bound for all flat-histogram methods such as Wang-Landau sampling, multicanonical sampling, tempering and broad histograms. For the 2D spin glass we found severe limitations in the form of exponential scaling and fat-tailed Frechet distributions of the tunneling time, the relevant time scale when sampling the full energy range in a multicanonical simulation.

We then developed an optimized ensembles, gaining orders of magnitude over the flat histogram and multicanonical ensembles.

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- Simon Trebst, Emanuel Gull and Matthias Troyer, J. Chem. Phys. (2005), in press

Title: Simulations of novel exotic phases of matter

Researchers: F. Alet. S. Trebst, M. Troyer

Institute/Group: Theoretische Physik, ETH Zürich

Description:

Novel states of matter with fractional quantum numbers, where an electron effectively splits up into smaller parts, each carrying only parts of the mass or charge of the original electron, have been a vivid research topic within condensed matter physics, propelled by the discovery of high temperature superconductivity and the fractional quantum hall effect.

The central role of excitations carrying a fractional charge in these novel quantum phases has been addressed in theoretical works over the years. Related topological states have recently been found to be promising candidates for the physical implementation of qubits, the elementary building units of a quantum computer. What has been missing so far are detailed numerical investigations if these proposed exotic phases are actually realized in realistic model.

We develop novel quantum simulation algorithms to study microscopic models and search for these fractionalized states with explicit macroscopic topological order to obtain the needed definitive proof of existence of these phases through high-performance numerical work.

References:

F. Alet, J. L. Jacobsen, G. Misguich, V. Pasquier, F. Mila and M. Troyer,. Rev. Lett. **94**, 235702 (2005)

Title: NP-hardness of the negative sign problem of quantum Monte Carlo simulations

Researchers: M. Troyer [*]
U.-J. Wiese [**]

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

Description:

Quantum Monte Carlo simulations, while being efficient for bosons and non-frustrated quantum magnets, suffer from the infamous ``negative sign problem'' when applied to fermions or frustrated magnets -- causing an exponential increase of the computing time with the number of particles. A polynomial time solution to the sign problem is highly desired, since it would provide an unbiased and numerically exact method to simulate correlated quantum systems. Here we argue, however, that such a solution is almost certainly unattainable, by showing that it is NP-hard, implying that a generic solution of the sign problem would also solve all NP-complete problems in polynomial time.

References:

- M. Troyer and U.-J. Wiese, Phys. Rev. Lett. **94**, 170201 (2005).

Title: Simulations of trapped ultra-cold atoms

Researchers: A. Esposito, H.G. Katzgraber, S. Trebst, M. Troyer [*]
G.G. Batrouni [**]
F. Alet [***]
S. Wessel [****]
P. Zoller [*****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Nice, France
[***] Université de Toulouse, France
[****] Universität Stuttgart, Germany
[*****] Universität Innsbruck, Austria

Description:

In order to study the Mott-transition observed in trapped atomic gases within an optical lattice we perform Monte Carlo simulations of the bosonic Hubbard model, which is an appropriate lattice model in the strongly interacting regime. We have improved the efficiency of the underlying algorithm, by using a directed loop scheme, which is has bounce-free regions also for the soft-core bosonic case. In addition to studying trapping geometries in various dimensions (1, 2, and 3), we are also investigating the dimensional crossover observed within optical lattices with anisotropic hopping matrix elements, investigating the "Tonks gas" limit of strong repulsion, and properties of fermionic atoms loaded into optical lattices.

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Simon Trebst, Ulrich Schollwöck, Matthias Troyer and Peter Zoller, Preprint,

Helmut G. Katzgraber, A. Espositio and Matthias Troyer, Preprint,

Title: Simulations of dissipative quantum systems

Researchers: P. Werner, M. Troyer [*]
S. Chakravarty [**]
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Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California, Los Angeles
[***] Yale University

Description:

Dissipation effects due to coupling to the environment can substantially alter the nature and universality class of a quantum phase transition. In this project we develop new quantum Monte Carlo algorithms for the simulation of dissipation-driven quantum phase transitions, exceeding the performance of standard methods by orders of magnitudes. This allows for the first time the accurate investigation of these quantum phase transitions in systems such as dissipative spin chains, quantum wires, single electron boxes or shunted Josephson junctions.

References:

S. Sachdev, P. Werner, M. Troyer, Phys. Rev. Lett. **92**, 237003 (2004)

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P. Werner and M. Troyer, Preprint, J. Stat. Mech. P01003 (2005).

Philipp Werner, Gil Refeael and Matthias Troyer J. Stat. Mech. (2005), in press

Title: The ALPS project

Researchers: F. Alet, P. Dayal, M. Körner, S. Trebst, M.Troyer, P. Werner [*]
M. Rütti, W.P. Petersen [**]
and the ALPS collaboration (http://alps.comp-phys.org/) [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] SAM, ETH Zürich
[***] and many other institutions

Description:

Unlike in other physics communities there have been no "community codes" available to study strongly correlated quantum mechanical systems with researchers writing individual codes, adjusting them for specific needs of new projects and thereby investing weeks to months in software development. The ALPS project (Algorithms and Libraries for Physics Simulations) is an open source effort aiming at simplifying the development of simulation codes for strongly correlated quantum mechanical systems. A set of libraries of differing technical level have been implemented to support researchers to develop model independent, generic software, including basic libraries for lattice structures, quantum models, error analysis, parallelization of simulations and XML tools. On top, generic application programs are offered to non-experts, such as Monte Carlo for classical magnets, Quantum Monte Carlo for quantum magnets and bosons (stochastic series expansion (SSE), continuous time worm algorithm) as well as exact and full diagonalization. Future applications will include Density Matrix Renormalization Group (DMRG) and Linked Cluster Series Expansions.

References:

F. Alet, P. Dayal, H.G. Evertz, A. Grzesik, A. Honecker, M. Körner, A. Läuchli, S. Manmana, I. McCulloch, R. Noack, G. Schmid, U. Schollwöck, S. Todo, S. Trebst, Matthias Troyer, P. Werner, S. Wessel (ALPS collaboration), J. Phys. Soc. Jpn. Suppl. **74**, 30 (2005).

http://alps.comp-phys.org/

Title: Simulation of Electron Source
for Next-Generation X-ray Free Electron Laser

Researchers: A. Candel, M. Troyer [*]
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Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Paul Scherrer Institut, PSI Villigen

Description:

Advanced next-generation synchrotron radiation sources are needed for future scientific research. To keep costs low, while delivering highest possible brilliance beams, elaborate compact setups are necessary. A new type of compact X-ray free electron laser under consideration at PSI demands very high quality standards of the electron beam. This is far beyond current possibilities and expected only to be realizable with a new generation of electron source, consisting of nanostructured microcathodes, paired with extremely high accelerating gradients.
In order to gain theoretical understanding of this physically extreme regime, we need unpreceded simulation accuracy. We have developed a massive parallel relativistic 3D particle-in-cell code, based on the finite integration technique. First studies on the optimal electron source setup have been conducted and show the suitability of the code for our purposes.

References:

A. Candel, M. Dehler, M. Troyer, Preprint, Submitted to Nuclear Instruments and Methods in Physics Research

Title: Ramping fermions in optical lattices across a Feshbach resonance

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

Institute/Group: *Theoretische Physik, ETH Zürich

Description:

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

References:

H. G. Katzgraber, A. Esposito, and M. Troyer, Phys. Rev. B, submiited.

Title: Spin glasses in a field

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

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

Description:

In order to test the existence of a spin-glass phase in a field at finite temperatures, we perform Monte Carlo simulations of the one-dimensional long-range Ising spin glass with power-law interactions in the presence of a (random) field. By tuning the exponent of the power-law interactions, we are able to scan the full range of possible behaviors from the infinite-range (Sherrington-Kirkpatrick) model to the short-range model. A finite-size scaling analysis of the correlation length indicates that there is no transition in a field with non-mean field critical behavior at zero field. This suggests that there is no Almeida-Thouless line for short-range Ising spin glasses away from the mean-field regime.

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

References:

A. P. Young and H. G. Katzgraber, Phys. Rev. Lett. 93, 207203 (2005)

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

H. G. Katzgraber and G. T. Zimanyi, Phys. Rev. Lett, submitted.

Title: Simulation and optimization of photonic crystals and metamaterials

Researchers: Christian Hafner
Jasmin Smajic
Cui Xudong
Rüdiger Vahldieck
Kakhaber Tavzarashvili
Nicolas Guérin.

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

Description:

Photonic crystals or more general metamaterials are promising concepts for electromagnetics and optics. By a proper design of such micro- and nanostructures one may obtain material properties that do not exist in nature, for example, a negative index of refraction or that are much more pronounced than the properties observed in natural media, for example, chirality. By combining and doping of metamaterials, new devices may be obtained. The design of such structures is numerically very demanding and requires accurate and reliable software for the analysis and optimization. Currently, we are developing various codes for these tasks based on different techniques, namely for the simulation: The Multiple Multipole Program (MMP), a frequency-domain boundary method, Method of Moments (MoM) codes, and time-domain methods such as FDTD; and for the optimization: Genetic Algorithms (GA) including microGA and Evolutionary Strategies (ES) with special table-based statistical analysis for efficient real and binary optimizations. We apply these codes to various applications such as perfect waveguide bends, light splitters, filters, mode converters, etc.

References:

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[4] Christian Hafner, "Drude Model Replacement by Symbolic Regression", *J. Comp. Theo. Nanoscience*, Vol. 2, No. 1, March 2005, pp 88-980.
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Title: A hybrid drift-diffusion—TLM method for analysis of traveling-wave photodetectors

Researchers: Damir Pasalic
Rüdiger Vahldieck

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

Description:

Traveling-wave photodetectors (TWPDs), having broad bandwidth and high output saturation current, are key components of modern optical communication systems. As optical amplification becomes more widely employed in such systems, the photodetectors capable of maintaining high efficiency and broad bandwidth under high optical illumination are of special interest. As complexity of the TWPDs increases, the standard means of their analysis, such as the equivalent circuit model, are not adequate any more. Therefore, there is an increased interest for a more general, numerical approach to their analysis. In this project, we are developing a new, hybrid method for rigorous analysis of TWPDs of general geometry. The method is a combination of a 2D drift-diffusion semiconductor analysis and a full-wave EM simulator. As a result of the semiconductor analysis, currents at the device's cross-section are obtained. Then, they are used as the source currents in a full-wave EM simulation of the structure to obtain microwave parameters of interest, such as microwave phase velocity and S-parameters at the interface with the embedding microwave circuit. For full-wave EM simulations, the frequency-domain TLM method is employed.

References:

D. Pasalic and R. Vahldieck, "A hybrid drift-diffusion—TLM analysis of traveling-wave photodetectors," accepted for publication in *IEEE Trans. Microwave Theory Tech.*

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

Researchers: Christophe Fumeaux
Dirk Baumann
Krishnaswamy Sankaran
Rüdiger Vahldieck

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

Description:

In this project, a 3D solver for accurate numerical simulations of electromagnetic (EM) fields is developed based on the Finite-Volume Time-Domain (FVTD) method. As opposed to the Finite-Difference Time-Domain (FDTD) method applied in a Cartesian grid, the FVTD method allows the use of fully unstructured meshes (e.g. made of tetrahedrons). This represents a significant advantage for the resolution of small details within larger structures, for the conformal modeling of curved surfaces, and in connection with different materials. For a general EM problem, most of the FVTD computational domain is meshed with cells of typical linear dimensions corresponding to a tenth of the shortest wavelength of interest, while smaller cells are only required in restricted areas where fine structural details need to be resolved.
The present project considers the development of the FVTD method in two complementary lines of investigation. The first aspect of the project regards the theoretical development of the method: FVTD is characterized by a great diversity of related algorithms with potentially superior accuracy and/or increased computational efficiency. Along this line, different variations of the spatial and temporal approximations (e.g. local time stepping [1]) are investigated. Other aspects, such the definition of ports for S-parameter extraction [5] and the development of accurate absorbing boundary conditions (ABC) are also considered. In the second line of investigation, the FVTD method is applied to the solution of challenging EM problem, in particular to the characterization of complex antenna structures [2][3][4].

References:

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[2] D. Baumann, C. Fumeaux, P. Leuchtmann, R. Vahldieck, "Finite-Volume Time-Domain (FVTD) modeling of a broadband double-ridged horn antenna", *International Journal of Numerical Modelling: Electronic Networks, devices and fields*, vol. **17**, 285-298 (April 2004)
[3] C. Fumeaux, D. Baumann, R. Vahldieck, "Advanced FVTD simulation of dielectric resonator antennas and feed structures", *ACES Journal*, vol. **19**(3), 155-164 (November 2004) (Awarded ACES 2004 best journal paper)
[4] C. Fumeaux, D. Baumann, R. Vahldieck, "FVTD Characterization of Substrate Effects for Archimedean Spiral Antennas in Planar and Conformal Configurations", Accepted for publication in the *ACES Journal* (2005)
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Title: Methane clustering in explicit water: Effect of urea on hydrophobic interactions

Researchers: Chris Oostenbrink
Wilfred F. van Gunsteren

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

Description:

Methane aggregation in water has been studied by simulation for thirteen systems of different sizes and compositions. It was found that favourable cluster formation only occurs after a certain critical cluster size has been reached. The effect of urea on hydrophobic clustering was studied for two urea concentrations. High urea concentrations result in slightly enhanced methane cluster formation, rather than a reduction of the hydrophobic effect. Structural analysis of the Kirkwood–Buff excess coordination and preferential solvation points at a mechanism in which urea pushes the methane into the water, locally increasing methane concentration and hence promoting cluster formation.

References: Phys.Chem.Chem.Phys. **7** (2005) 53-58

Title: Molecular Dynamics simulations and free energy calculations of netropsin and distamycin binding to an AAAAA DNA binding site

Researchers: Jozica Dolenc*
Chris Oostenbrink
Joze Koller*
Wilfred F. van Gunsteren

Institute/Group: *Faculty of Chem. Techn., University of Ljubljana, Ljubljana, Slovenia
Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland

Description:

Molecular dynamics simulations have been performed on netropsin in two different charge states and on distamycin binding to the minor groove of the DNA duplexd(CGCGAAAAACGCG)·d(CGCGTTTTTCGCG). The relative free energy of binding of the two noncovalently interacting ligands was calculated using the thermodynamic integration method and reflects the experimental result. From 2 ns simulations of the ligands free in solution and when bound to DNA, the mobility and the hydrogen-bonding patterns of the ligands were studied, as well as their hydration. It is shown that even though distamycin is less hydrated than netropsin, the loss of ligand–solvent interactions is very similar for both ligands. The relative mobilities of the ligands in their bound and free forms indicate a larger entropic penalty for distamycin when binding to the minor groove compared with netropsin, partially explaining the lower binding affinity of the distamycin molecule. The detailed structural and energetic insights obtained from the molecular dynamics simulations allowfor a better understanding of the factors determining ligand–DNA binding.

References: Nucleic Acids Research **33** (2005) 725-733

Title: An Improved Nucleic-Acid Parameter Set for the GROMOS Force Field

Researchers: Thereza A. Soares
Philippe H. Hünenberger
Mika A. Kastenholz
Vincent Kräutler
Thomas Lenz
Roberto D. Lins
Chris Oostenbrink
Wilfred F. van Gunsteren

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

Description:

Over the past decades, the GROMOS force field for biomolecular simulation has primarily been developed for performing molecular dynamics (MD) simulations of polypeptides and, to a lesser extent, sugars. When applied to DNA, the 43A1 and 45A3 parameter sets of the years 1996 and 2001 produced rather flexible double-helical structures, in which the Watson–Crick hydrogen-bonding content was more limited than expected. To improve on the currently available parameter sets, the nucleotide backbone torsional-angle parameters and the charge distribution of the nucleotide bases are reconsidered based on quantum-chemical data. The new 45A4 parameter set resulting from this refinement appears to perform well in terms of reproducing solution NMR data and canonical hydrogen bonding. The deviation between simulated and experimental observables is now of the same order of magnitude as the uncertainty in the experimental values themselves.

References: J. Comput. Chem. **26** (2005) 725-737

Title: Free energies of ligand binding for structurally diverse compounds

Researchers: Chris Oostenbrink
Wilfred F. van Gunsteren

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

Description:

The one-step perturbation approach is an efficient means to calculate many relative free energies from a common reference compound. Combining lessons learned in previous studies, an application of the method is presented that allows for the calculation of relative binding free energies for structurally rather diverse compounds from only a few simulations. Based on the well known statistical-mechanical perturbation formula, the results do not require any empirical parameters, or training sets, only limited knowledge of the binding characteristics of the ligands suffices to design appropriate reference compounds. Depending on the choice of reference compound, relative free energies of binding rigid ligands to the ligand-binding domain of the estrogen receptor can be obtained that show good agreement with the experimental values. The approach presented here can easily be applied to many rigid ligands, and it should be relatively easy to extend the method to account for ligand flexibility. The free-energy calculations can be straightforwardly parallelized, allowing for an efficient means to understand and predict relative binding free energies.

References: PNAS **102** (2005) 6750-6754

Title: The Relative Stability of Homochiral and Heterochiral Alanine Dipeptides. Effects of Perturbation Pahtways and Force-Field Parameters on Free Energy Calculations

Researchers: Yu Zhou*/**
Chris Oostenbrink
Wilfred F. van Gunsteren
Wilfred R. Hagen*
Simon R. de Leeuw**
Jaap A. Jongejan*

Institute/Group: Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
*Dept. of Biotechnology, Delft University of Technology, Delft, The Netherlands
**Physical Chemistry and Molecular Thermodynamics, Delft University of Technology, Delft, The Netherlands

Description:

The relative stability of homochiral (*D,D* or *L,L*) and heterochiral (*D,L* or *L,D*) dipeptides may have been a decisive factor in the evolutionary propagation of a symmetry-breaking event leading to the present-day predominance of L-amino acids in natural proteins. Kinetic resolution in the solid-phase peptide synthesis of blocked dialanine suggests the activation free energy difference of formation of (*D,D* or *L,L*)- and (*D,L* or *L,D*)-dialanine to be 0.22 $kJmol^{-1}$ in favour of the formation of the homochiral dipeptide. Computer simulation studies were performed on water-solvated dialanine, applying a thermodynamic integration protocol using the GROMOS force field. Five different pathways and three force-field parameter sets have been used to assess the possibility of a computational prediction of the chiral preference. Inversion of the configuration around either one of the C_α-atoms by changing the improper dihedral angle with concomitant relaxation of the bond angles, leads to an excellent reproduction of the experimental result.

References: Mol. Phys. **103** (2005) 1961-1969

Title: Efficient Calculation of Many Stacking and Pairing Free Energies in DNA from a Few Molecular Dynamics Simulations

Researchers: Chris Oostenbrink
Wilfred F. van Gunsteren

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

Description:

Through the use of the one-step perturbation approach, 130 free energies of base stacking and 1024 free energies of base pairing in DNA have been calculated from only five simulations of a nonphysical reference state. From analysis of a diverse set of 23 natural and unnatural bases, it appears that stacking free energies and stacking conformations play an important role in pairing of DNA nucleotides. On the one hand, favourable pairing free energies were found for bases that do not have the possibility to form canonical hydrogen bonds, while on the other hand, good hydrogen-bonding possibilities do not guarantee a favourable pairing free energy if the stacking of the bases dictates an unfavourable conformation. In this application, the one-step perturbation approach yields a wealth of both energetic and structural information at minimal computational cost.

References: Chem. Eur. J. **11** (2005) 4340-4348

Title: A Photoinducible β-Hairpin

Researchers: Andreas Aemisseger*
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Wilfred F. van Gunsteren
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*Laboratory of Organic Chemistry, ETH Hönggerberg, Zürich, Switzerland

Description:

A photochromic azobenzene linker was incorporated as a turn element into an amino acid sequence known to fold into a *β*-hairpin structure in aqueous solution. Oligomer formation when the linker was in its thermodynamically favored trans form prohibited structure determination. Light-induced conformational change of the linker to the cis form led to the formation of monomers which exhibited a well-defined *β*-hairpin structure as determined by ^{1}H NMR. The rate of the light-induced cis-to-trans isomerization of the azobenzene-containing peptide was 30% slower compared to the unsubstituted chromophore. These results suggest that suitably substituted azobenzenes can be used as photoinducible turn elements to investigate and control the folding and stability of *β*-sheets.

References: JACS 127 (2005) 2929-2936

Title: Use of Molecular Dynamics in the Design and Structure Determination of a Photoinducible β-Hairpin

Researchers: Vincent Kräutler
Andreas Aemissegger*
Philippe H. Hünenberger
Donald Hilvert*
Tomas Hansson
Wilfred F. van Gunsteren

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

Description:

The study presented here consists of three parts. In the first, the ability of a set of differently substituted diazobenzene-based linkers to act as photoswitchable β-turn building blocks was assessed. A 12-residue peptide known to form β-hairpins was taken as the basis for the modeling process. The central (β-turn) residue pair was successively replaced by six symmetrically ((*o,o*), (*m,m*), or (*p,p*)) substituted (aminomethyl/carboxymethyl or aminoethyl/carboxyethyl) diazobenzene derivatives leading to a set of peptides with a photoswitchable backbone conformation. The folding behavior of each peptide was then investigated by performing molecular dynamics simulations in water (4ns) and in methanol (10ns) at room temperature. The simulations suggest that (*o,o*)- and (*m,m*)-substituted linkers with a single methylene spacer are significantly better suited to act as photoswitchable β-turn building blocks than the other linkers examined in this study. The peptide containing the (*m,m*)-substituted linker was synthesized and characterized by NMR in its *cis* configuration. In the second part of this study, the structure of this peptide was refined using explicit-solvent simulations and NOE distance restraints, employing a variety of refinement protocols (instantaneous and time-averaged restraining as well as unrestrained simulations). We show that for this type of systems, even short simulations provide a significant improvement in our understanding of their structure if physically meaningful force fields are employed. In the third part, unrestrained explicit-solvent simulations starting from either the NMR model structure (75ns) or a fully extended structure (25ns) are shown to converge to a stable β-hairpin. The resulting ensemble is in good agreement with experimental data, indicating successful structure prediction of the investigated hairpin by classical explicit-solvent molecular dynamics simulations.

References: JACS 127 (2005) 4935-4942

Title: An approximate but fast method to impose flexible distance constraints in molecular dynamics simulations

Researchers: Markus Christen
Wilfred F. van Gunsteren

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

Description:

A fast but approximative method to apply flexible constraints to bond lengths in molecular dynamics simulations is presented and the effects of the approximation are investigated. The method is not energy conserving, but coupling to a temperature bath results in stable simulations. The high frequencies from bond-length vibrations are successfully removed from the system while maintaining the flexibility of the bonds. As a test liquid neopentane is simulated at different pressures. Energetic and dynamic properties are not affected by the new flexible constraint simulation method.

References: J. Chem. Phys. **122** (2005) on-line

Title: Accounting for polarization in molecular simulation

Researchers: Haibo Yu*
Wilfred F. van Gunsteren

Institute/Group: Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland
*Dept of Chemistry, University of Wisconsin, Madison, Wisconsin, USA

Description:

Polarization plays an important role in the energetics of molecular systems, not the least in biomolecular systems. Most computer simulation studies of such systems do not treat electronic polarisability explicitly, but only implicitly using effective charges, dielectric permittivities or continuum electrostatics methods. Yet, the introduction of explicit polarisability into biomolecular models and force fields is unavoidable when more accurate simulation results are to be obtained. Various ways to account for polarisability in (bio)molecular simulation are reviewed with an eye to striking a balance between accuracy on the one hand and simplicity and computational efficiency on the other. The various choices to be made are listed and discussed. The most promising approach, the so-called Charge-On-Spring type of models, is treated in more detail and applied to liquid water as an example. Its implementation in the GROMOS biomolecular simulation software is sketched.

References: in press (*Comput.Phys.Commun.)*

Title: Interpreting NMR Data for β-peptides using Molecular Dynamics Simulations

Researchers: Daniel Trzesniak
Alice Glättli
Bernhard Jaun*
Wilfred F. van Gunsteren

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

Description:

NMR is one of the most used techniques to resolve structure of proteins and peptides in solution. However, inconsistencies may occur due to the fact that a polypeptide may adopt more than one conformation. Since the NOE distance bounds and ^{3}J-values used in such structure determination represent a non-linear average over the total ensemble of conformers, imposition of NOE or ^{3}J-value restraints to obtain one unique conformation is not an appropriate procedure in such cases. Here we show that unrestrained MD simulation of a solute in solution using a high-quality force field yields a conformational ensemble that is largely compatible with the experimental NMR data on the solute. Four 100 ns MD simulations of two forms of a nine residue *β*-peptide in methanol at two temperatures produced conformational ensembles that were used to interpret the NMR data on this molecule and resolve inconsistencies between the experimental NOEs. The protected and unprotected forms of the *β*-peptide adopt predominantly a *12/10*-helix in agreement with the qualitative interpretation of the NMR data. However, a particular NOE was not compatible with this helix indicating the presence of other conformations. The simulations showed that 3_{14}-helical structures were present in the ensemble of the unprotected form and that their presence correlates with the fulfillment of the particular NOE. The MD conformational ensembles allowed for a detailed and consistent interpretation of the experimental data and showed the small but specific conformational differences between the protected and unprotected forms of the peptide.

References: in press (*JACS)*

Title: On the Influence of Charged Side Chains on the Folding–Unfolding Equilibrium of β-Peptides: A Molecular Dynamics Simulation Study

Researchers:
Alice Glättli
Xavier Daura*
Pascal Bindschädler**
Bernhard Jaun**
Yogesh R. Mahajan**
Raveendra I. Mathad**
Magnus Rueping**
Dieter Seebach**
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Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
*Universitat Autonoma de Barcelona, Bellaterra, Spain
**Laboratory of Organic Chemistry, ETH Hönggerberg, Zürich, Switzerland

Description:

The influence of charged side chains on the folding–unfolding equilibrium of β-peptides was investigated by means of molecular dynamics simulations. Four different peptides containing only negatively charged side chains, positively charged side chains, both types of charged side chains (with the ability to form stabilizing salt bridges) or no charged side chains were studied under various conditions (different simulation temperatures, starting structures and solvent environment). The NMR solution structure in methanol of one of the peptides (A) has already been published; the synthesis and NMR analysis of another peptide (B) is described here. The other peptides (C and D) studied herein have hitherto not been synthesized. All four peptides A–D are expected to adopt a lefthanded 3_{14}-helix in solution as well as in the simulations. The resulting ensembles of structures were analyzed in terms of conformational space sampled by the peptides, folding behavior, structural properties such as hydrogen bonding, side chain–side chain and side chain–backbone interactions and in terms of the level of agreement with the NMR data available for two of the peptides. It was found that the presence of charged side chains significantly slows down the folding process in methanol solution due to the stabilization of intermediate conformers with side chain–backbone interactions. In water, where the solvent competes with the solute–solute polar interactions, the folding process to the 3_{14}-helix is faster in the simulations.

References: in press (*Chemistry – A European Journal*)

Title: Molecular Dynamics Study of the Stabilities of Consensus Designed Ankyrin Repeat Proteins

Researchers: Haibo Yu*
Andreas Kohl**
H.Kaspar Binz**
Andreas Plückthun**
Markus G. Grütter**
Wilfred F. van Gunsteren

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*Dept. of Chemistry, University of Wisconsin, Madison, Wisconsin, USA
**Biochem. Institut, Universität Zürich, Zürich, Switzerland

Description:

Homology modelling and molecular dynamics (MD) simulations with explicit solvent have been performed for two designed ankyrin repeat (AR) proteins (E3_5 and E3_19). These two proteins are highly homologous (with about 87% sequence identity) and their crystal structures have a Cα atom-positional root-mean-square difference of about 0.14nm. Experimentally it was found that E3_5 is considerably more stable than E3_19 in guanidinium hydrochloride and thermal denaturation experiments.
Since the crystal structure of E3_19 was solved later than that of E3 5, a homology model of E3_19 based on the crystal structure of E3_5 was also used in the simulations. E3 5 shows a very stable trajectory in both crystal and solution simulations. In contrast, the C-terminal repeat of E3_19 unfolds in the simulations starting from either the modelled structure or the crystal structure, although it has a sequence identical to that of E3_5. A continuum electrostatic model was used to estimate the effect of single mutations on protein stability and to study the interaction between the internal ARs and the C-terminal capping AR. Mutations involving charged residues were found to have large effects on stability. Due to the difference in charge distribution in the internal ARs of E3_19 and E3_5, their interaction with the C-terminal capping AR is less favorable in E3_19. The simulation trajectories suggest that the stability of the designed AR proteins can be increased by optimizing the electrostatic interactions within and between the different repeats.

References: in press (*Proteins*)

Title: Molecular Dynamics Simulation of Lipid Bilayers with GROMOS96: Application of Surface Tension

Researchers: Indira Chandrasekhar
Dirk Bakowies
Alice Glättli
Philippe H. Hünenberger
Cristina Pereira
Wilfred F. van Gunsteren

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

Description:

The GROMOS96 force fields 45A3 and 53A5, when applied to DPPC membranes, have a tendency to a reduced area per lipid in constant pressure simulations. The application of surface tension is effective in increasing the area per lipid, a measure of the phase of the membrane, but only if the area is already close to the experimental range. Therefore the surface tension cannot compensate for strong inadequacies in the force-field parameters. The behaviour of the 45A3 force field from long $NP_n\gamma T$ simulations of tens of nano-seconds is analysed over a range of different surface tensions. Comparisons are made with the corresponding NP_nAT simulations.

References: in press (*Mol. Simulation*)

Title: Calculating zeros: non-equilibrium free energy calculations

Researchers: Chris Oostenbrink*
Wilfred F. van Gunsteren

Institute/Group: *Vrije Universiteit, Pharmaceut. Sci. / Pharmacochem., Amsterdam, The Netherlands
Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland

Description:

Free energy calculations on three model processes with theoretically known free energy changes have been performed using short simulation times. A comparison between equilibrium (thermodynamic integration) and non-equilibrium (fast growth) methods has been made in order to assess the accuracy and precision of these methods. The three processes have been chosen to represent processes often observed in biomolecular free energy calculations. They involve a redistribution of charges, the creation and annihilation of neutral particles and conformational changes. At very short overall simulation times, the thermodynamic integration approach using discrete steps is most accurate. More importantly, reasonable accuracy can be obtained using this method, which seems independent of the overall simulation time. In cases where slow conformational changes play a role, fast growth simulations might have an advantage over discrete thermodynamic integration where sufficient sampling needs to be obtained at every λ-point, but only if the initial conformations do properly represent an equilibrium ensemble. From these three test cases practical lessons can be learned that will be applicable to biomolecular free energy calculations.

References: in press (*Chem. Phys.*)

Title: Acetonitrile revisited: a molecular dynamics study of the liquid phase

Researchers: Peter J. Gee
Wilfred F. van Gunsteren

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

Description:

The subject of this report is the calibration of a model of the liquid state of acetonitrile (methyl cyanide). The model describes the liquid in terms of molecular mechanics with each molecule of the liquid treated as a rigid body that is composed of three interaction-sites, between which Coulomb and dispersion interactions are computed. A brief overview of the literature on such models is given and a set of parameters for the model is presented. The representation of liquid acetonitrile produced by the parameters is compared to that produced by several other parameter-sets available in the literature. It is concluded that, of the parameter-sets for the three-site molecular mechanics model which currently are available, under the simulation conditions used, the one presented produces the most rounded representation of the properties of liquid acetonitrile.

References: in press (*Molecular Physics*)

Title: Numerical simulation of the effect of solvent viscosity on the motions of a beta-peptide heptamer

Researchers: Peter J. Gee
Wilfred F. van Gunsteren

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

Description:

This report examines the effect of a decrease in solvent viscosity on the simulated folding behaviour of a beta-peptide heptamer in methanol solution. Simulations of the molecular dynamics of the heptamer H-β^3-HVal-β^3-HAla-β^3-HLeu-(S,S)-β^3-HAla(αMe)-β^3-HVal-β^3-HAla-β^3-HLeu-OH (Figure 1) in methanol, with an explicit representation of the methanol molecules, have been performed to 80ns with the viscosity of the solvent varied. The simulations indicate that at a solvent viscosity which is one third that of methanol, only the dynamic aspects of the folding process are altered, and that the rate of folding is increased. At a viscosity of a tenth that of methanol, insufficient statistics are obtained within an 80ns period. It is suggested that the fact that 80ns is insufficient time to reach conformational equilibrium at very low viscosity may indicate that the dependence of the folding rate of a beta-peptide on solvent viscosity has two regimes, a result noted for alpha-peptides in another computational study.

References: in press (*Chemistry – A European Journal*)

Title: Numerical simulation of the pressure-denaturation of a helical beta-peptide heptamer solvated in methanol

Researchers: Peter J. Gee
Wilfred F. van Gunsteren

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

Description:

The effect of elevated pressure on the conformational behaviour of a beta-peptide heptamer in methanol solution is considered. The response of the peptide to elevated pressure is probed by means of molecular dynamics simulations and is described in atomic terms. The most striking features of the response are that the region of the unfolded state of the peptide which is accessible at elevated pressure is narrow and that thermal and pressure denaturation produce similar unfolded states in the case of this beta-peptide.

References: manuscript submitted (*Helv. Chim. Acta*)

Title: Terminal-group effects on the folding behaviour of selected beta-peptides

Researchers: Peter J. Gee
Wilfred F. van Gunsteren

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

Description:

It has been suggested that the stability of a beta-peptide helical fold is affected by the interplay between the electrical charge of terminal groups and the dipole due to the helical conformation; the numerical simulations presented herein test that suggestion. The motions of two beta-peptide oligomers, each of which has been shown by NMR-spectroscopy to fold into a different helical conformation, have been simulated. The simulated motions bear out empirical observations as to the effect of chemical protection of terminal groups on the stability of beta-peptide helical folds and they support the hypothesis of "charge-dipole stabilization".

References: in press (*Proteins*)

Title: A molecular dynamics study of the bee venom melittin in aqueous solution, in methanol, and inserted in a phospholipid bilayer

Researchers: Alice Glättli
Indira Chandrasekhar
Wilfred F. van Gunsteren

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

Description:

The structural properties of melittin, a small amphipathic peptide found in the bee venom, are investigated in three different environments by molecular dynamics simulation. Long simulations have been performed for monomeric melittin solvated in water, in methanol, and inserted in a dimyristoylphosphatidylcholine bilayer. The resulting trajectories were analysed in terms of structural properties of the peptide and compared to the available NMR data. While in water and methanol solution melittin is observed to partly unfold, the peptide retains its structure when embedded in a lipid bilayer. The latter simulation shows good agreement with the experimentally derived ^{3}J-coupling constants. Generally, it appears that the stability of the helical conformation of melittin is higher the lower the dielectric permittivity of the environment is. In addition, peptide-lipid interactions were investigated showing that the C-terminus of the peptide provides an anchor to the lipid bilayer by forming hydrogen bonds with the lipid head groups.

References: manuscript submitted (*Eur. Biophys. J.*)

Title: Comparing atomistic simulation data with the NMR experiment: How much can NOE's actually tell us?

Researchers: Bojan Zagrovic
Wilfred F. van Gunsteren

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

Description:

Simulated molecular dynamics trajectories of proteins and nucleic acids are often compared with nuclear magnetic resonance data for the purposes of assessing the quality of the force field used or, equally important, trying to interpret ambiguous experimental data. In particular, NOE intensities or atom-atom distances derived from them are frequently calculated from the simulated ensembles since the distance restraints derived from NOEs are the key ingredient in NMR-based protein structure determination. In this study, we ask how diverse and non-native-like an ensemble of structures can be and still match the experimental NOE distance upper bounds well. We present two examples in which simulated ensembles of highly non-native polypeptide structures (an unfolded state ensemble of the villin headpiece and a high-temperature denatured ensemble of lysozyme) are shown to match rather well the experimental NOE distance upper bounds from which the corresponding native structures were derived. For example, the unfolded ensemble of villin headpiece, which is on average 0.90 ± 0.13 nm RMSD away from the native NMR structure, deviates from the experimental restraints by only 0.027 nm on average. However, this artificially good agreement is largely a consequence of 1) the highly non-linear effects of r^{-6} (or r^{-3}) averaging and 2) focusing only on the experimentally observed set of NOE bounds. Namely, in addition to the experimentally observed NOEs, both simulated ensembles (especially the villin ensemble) also predict a large number of NOEs which are not seen in the experiment. If these are taken into account, the agreement between simulation and experiment gets markedly worse, as it should, given the non-native nature of the underlying simulated ensembles. In light of the examples given, we conclude that comparing experimental NOE distance restraints with large simulated ensembles provides just by itself only limited information about the quality of simulation.

References: in press (*Proteins*)

Title: Orientation and Conformational Preference of Leucine-Enephalin at the Surface of a Hydrated Dimyristoylphosphatidylcholine Bilayer: NMR and MD Simulation

Researchers: Indira Chandrasekhar
Giorgia Zandomeneghi
Philip T.F. Williamson
Beat Meier
Wilfred F. van Gunsteren

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

Description:

The morphogenic opiate pentapeptide Leucine-enkephalin (lenk) in a hydrated dimyristoylphosphatidylcholine (DMPC) bilayer is studied using NMR spectroscopy and molecular dynamics simulation. Contrary to the frequent assumption that the peptide attains a single fixed conformation in the presence of membranes, we find that the lenk molecule is flexible, switching between specific bent conformations. The constraints to the orientation of the aromatic rings that are identified by the NMR experiment are found by the MD simulation to be related to the depth of the peptide in the bilayer. The motion of the N-H vectors of the peptide bonds with respect to the magnetic field direction as observed by MD largely explain the magnitude of the observed residual dipolar coupling (RDC), which are much reduced over the static ^{15}N-^{1}H coupling. The measured RDC's are nevertheless significantly larger than the predicted ones, possibly due the absence of long time motions in the simulations. The conformational behaviour of lenk at the DMPC surface is compared to that in the aqueous solution, both in the neutral and in the zwitterionic forms.

References: manuscript submitted (*JACS*)

Title: The GROMOS software for biomolecular simulation: GROMOS05

Researchers:
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*Swissre, Zürich, Switzerland
**Vrije Universiteit, Pharmaceut. Sci. / Pharmacochem., Amsterdam, The Netherlands
***Max-Planck-Institute for Polymer Research, Mainz, Germany

Description:

We present the latest version of the Groningen Molecular Simulation program package, GROMOS05. It has been developed for the dynamical modelling of (bio)molecules using the methods of molecular dynamics, stochastic dynamics, and energy minimisation. An overview of GROMOS05 is given, highlighting features not present in the last major release, GROMOS96. The organisation of the program package is outlined and the included analysis package GROMOS++ is described. Finally, some applications illustrating the various available functionalities are presented.

References: manuscript submitted (*J. Comput. Chem.)*

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

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

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

Description:

The most powerful tools to investigate the sensitivity of the Earth's climate to anthropogenic perturbations are three dimensional numerical models of the climate system (GCMs). In the framework of National Competence Centre for Climate Research (NCCR Climate), we are maintaining and running a global climate model (ECHAM5) at the Swiss Centre for Scientific Computing (CSCS).

In general, progress in global climate modeling can be expected from an increase in resolution as well as improvements in understanding and parameterization of inadequately represented or entirely missing key climate processes. We investigate selected aspects of both issues.

In previous years, the focus was on the improvements gained with increase in resolution. One advantage of global high-resolution experiments is an improved representation of topography and associated effects, such as orographically induced precipitation, which is of key importance for mountainous areas as well as high latitude regions. This enables a more realistic simulation of the accumulation changes under greenhouse forcing for estimates of mass balance changes on mountain glaciers and polar ice sheets, and their respective impact on global sea level (Wild, Ohmura IPCC Third Assessment Report 2001, Chapter 11).

The results of new high resolution simulations with ECHAM5 will provide a database for various climate change related studies within the NCCR community as well as for nesting of regional models over Europe. Preliminary comparisons of our results with high resolution GCM experiments performed in other modeling groups suggest that the latest generation of high resolution GCMs may be quite consistent in their regional climate change projections under greenhouse forcing.

In addition to the aspect of higher resolution, we address also the issue of neglected or crudely represented processes in GCMs. In several studies of our studies serious limitations in the radiation budgets and in the surface exchange processes of climate models were detected (e.g, Wild 2005, Wild et al. 2005b, Roesch and Roeckner 2005, Wild and Roeckner 2005). In addition, evaluations of the radiation databases available at our institute revealed significant trends in surface radiation, some of them now referred to as 'global dimming' (Gilgen et al. 1998, Wild et al. 2004, 2005a). These trends are not adequately reproduced in climate models, and may largely affect surface climate as well as the global hydrological cycle (Ohmura and Wild 2002, Wild et al. 2004, 2005a). A key factor for the explanation of the cited GCM biases as well as the observed trends may be aerosol, with its direct and indirect radiative effects. However, these effects are still very crudely represented in climate models. We investigate this issue based on the ECHAM5 GCM, updated with comprehensive aerosol and cloud microphysics module.

References: See separate list.

Title: Computational Optoelectronics

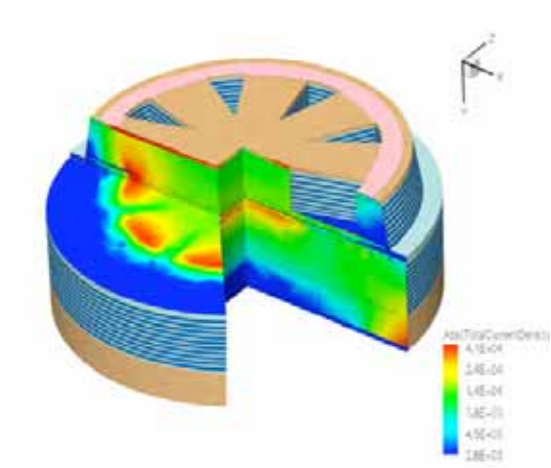
Researchers: Bernd Witzigmann
Friedhard Römer
Stefan Odermatt
Dölf Aemmer

Institute/ Group: Integrated Systems Laboratory/
Computational Optoelectronics Group

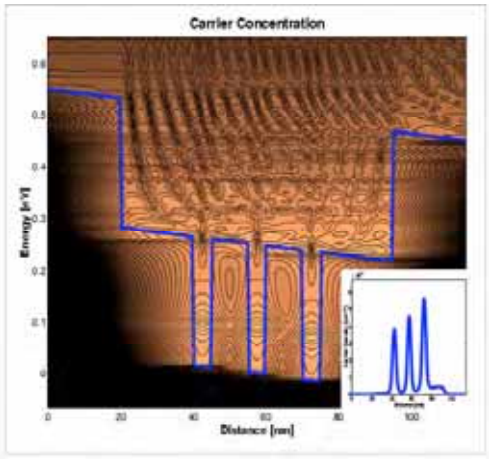
Description:

Optoelectronics continue to have a tremendous impact in fields such as information technology, sensing, lighting, and materials processing. At present, high capacity fiber optic communication networks are the backbone of the internet. As an example of future technology with disruptive potential, incandescent light sources ('light bulbs') might be replaced by ten times more efficient high brightness solid-state light-emitting diodes (LED). Key ingredients to these developments are high performance, low-cost optoelectronic devices and systems. Their design poses a special challenge, as stringent electrical and optical specifications need to be met at the same time. The research of the computational optoelectronics group is devoted to the design and analysis of optoelectronic devices and systems, in close collaboration with industry and academia. Our activities include the development of physics-based simulation models, design and analysis of optoelectronic devices and systems, and device level characterization.

Our projects include electro-opto-thermal simulation of Vertical Cavity Surface Emitting Lasers (VCSELs), Electromagnetic Simulation of Microcavities, and a first-principle calculation of the optical properties of novel composite materials. The simulations are run on high-performance compute-servers at Integrated Systems Laboratory. The figures below illustrate some of the project results.



Three-dimesional simulation of a Vertical-Cavity Surface Emitting Laser (VCSEL).



Quantum-kinetic calculation of the electron density in a multiple quantum-well structure.

Title: Automated NOESY spectral analysis and NMR structure determination using the new software RADAR

Researchers: Torsten Herrmann
Francesco Fiorito
Pascal Bettendorff
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
This project is focused on automated NMR data analysis for three-dimensional structure determination of biological macromolecules in solution, with the prime objectives of increasing the efficiency and the reliability of protein structure determination by NMR. In this process, the presently used software for interactive analysis of multidimensional NMR spectra is being replaced by the fully automated routine RADAR. The software package RADAR will combine and tightly merge the functionalities of the two algorithms ATNOS for automated NOESY peak picking and CANDID for automated NOE assignment, and it should enable direct refinement of NMR structures of proteins against the raw NMR data.
RADAR is based on an input of experimental 2D and heteronuclear-resolved 3D [1H,1H]-NOESY spectra and a chemical shift list from previous, independently performed sequence-specific resonance assignment.
Further developments will include attempts to add automated sequence-specific assignment from minimal sets of NMR spectra.

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

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

Fadel, V., Bettendorff, P., Herrmann, T., de Azevedo Jr, W.F., Oliveira, E.B., Yamane, T. & Wüthrich, K.
"Automated determination of the solution NMR structure and disulfide connectivity of crotamine, a myotoxin from Crotalus durissus terrificus venom."
Toxicon (in press)

Title: Structural studies of prion proteins

Researchers: Dominik Lysek
Barbara Christen
Daniel Roberto Perez Lagos
Francesco Fiorito
Christine von Schroetter
Simone Hornemann
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

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 three-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.

References:

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

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

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

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

Title: Structural studies of pheromone-binding protein from Bombyx mori (BmPBP)

Researchers: Fred Damberger
Erich Michels
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
Odorant-binding proteins (OBPs) occur at high concentrations in the lymph of insect olfactory sensilla and transport the hydrophobic odorant molecules from the periphery of the sensillum to the olfactory receptors. The pheromone binding proteins (PBPs) are a subclass of the OBPs which bind pheromones used in insect communication. Our work so far shows that the pheromone binding protein from the silkmoth Bombyx mori, (BmPBP), undergoes a pH-dependent conformational transition between two forms (BmPBPA observed at pH 4.5 and BmPBPB at pH 6.5) which is likely to relate to biological function. To obtain a more complete picture of the function of BmPBP, we have determined the solution structure of BmPBPA 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, which might be applicable to an entire class of proteins with pheromone-binding function.

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

Title: Structural aspects of the type-1 pilus assembly

Researchers: Reto Horst
Pascal Bettendorff
Torsten Herrmann
Rudi Glockshuber
Markus G. Grütter
Guido Capitani
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:
Type-1 pili ("Fimbrae") are large, heterooligomeric protein filaments of uropathogenic E. coli strains that are required for the attachment of the bacteria to host cell surfaces and that enable survival inside of macrophages. These pili are constituted by up to 2000 protein subunits, where FimA is the most abundant one (>98%), with FimF, FimI, FimG and the mannose-binding subunit FimH making up the rest. We aim at contributing to the understanding of the mechanisms of pilus assembly, which involve additional proteins in the periplasm and the bacterial membrane. Thus, in a previous collaboration with the group of Prof. R. Glockshuber, we solved the solution structure of FimC, a periplasmic assembly factor which is not a structural component of the pili but is required for pilus assembly in vivo. The actual pilus assembly on the cell surface is performed by the membrane protein FimD, which is another target for obtaining structural information. The application of new, TROSY-based NMR techniques will provide insights into the interactions of the different proteins involved and their structures.

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

6

High-performance Hardware

6.1 C4: Competence Center for Computational Chemistry

At the 2004 C4 Annual Workshop, after ten years of leadership, Prof. Wilfred van Gunsteren handed the directorate of C4 over to PD Hans P. Lüthi. Wilfred van Gunsteren still serves as a member of the new C4 Steering Committee, together with Dr. Wanda Andreoni (IBM Research) and Jürg Hutter (University of Zürich).

C4 is seeking new challenges and opportunities not just within chemistry, but also in materials science and in the biosciences: the "C" standing for "Chemistry" in C4 shall be replaced by "molecular science". C4 shall keep its role as a major contributor to computational science at ETH Zürich and at the University of Zürich. And, very importantly, it shall also serve as a platform for the interaction with external partners (academic and industrial) to cater to the flow of know-how.

For this matter C4 was offered a one-week tutorial on Car-Parrinello molecular dynamics presented by Prof. J. Hutter and Dr. M. Iannuzzi. It was the first tutorial of its kind with attendance from ETH, the University of Zurich, the Paul Scherrer Institute, EPFL, and the University of Bern. The 2005 C4 annual workshop was hold jointly with the computer aided drug design group of the Novartis corporation lead by Dr. R. Lewis. To cater to the exchange of students and researchers between Novartis and the members of C4, an internship program was developed and presented at the workshop. C4 also entered a partnership with its counterpart at the University of California in Berkeley, the Kenneth S. Pitzer Center for Theoretical Chemistry. This is a program developed under the "umbrella" of the ETH – UC Berkeley Memorandum of Understanding for the exchange of students and researchers.

More information about these and other activities can be found at
www.c4.ethz.ch

Hans P. Lüthi
Leiter C4

6.2 CSCS – Swiss National Supercomputing Centre

Jari Järvinen
Dominik Ulmer

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

1. CSCS' High-Quality Services for National Research Community

Due to its mission formulated by ETH Board, CSCS provides, develops and promotes technical and scientific services for the Swiss research community in high-performance and high-throughput computing. It is a centre of competences that pioneers new information technologies, collaborates with domestic and foreign researchers, and carries out its own research in computational sciences and scientific computing.

The mission of CSCS is target-oriented in challenging research environment consisting of world-wide recognized research organizations and individual researchers. CSCS' infrastructural services, high performance and scientific computing competences must fulfill high quality criteria and customers' needs.

CSCS invests in its high performance computing (HPC) services. Also, a specific emphasis is put on hiring experienced personnel for critical scientific computing duties. It is planned that by 2007, about 15 persons are working in HPC operations and 30 in scientific computing services.

Extensive and powerful high performance and high-throughput computing services combined with in-depth knowledge and experience on computational sciences and scientific computing offer CSCS' customers a concept for successful research. CSCS will collaborate with its customers in challenging research projects to enable new discoveries in science and research.

2. CSCS' National Computing Infrastructure

CSCS offers customers a most competitive, performing, reliable and easy-to-use computing infrastructure, Figure 2.1. The infrastructure is based on the integration of supercomputers, clusters, high-speed networks and data management resources. It is completed with extensive variety of scientific software.

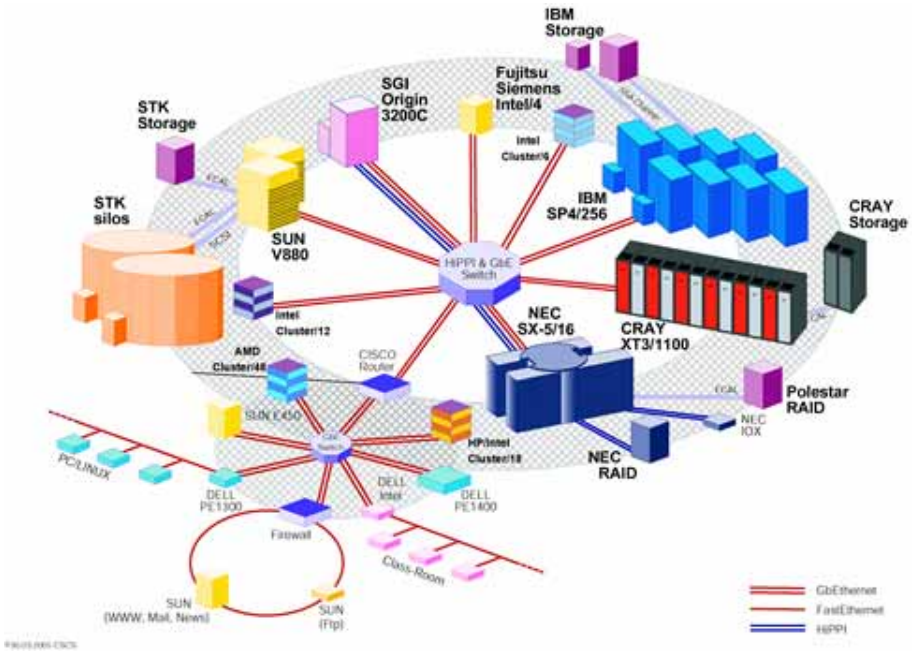


Figure 2.1 CSCS High Performance Computing and Networking Infrastructure

2.1 High Performance Computing and High-Throughput Computing Infrastructure at CSCS

Currently, CSCS offers supercomputing services to the national user community on parallel vector processing, massively parallel processing and cluster computing environments.

As a parallel vector processing environment, CSCS maintains NEC SX-5 single node system with 16 CPUs and 64 Gbytes of shared main memory running under Super-UX with NQS scheduler. The network connections are provided via HiPPI and GigabitEthernet and the peak performance of the system is 128 Gigaflops.

For massively parallel processing, CSCS offers 8 IBM Regatta p690 SMPs for a total of 256 Power4 CPUs, 768 GBytes of main memory, totaling a theoretical peak performance of 1.38 TFlops. The SP frames are tightly coupled by a Double Colony switch in order to provide a parallel environment with a Global Parallel File System of 4 TB. The overall system runs on AIX with job management based on LoadLeveler. The system is complemented by 2 NightHawks (Power3 nodes, total of 32 CPUs and 32 GBytes main memory) with a peak performance of 48 GFlops.

Besides parallel vector processing and massively parallel processing environments, CSCS offers cluster computing capacity to the Swiss research community. As an example, CSCS hosts Tier-2 level computing cluster for Large Hadron Collider Computing Grid. The CSCS LHC Computing

Grid consists of 20 dual-processor AMD0-Athlon-MP processors and operates on Linux. The system offers main memory of about 20 GB and 4.8 TB disk space.

CSCS' computational environment is completed by extensive Horizon and Zenith projects in 2005 and 2006, see Chapter 4.

2.2 Data Management Environment at CSCS

The CSCS data archive facility is based on the SAM-FS Hierarchical Storage Management (HSM) software running on a high-availability SUN cluster (two SUN V880 servers), which transparently controls data movement between the fast LSI Logic D280/9176 raid disk cache of 8 TB and two high-capacity StorageTek "Powderhorn" tape silos with mixed SCSI / FC tape drive technology. Redundant Brocade switches ensure a fully-switched FiberChannel archive environment. A recent major upgrade of selected hardware and software components allow users to benefit from higher archive access performance and increased service availability, while still ensuring seamless growth of the archive capacity, currently exceeding 260 TB.

3. Who Uses CSCS Computing Infrastructure?

CSCS' clientele consists of researchers in bioscience/chemistry, engineering, environment, materials science, and physics. Most of the computing resources offered by CSCS are used by bioscientists/chemists, engineers, and environmental scientists, see Figure 3.1 (usage by discipline on IBM). The allocation for organizations is presented in Figures 3.2 and 3.3.

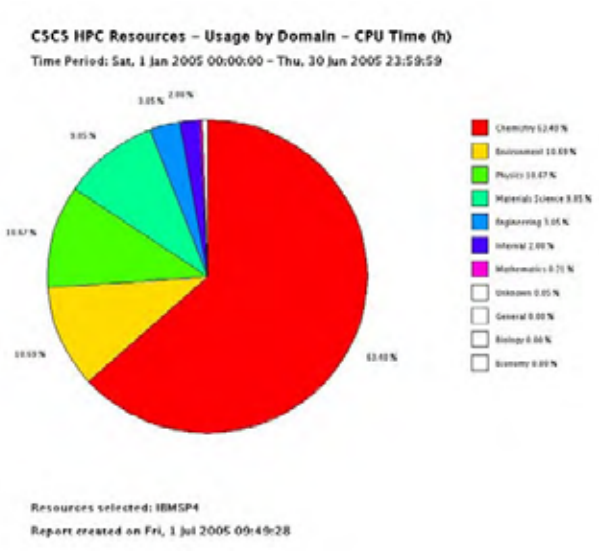


Figure 3.1 Usage by Discipline on IBM SP4 (1H/2005)

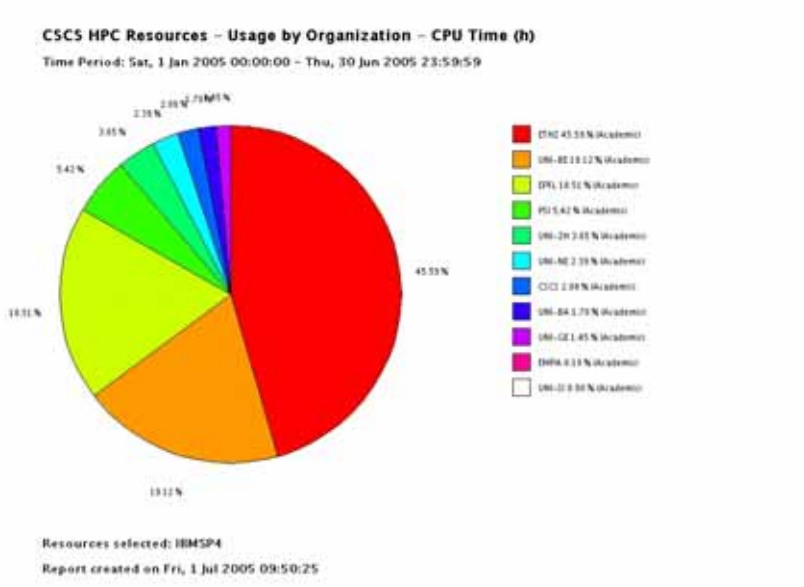


Figure 3.2 Usage by Organizations on IBM SP4 (1H/2005)

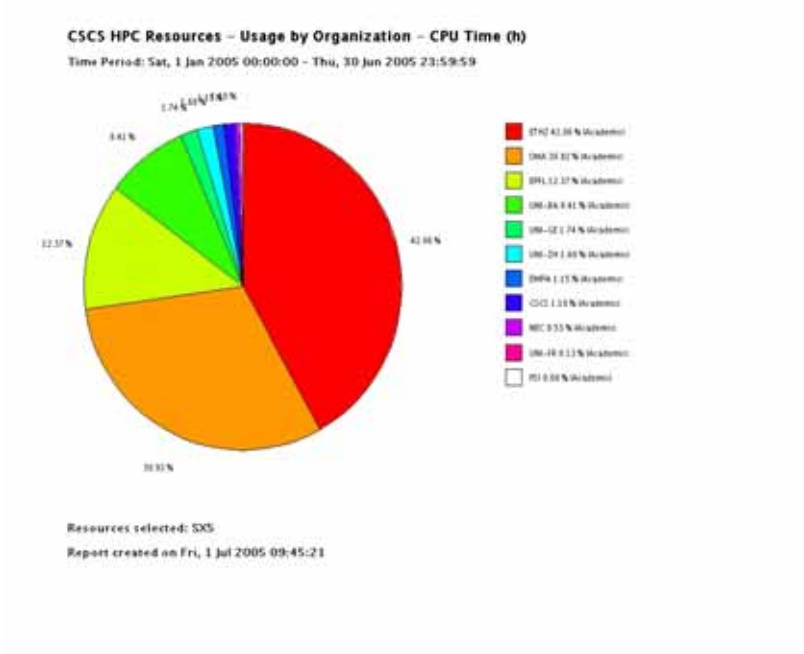


Figure 3.3 Usage by Organizations on NEC SX-5 (1H/2005)

High performance computing resources are allocated to research projects on competitive basis. The resources are shared between projects, which have outstanding impact to science, research and development and society. The Large User Projects (LUPs) for 2005 are presented in Table 3.1.

Project Leader	**Domain**	**Large User Project**
Arbenz P.	ETHZ	Large scale eigenvalue problems in opto-electronic semiconductor lasers and accelerator cavities
Baiker A.	ETHZ	Hydrogenation reactions in heterogeneous enatioselective catalysis and homogeneous catalysis in supercritical CO2
Bakowies D.	ETHZ	Atomization energies from ab initio calculations without empirical correction
Beniston M.	Uni FR	Global and regional climate modelling
Besson O.	Uni NE	Numerical solution of navier-stokes equations in shallow domains on MPP
Bey I.	EPFL	Coupling tropospheric chemistry and aerosols in the general circulation model ECHAM
Bürgi Th.	Uni NE	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper W.A.	EPFL	Computation of Stellarator Coils, Equilibrium and Stability
Davies H.C.	ETHZ	ERA40 for NCCR-Climate
Deubel D.	ETHZ	Quantum studies of inorganic anticancer drugs
Fäh D.	ETHZ	Numerical Modelling of seismic local effect extimation of complex sites
Fichtner W.	ETHZ	Computational science and engineering in microelectronics and optoelectronics
Folini D.	EMPA	Inverse modeling to monitor source regions of air pollutants in Europe
Hasenfratz P.	Uni BE	Chiral Symmetric Dirac operator in lattice QCD
Hauser A.	Uni GE	Photophysics and photochemistry of transition metal compounds: Theoretical Approaches
Helm L.	EPFL	Hyperfine interaction anisotropy on first and second coordination sphere water molecules in paramagnetic metal ion solution
Hutter J.	Uni ZH	Development and application of ab-initio molecular dynamics methods
Jakob A.	PSI	Molecular modelling of radionuclide mobility and retardation in clay materials
Joos F.	UNI BE	Carboclime: modelling carbon cycles climate

		feedback
Keller J.	PSI	Air quality modeling in Switzerland
Kleiser L.	ETHZ	Numerical simulation of transitional, turbulent and multiphase flows
Koumoutsakos P.	ETHZ	Simulations using particle methods, Optimization of real world problems using evolutionary algorithms Multiscale modeling, simulation and optimization of complex systems
Leriche E.	EPFL	Direct numerical simulation ot the buoyancy-driven turbulence in a cavity: the DNSBDTC project
Leutwyler S.	Uni BE	Proton transfer and hydrogen bonding in microsolvent clusters and nucleic acid base pairs: theroy and dynamics
Leyland P.	EPFL	Aerothermodynamic simulations in aerospace and aeronautic applications
Lohmann U.	ETHZ	Effects of aerosols on clouds and climate
Lüthi H.P.	ETHZ	Computational quantum chemistry of large molecules
Meuwly M.	Uni BS	Electronic structure calculations for molecular dynamics simulations of iron-containing, reactive centers of biomolecules Theoretical investigations of iridium-catalyzed reactions
Oganov A.	ETHZ	Computational mineral physics and crystallography
Ohmura A.	ETHZ	Global climate change: modelling atmosphere/ocean variability on decadel time scales
Parlange M.	EPFL	Large Eddy Simulation of atmospheric boundary layer flow over complex terrain
Pasquarello A.	EPFL	Disordered network-forming materials
Posternak M.	EPFL	Computational Physics in condensed matter
Poulikakos D.	ETHZ	Biothermpfluidics for cerebrospinal fluid diagnostic and control, Explosive vaporization phenomena in microenclosures
Röthlisberger U.	EPFL	Mixed quantum mechanics / molecular mechanics study of systems of biological interest
Samland M.	Uni BS	The Milky way and its satellite dwarf galaxies
Schär Ch.	ETHZ	Modelling weather and climate on european and alpine scales
Sennhauser U.	EMPA	Nanoxid
Stocker Th.	Uni BE	Monalisa: modelling and reconstruction of

		north Atlantic climate system variability
Van Lenthe H.	ETHZ	Identifying genetics determinants of bone strength
Van Swygenhoven H.	PSI	Modelling dynamics computer simulation of nanostructured materials
Vogel P.	EPFL	New organic chemistry with Sulfur Dioxide: the electron releasing conjugated Carbonyl Group

Table 3.1 Large User Projects at CSCS in 2005

4. Extensions in CSCS' Computing Environment

The need of computing resources is rapidly growing in the user community of CSCS. In the last calls for LUPs, the resource allocation committee had to cut back or even completely turn down scientifically competent research projects because of the restrictions in compute capacity. The situation is tightened further by the age of the SX-5 which is now more than 5 years old.

Over the last years, CSCS has observed a revitalization of supercomputing technology development. This situation has given CSCS the possibility to explore new HPC architectures for better matching applications and system architectures and also for attracting new application areas. CSCS has developed a strategy for managing the computer portfolio of CSCS. It is based on a technology innovation cycle and maps out, in qualitative fashion, four different basic areas between the two coordinate axes "scientific output productivity" and "support effort" ("time to solution" from a user point of view). The duration of the cycle is typically longer than the lifetime of a given system, which travels with an individual speed on this cycle. It is the goal of CSCS to have at least systems in the right half of the coordinate square, where system with high productivity reside, either based on mature, well-known technology with short time to solution, or with leading edge technology that require higher support effort by CSCS.

Currently, CSCS has two projects underway for the extension and renewal of the computing infrastructure. Horizon, a joint project with PSI, installs a massively parallel processor Cray XT3 computer system based on the Red Storm technology at CSCS. The new supercomputer is able to deliver peak performance of 5.9 Tflop/s. Horizon consists of 1'100 2.6 GHz AMD Opteron processors, connected by the Cray SeaStar high-bandwidth, low-latency interconnect using a 3D torus topology. The Horizon will be opened for all CSCS' customers in the beginning of 2006.

The other project, called Zenith, targets at a highly integrated system with powerful single processors and a globally addressable memory. The system will have a balanced architecture between processor and memory bandwidth and will provide a high sustained performance for some key applications. The system will be installed at CSCS in the first half of 2006.

Both projects together target at a minimal five fold increase of the computing power presently at CSCS. The NEC SX 5 will be decommissioned during the second half of 2005.

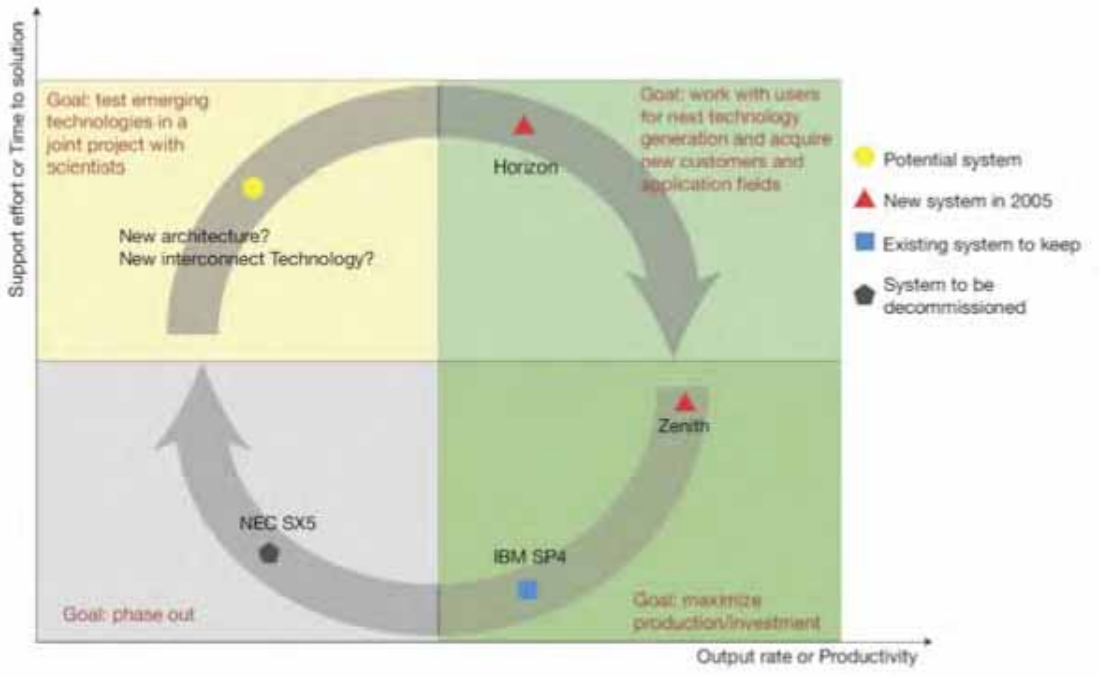


Figure 4.1 Exploring HPC Architectures for Satisfying Customers' Needs

6.3. The Beowulf Clusters “Asgard” and “Hreidar” and “Gonzales”

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 502-CPU Asgard Beowulf cluster built from 500 MHz Pentium-III CPUs, which was installed early in the year 2000 has been converted to a special-use cluster for particle physics, to be integrated into the CERN data grid, and to be available for Monte Carlo simulations in particle physics.

The installation of he two successor clusters has also been finished. The Hreidar cluster, connected by Ethernet, has been upgraded to 320 AMD Opteron CPUs, with startup funds of Prof. Äbersold in D-BIOL. A second cluster “Gonzales”, also consisting of 320 AMD Opteron CPUs but connected by a fast Quadrics network has been organized and installed by the Informatikdienste and is mainly used for applications requiring a fast network.

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

6.4 Information Technology Services

The following resources are available:

- Hewlett Packard Superdome Cluster consisting of
    - 1 HP Superdome (Stardust): 64 Itanium2 CPUs (1500 MHz), 128 GB Memory, 400 GB local Disk, 2 TB SAN Disk, HP/UX Operating System
    - 1 HP Superdome (Pegasus): 32 Itanium2 CPUs (1500 MHz), 64 GB Memory, 400 GB local Disk, 2 TB SAN Disk, HP/UX Operating System

  The cluster is used for parallel code taking advantage of the shared memory programming model offered by the cc-numa architecture of these systems. Many standard applications (finite element modeling, mathematics, simulations, etc.) are in this category.

  The systems major usage is in the fields of thermodynamics, fluiddynamics, virtual production (FEM) and theoretical physics.

  The following software is available on the Superdome cluster:

  HP Fortran: Compiler and associated products
  HP Fortran 90: Compiler and associated products
  HP C/ansi: C Developer's Bundle for HP-UX 11.00
  HP C++: Compiler
  KAI Guide C++: Open MP
  Abaqus 5.8: General-purpose finite element analysis
  ACSL: Advanced continuous simulation language
  Ampl 9.5.13: Modeling language for Mathematical Programming
  ANSYS 5.5: Finite element analysis
  AVS: Advanced visual system
  CPLEX 65: Linear optimization solver
  CFX Tascflow: CFD analysis and design tool
  Diana 7.2: Finite element analysis
  Gaussian 98: semi empirical and ab initio molecular orbital (MO) calculations.
  MARC/MENTAT K7.3: Nonlinear finite element program
  Matlab 11.1: Language for technical computing
  Molcas 5: Quantum chemistry software
  NAG F95: Fortran library
  IMSL: Fortran Numerical Libraries
  Para Phoenics 32: CFD
  Patran 9.0: Finite element (Modeling, Analysis, Results evaluation)
  Tecplot 8.0: Tool for visualizing a wide range of technical data
  PV-Wave: Signal Processing Toolkit

- The Information Technology Services operate two Beowulf Clusters co-owned with the Departments Physics, Mathematics, Material Sciences and Computer Science. One cluster (“Hreidar”) consists of 160 dual processor AMD Opteron 244 systems with 4 GB memory and Ethernet network, the other (“Gonzales”) consists of 160 dual processor AMD Opteron 250 systems with 8 GB memory and Quadrics High Bandwidth/Low Latency network. By the end of 2005 the Gonzales cluster will be extended

by 128 nodes and the Hreidar cluster by 16 nodes. Parts of the Gonzales cluster are operated as a central resource, which can be used on a fair share base by the ETH community without being co-owner of the cluster.

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

7

Outlook

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

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

This year we have started with the new Master program in CSE. For this, new courses had to be designed and some newly designed ones will be improved. Since procedures for accepting students from outside ETH had not been in place in the period of this report we have not yet advertised the Master program. However, we are about to setting up a body to handle the admission of students from outside ETH. Hence, we shall advertise our CSE Master program in the next year and we expect to receive a larger international student body next fall. As the curriculum becomes more international the course material will have to be more and more in English and of course the lectures as well. The tailoring of courses to the needs of students in CSE will continue.

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

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

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

Zürich, December 2005
Rolf Jeltsch

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