Fast Methods for Long-Range Interactions in Complex Systems

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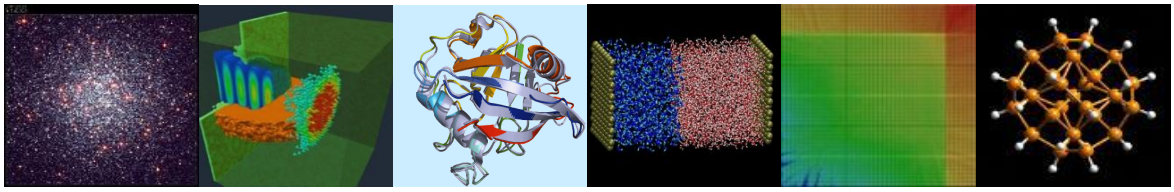

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Poster Presentations

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Preface

Computer simulations of complex particle systems play an important role in a broad field of physics, e.g. astrophysics, statistical physics, plasma physics, material sciences, physical chemistry or biophysics, to name a few. Current leading parallel hardware systems, which show a performance in the PFlop/s range, have made it possible to increase strongly the problem size of simulation systems. However, it is not only the development of more powerful hardware, but at the same time the development of numerical algorithms, which enable mapping of complex problems onto limited hardware memory and which have nearly optimal scaling properties, which increase the computational effort proportionally with the number of particles.
Especially in fields, where long-range interactions between particles have to be taken into account the numerical effort is usually very large. Since most of the interesting physical phenomena involve electrostatic, gravitational or hydrodynamic effects, the proper inclusion of long range interactions is essential for the correct description of systems of interest. Since in principle, long range interactions have $\mathcal{O}(N^2)$-complexity, fast implementations have to rely on approximations. Although, in principle, various methods might be considered as *exact representations* of the problem, approximations with controlable error thresholds are developed. Since different boundary conditions or dielectric properties require the application of appropriate methods, there is not only one method, but various classes of methods developed. E.g. the inclusion of different symmetries in the system (1d-, 2d- or 3d-periodic systems), the presence of interfaces or the inclusion of inhomogeneous dielectric properties, require the implementation of different electrostatic methods. Since long-range interactions are fundamental in a variety of disciplines there was sometimes an independent parallel development of similar methods or a *re-discovery* of methods in distinct research areas.
Because of the importance of long-range interactions under various conditions in science, the present school does not only focus on one given method method, but introduces a spectrum of different fast algorithms:

- Fourier transform based methods
  - Particle-particle particle-mesh method (P^3M)
  - MMM-methods (MMM1d, MMM2d)
  - Fast summation based on non-equidistant Fast Fourier Transform (NFFT)
- Hierarchical methods
  - Fast Multipole Method (FMM)
  - Barnes-Hut Tree method
  - Multigrid based methods
- Local cutoff-approximations
  - Wolf summation
  - Maggs solver for Maxwell equations

In addition to the mathematical description of the methods, focus is given to the parallelization and implementation on parallel computers. To give a more general introduction into parallel programming, a special session is organized where different libraries and paradigms (MPI, OpenMP) are introduced and participants are able to train their skills in a practical session. Furthermore, hands-on sessions are organized in the afternoons, which complement the talks on theoretical foundations and implementation issues of different algorithms.

This CECAM summer school, organized by the CECAM Jülich-Node, on *Fast Methods for Long-Range Interactions in Complex Systems* brings together a number of German experts in the fields of mathematical methods and development of algorithms. The presented methods and their efficient parallel implementation are part of the German network project *ScaFaCoS* (Scalable Fast Coulomb Solvers), supported by the German Ministry for Education and Science (BMBF), which aims to build a publicly accessible parallel library.

This preface also gives the opportunity to thank all the speakers, having prepared the lectures and practical sessions. Also we would like to express most cordial gratitudes to Monika Marx, who has put tremendous effort in the realization of the present poster abstracts, WEB pages and lots of plannings. We are also most grateful to Elke Bielitza and Martina Werner who were indispensable for this school by taking care of logistical details, transports, registration, catering and a lot more. Furthermore, thanks are expressed to Oliver Bücker, René Halver for lots of detailed work, technical and administrational support as well as to Jan Meinke and Ulrich Detert for offering presentations and guided tours through JSC.

Jülich, September 2011

Godehard Sutmann
Paul Gibbon
Thomas Lippert

CECAM - Jülich Summer School 2011

Fast Methods for Long-Range Interactions in Complex Systems

	Monday 12 September	Tuesday 13 September	Wednesday 14 September	Thursday 15 September	Friday 16 September
9:00 – 10:30	**Registration**	*F. Gähler* **Local Cutoff-Methods**	*D. Potts* **NFFT and Fast Summation**	*P. Gibbon* **Barnes-Hut Treecode**	Practical Session **Applications**
10:30 – 10:45	**Welcome**	**Coffee Break**			
10:45 – 12:15	*N. Attig* **Challenges in High Performance Computing** *G.Sutmann* **Classical Particle Simulations**	*M. Bolten* **Multigrid Methods**	*A. Arnold* **Fourier Transform-Based and Optimal Methods P^{3}M**	*I. Kabadshow* **Fast Multipole Method**	Practical Session **Applications** N. Eicker **The Future of Cluster Computing**
12:15 – 13:30	**Lunch Break**				**Final Remarks** **Lunch Break**
13:30 – 14:15	*L. Arnold* **Introduction to MPI**	*R. Halver* **ScaFaCoS Interface**	B. Duenweg **Local Approaches to Electrostatics**	*M. Hofmann* **Parallel Sorting**	**Departure**
14:15 – 15:00	*L. Arnold / F. Janetzko* Practical Session **MPI Tutorial**	*R. Halver / F. Gähler* Practical Session **ScaFaCoS Interface**		*P. Gibbon / M. Winkel* Practical Session **Barnes-Hut Treecode**	
15:00 – 16:00			*D. Potts / M. Pippig* *Practical Session* **NFFT and Fast Summation**		
16:00– 17:00			*O. Lenz / F. Fahrenberger* *Practical Session* **Fourier Transform-Based and Optimal Methods and MEMD**	*I. Kabadshow* Practical Session **Experiences with FMM**	
17:00– 17:30	**Get-Together**	**Poster Presentation**			
17:30 – 19:00		**Poster Session**			

Contents

A Survey of the Performance of Classical Potential Solvers for Charge Distributions

Joseba Alberdi Rodriguez and Pablo García-Risueño

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We perform a survey of different methods to calculate the classical electrostatic Hartree potential, created by charge distribution ($\rho(\vec{r})$) in a mesh. Our goal is to provide the reader with a estimation on the performance -both in numerical complexity and in accuracy- of popular solvers (e.g. Conjugate Gradients[1] or Multigrid methods[2–6]), and to give her an intuitive idea about the way these solvers operate. Highly parallelizable new routines (using PFFT[7] and FMM[8] external libraries) have been implemented to be used in our tests, so that reliable conclusions about the capability of methods to tackle large systems in cluster computing can be obtained from our work. For this work the Octopus[9] code has been used and the methods that we compare are the following: (1) FMM, (2) serial FFT, (3) ISF, (4) Parallel FFT, (5) multigrid and (6) conjugate gradients.

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Fractional-step Kinetic Monte Carlo Algorithms and Hierarchical Parallelization

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We present a mathematical framework for constructing and analyzing parallel algorithms for lattice Kinetic Monte Carlo (KMC) simulations[1]. The resulting algorithms have the capacity to simulate a wide range of spatio-temporal scales in spatially distributed, non-equilibrium physiochemical processes with complex chemistry and transport micromechanisms. Our methodology relies on a spatial decomposition of the Markov operator underlying the KMC algorithm into a hierarchy of operators corresponding to the processors structure in the parallel architecture. Based on this operator decomposition, we formulate Fractional Step Approximation schemes by employing the Trotter Theorem[2] and its random variants; these schemes, (a) determine the communication schedule between processors, and (b) are run independently on each processor through a serial KMC simulation on each fractional step time-window.
Furthermore, the proposed mathematical framework allows us to rigorously justify the numerical and statistical consistency of the proposed algorithms, showing the convergence of our approximating schemes to the original serial KMC. The approach also provides a systematic evaluation of different processor communicating schedules. We carry out a detailed benchmarking of the parallel KMC schemes using available exact solutions, for example, in Ising-type systems and we demonstrate the capabilities of the method to simulate complex spatially distributed reactions at very large scales on GPUs.

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Modulation of Band Gap with External Perturbations of Functionalized Graphene Bilayers

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Pristine graphene is a semimetal with zero gap at the Dirac point[1]. The gap can be opened by external perturbations such as strain, electric field[2], and chemical modifications. We have investigated the band structure of bilayer systems having graphene layers functionalized with halogens under external perturbations. We used first principles calculations within the framework of density functional theory (DFT) to describe the dispersion of bands closer to Fermi level using the DFT package FLEUR[3] by applying periodic conditions in two dimensions. Our results show the possible selective modulation of conduction and valence bands of bilayer systems that result in interesting band gap features.

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Capillary Collapse of Colloids: Appearance of Shock–Waves in a Model System for Two–Dimensional Screened Gravity

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Using Brownian dynamics simulations, density functional theory and an analytical perturbation theory, we study the collapse of a finite patch of interfacially trapped colloidal particles of micrometer size, driven by long–ranged capillary attractions. Since these attractions vary logarithmically with the distance, the system is analogous to a two–dimensional (2D) self gravitating one[1]. A crucial difference is the appearance of a tunable screening length through the capillary length λ (typically ~ 1 mm) which strongly influences the dynamics. In the limit $\lambda \to \infty$ the system behaves like a 2D self gravitating fluid, leading to a uniform collapse of the particles towards the center. For finite values of λ, however, theory predicts a ringlike density peak at the outer rim of the collapsing disc moving as a shock wave towards the center. For point particles in a "cold" system, the shockwave becomes singular at finite times, but for particles with a finite size in a "hot" system the singularity is regularized and the shock wave travels inward until the system is compactified[2]. In the simulations, the ringlike peak is resolved into competing smaller clusters. Finally, the influence of hydrodynamic interactions on this capillary collapse will be discussed.

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TRAVIS - A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories

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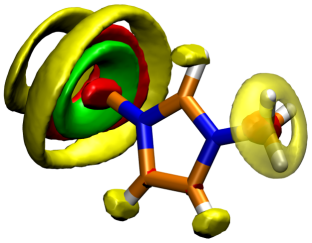
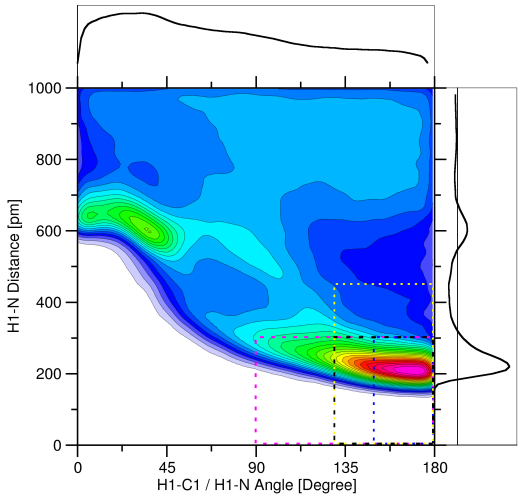


We present TRAVIS (TRajectory Analyzer and VISualizer), a free program package for analyzing and visualizing Monte Carlo and molecular dynamics trajectories. The aim of TRAVIS is to collect as many analyses as possible in one program, creating a powerful tool and making it unnecessary to use many different programs for evaluating simulations. This should greatly rationalize and simplify the workflow of analyzing trajectories. TRAVIS is written in C++, open-source freeware and licensed under the terms of the GNU General Public License (GPLv3). It is easy to install (platform independent, no external libraries) and easy to use. On this poster, we present some of the algorithms that are implemented in TRAVIS - many of them widely known for a long time, but some of them also to appear in literature for the first time. All shown analyses only require a standard MD trajectory as input data.



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2. `http://www.uni-leipzig.de/ travis`

Parallelization of an Efficient Method for Calculating Born Radii

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The Generalized Born Model[1] is one of the most widely used implicit solvent models for simulating biomolecules. Its accuracy and speed crucially depend on the correct calculation of the Born radii used for estimation of the polar solvation free energy[2]. While many improvements in accuracy have been reported over the last years, their implementation in an efficient method remains challenging[3].
Here we present results for the parallelization of a novel method for computing these Born radii on modern multi-core shared memory architectures. Our algorithm[4] constructs an octree reprensentation of the solute and solvent volume inside a bounding box of the molecule. To compute the Born radii an integration over the solvent octree is performed numerically, while the region outside the bounding box is integrated analytically and finally the integral is converted to the Born radius[5]. Parallelization[6] is done by splitting the bounding box into smaller boxes which are then assigned to different worker threads through a queue. Octree construction and integration are then performed independently for each thread. Finally the contributions to the total integral from each thread are summed up to compute the Born radius.
The parallelization performs very well for up to 5 threads, and moderately up to 17 threads, for which the computation of 220387 Born radii of the 70S Ribosome-tRNA complex is reduced to 0.62 seconds. However a further increase in the number of threads leads to longer computation times, thus requiring more code optimization for even better parallelization. The finished implementation of this algorithm will be made publicly available.

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Homology Modeling and Molecular Dynamics Simulations of the Human Wild Type and H1047R Mutant Form of the Catalytic Subunit of PI3K

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The PIK3CA gene is one of the most frequently mutated oncogenes in human cancers[1]. It encodes p110, the catalytic subunit of phosphatidylinositol 3-kinase (PI3K), which phosphorylates phosphatidylinositol 4,5-bisphosphate (PIP2) to convert it to phosphatidylinositol 3,4,5-trisphosphate (PIP3), using ATP. PIP3 activates a variety of downstream effectors that turn on signaling cascades, which lead to cell proliferation, survival, and cell growth[2]. One of the most frequent mutations in PI3K is a histidine changed to arginine in exon 20 (H1047R)[1]. Understanding how the p110 H1047R mutation causes tumorigenesis is central to developing new therapeutics for cancer[3]. To this end, atomistic models of the full-length wt and H1047R mutant p110 were created from the respective crystal structures[4,5], through a combination of homology and loop modeling. Molecular dynamics (MD) simulations in aqueous solution were subsequently carried out for 50 ns for both wt and mutant proteins. Mean square fluctuations were calculated from the last 30 ns, and in conjunction with hydrogen bond and salt bridge analysis, they were utilized to identify regions with different levels of mobility in the two variants. Moreover, predominant conformations of the kinase domain were produced through cluster analysis. Our results indicated three regions with different mobility: (i) the membrane binding loop region (residues 863-888), which is 30% less flexible in the mutant, (ii) the activation loop (939-952), which is 70% more flexible in the mutant, (iii) and the C-terminus (1046-1068), which is 20% more flexible in the mutant, all with respect to the wild type protein. Modeling efforts to construct the regulatory subunit (p85) of PI3K are under way, with the future goal to study the dynamics of the fully functional form of the kinase (p110/p85 heterodimer) and its interaction with the membrane bilayer.

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Development of a Melting Program for Ionic Liquids

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Ionic liquids are salts that are liquid at low temperature ($< 100^{\circ}$C). Even though the first representative has been known since 1914, the interest in ionic liquids has mainly grown in the last twenty years. They were extensively investigated with various experimental and theoretical methods to determine general physical properties as well as their applicability in industrial processes, especially as solvents and catalysts.
Typical examples for the cations are imidazolium, pyridinium as well as ammonium and phosphonium based ions. The anion can be a halogenide or a more complex ion such as bis(trifluoromethanesulfonyl)imide. These ions can be combined almost arbitrarily. Due to the huge amount of available combinations of anions and cations, the physical and chemical properties can be specifically varied over a wide range to obtain the characteristics needed. This is of special interest for their application in industrial processes. Therefore, the prediction of thermodynamic properties, especially the melting point is a task of major importance.
It was shown that classical molecular dynamics is an appropriate tool for the investigation of thermodynamic properties of ionic liquids. The program for simulating the melting process is based on a program to simulate the melting of argon and neon in an isoenthalpic-isobaric ensemble.[1,2] The melting curves for argon and neon calculated by molecular dynamics with forces obtained from an *ab initio* pair potential are in good agreement with the experiment over the whole investigated temperature range (i.e. from 30 to 280 K). The melting process is induced by a void centered in the simulation box. After the equilibration of the lattice a certain amount of atoms is removed from the system and the temperature is increased gradually. The criterion for melting is defined through a translational order parameter. In this contribution, we would like to present the approach used for this simulations in detail.

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Polymorphism in amorphous $Ge_2Sb_2Te_5$: comparison of melt-quenched and as-deposited structures

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The technological applicability of phase-change materials (PCM) for data storage and computer memory is based on the rapid amorphous-to-crystalline transition and subsequent changes in optical (and electrical) properties. The structure of the amorphous phase poses the main problem and is difficult to tackle both experimentally and theoretically. Our group has previously published results for the $Ge_2Sb_2Te_5$ (DVD-RAM alloy) and Ge_xTe_{1-x} alloys, which were obtained by performing massively-parallel density functional (DF) / molecular dynamics (MD) simulations[1]. We reported that atoms on GeTe-based materials can be classified into atomic types A (Ge,Sb) and B (Te), with strong AB alternation, and that the main structural motif of such materials is a four-membered $ABAB$ ring (ABAB square).

Atomistic simulations on phase-change materials have focused on melt-quenched (MQ) samples, and both system size and quench time have posed challenges. We present here results of massively-parallel DF simulations of the as-deposited (AD) amorphous structure of the prototype phase change material $Ge_2Sb_2Te_5$. We have studied a 648-atom sample generated by computer-aided deposition at 300 K and compare the results with those for a 460-atom MQ sample we reported previously[2]. The AD structure differs from MQ in essential ways: (1) Ge atoms are predominantly tetrahedrally coordinated, (2) homopolar and Ge-Sb bonds are more common and reduce the number of $ABAB$ squares, the characteristic building blocks of the material[3]. The first observation resolves the contradiction between measured and calculated Ge-Te bond lengths, and the latter explains the large differences in crystallization speeds. Sb and Te are more highly coordinated than expected from the 8-N rule (N is the number of valence electrons), and amorphous $Ge_2Sb_2Te_5$ cannot be regarded as a covalent network glass.

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Accuracy and Scaling of Raytracing Photoionisation Algorithms

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Modelling photoionisation in multidimensional hydrodynamics codes is an important but computationally intensive problem in Astrophysics. Three raytracing+photoionisation algorithms commonly used in hydrodynamics grid codes are compared in terms of accuracy, timestepping criteria, and parallel scaling. It is shown that explicit methods with first order time accuracy for photon conservation[1,2] must use very restrictive timestep criteria to accurately track hypersonic ionisation fronts. Second order accurate algorithms require more work per step but allow much longer timesteps and are consequently more efficient. The accuracy of both explicit algorithms as a function of timestep limit is evaluated in simple 1D test problems, clearly demonstrating the advantages of the second order algorithm. Moving to a second order algorithm would be a very simple modification to a number of fixed grid and AMR codes currently using explicit photoionisation methods.
Implicit methods (e.g. the C^2-ray method[3] and similar algorithms[4]) allow ionisation fronts to cross many grid cells per timestep while maintaining a high degree of photon conservation. They thus use only a fraction of the number of timesteps which an explicit algorithm requires to model fast moving ionisation fronts. For this reason, even though explicit methods scale more efficiently on parallel supercomputers, implicit methods remain competitive when total time to solution is considered. The parallel scaling of the implicit method and the second order explicit method are compared for different 2D and 3D problems using 8-512 cores. Both methods have comparable total runtime but, for 2D calculations modelling both fast winds and ionising radiation from massive stars, the explicit integration runs somewhat more efficiently than the implicit one.

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Worm Algorithm in Ordered and Disordered Media

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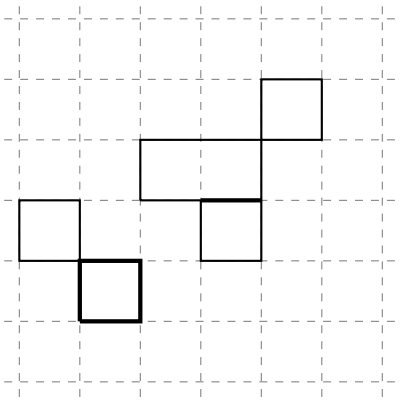
The Worm algorithm is a Monte Carlo method for simulating classical spin systems. It was introduced by Prokof'ev and Svistunov in 2001[1]. The algorithm based on the high-temperature expansion of the partition function

$$Z = \sum_{N_b \in \mathrm{CP}} \prod_b \frac{(\beta J)^{N_b}}{N_b!}, \tag{1}$$

where N_b denotes the bondstate of a single bond. The algorithm works only locally, but



A graphical representation of a state from the configuration space. The width of the solid line represents the corresponding bond state, dashed lines mean $N_b = 0$.

the works of Prokof'ev and Svistunov and a few others[2,3] suggest that it does not suffer from critical slowing down. We study the behavior of the worm algorithm for the Ising model for ordered and for diluted and disordered systems, especially at the critical point. We expanded the algorithm to such systems and introduced several estimators for common observables. We could confirm that the critical slowing down has no practical influence for the Worm algorithm. This also holds for disordered and diluted systems.

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Long-Range Coulomb Contributions to the Elastic Interactions in $KCuF_3$

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We have developed, within the harmonic approximation, a computational method to obtain the elastic constants for local lattice distortions. In particular we study the case of $KCuF_3$ whose lattice instability, given by the fluorines around copper, show the JT effect. The method consists in the next steps. Firstly, for the corresponding unit cell of the crystal, the energy of single and pair atomic distortions are calculated by means of density functional theory (DFT). Subsequently, we estimate the long-range Coulomb (LRC) energy using the Ewald summation. The difference between the DFT and the LRC energies leads to energetic variations within a small region of the lattice. Lastly, after fitting a polynomial to the "local-energy" curve as a function of displacement around the equilibrium position, we assign elastic constants to the local distortions.

NanoParticle Interactions with Pre-Stressed Lipid Bilayers

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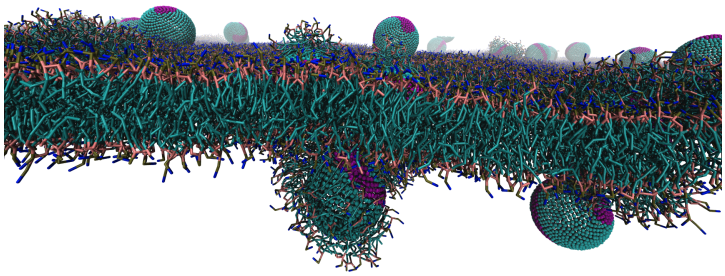
NanoParticles (NP) are widely used in biomedical applications ranging from directed drug delivery to tumor identification agents. Before one can exploit the NP properties, the nature of their interaction with the cell plasma membrane must be investigated. The translocation of NPs across the membrane depends upon many factors such like surface chemistry and size and membrane mechanical properties. However, the cell via the actin filaments regulates the surface tension of the plasma membrane, changing tis mechanical properties.
We employ a coarse grained molecular simulations using the Martini[1] model to clarify the effect of membrane pre-tension on the type of NP internalization. A constant surface tension (γ) ensemble ($N\gamma T$) is used to keep the membranes pre-tensed. Quantification of the effective interaction of a single NP with a Dipalmitoylphosphatidylcholine (DPPC) lipid bilayer is achieved through the use of Umbrella Sampling simulations combined with the weighted histogram method. We correlate the membrane surface tension to the permeability of the NP[2]. Unconstrained molecular dynamics simulations with multiple NPs over large membrane domains reaching into the μs timescales are used to investigate synergism in the NP update by lipid bilayers (Fig.1). Long range stress correlations, more than 100 nm are found to link the adsorbed amphiphilic NPs. NPs have been modeled to contain charged domains, affecting their interaction with the model bilayers.



Simulation snapshot of a 200×200 nm DPPC bilayer with multiple NPs. Cyan NP-beads denote hydrophobic sites whereas red ones hydrophilic. NPs have a diameter of 6nm.

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Azobenzenes Self Assembled Monolayers

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The photoisomerization process of azobenzene is widely studied both in solution and on metal surfaces[1,2], because of its efficiency and controllability. These features makes the azo-SAM a promising tool for controlling the movement of nano-objects with light. A preliminary study on the thio-azobenzene single molecule (thio-AZO) and on structural properties of a thio-AZO self assembled monolayer (SAM) on gold (111) surface is presented in this work. Both quantum mechanical calculations and classical simulations are used: electronic structure and geometry optimizations are performed with DFT methods whereas molecular dynamics (MD) simulations are run with pairwise potentials (OPLS/AA) and fixed charges. using models based on these approaches, we have studied the mechanical stiffness of the monolayer in the cis- and in the trans- form. calculated results agree with available experimental data, notwithstanding the use of a literature potential[3] which is not fully optimized for our systems. The testing of new reactive force fields and the optimization of a specific pairwise potential are in progress. For this purpose a wide sampling of the potential energy surfaces (PES) function has been done by means of QM methods. Preliminary tests show that QM-PES functions are well reproduced by our optimized force field.

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Magnetic Structures in Convecting Plasmas

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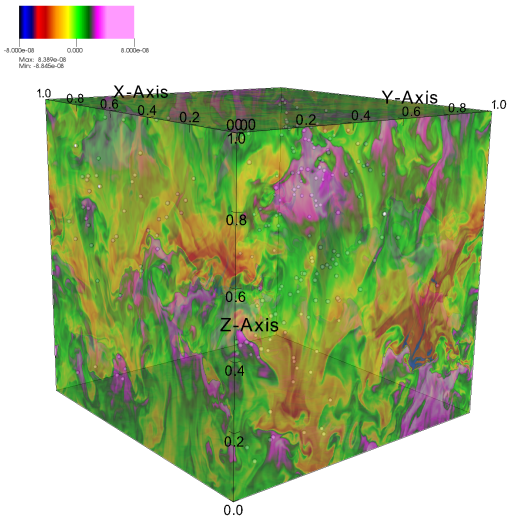
By tracking the movements of Lagrangian particles, we examine the formation of large-scale magnetic structures and current filaments in steady-state 3D turbulent magnetoconvection maintained by dynamo action. The movement of fluid particles evolves differently when large structures develop in the convecting plasma[1], and this difference is reflected in Lagrangian statistics[2]. Lagrangian statistics in the steadily convecting flow are calculated using the order-n method of Dubbeldam *et al.*[3] Our simulation employs the Boussinesq approximation to the MHD convection equations to allow for small differences in plasma density resulting from buoyancy. Pseudo-spectral simulations performed at a resolution of 512^3 solve these equations for a geometric cube of plasma with an imposed mean temperature gradient. Boundary conditions are fully periodic and disallow vertical streamers, specifically $k_z = 0$ modes.



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Thermoelectric Currents and their Role in Edge Localized Mode Formation in the JET Tokamak

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A recently developed numerical model[1], describing a self amplification and structure formation process which is used to model the initial nonlinear growth phase of edge localized modes (ELMs), is applied to the JET tokamak. Connection length simulations of the magnetic topology, including only error fields, for JET reveal the existence of small, so called short connection length flux tubes[2]. Such a configuration is used as starting point for the model. Thermoelectric currents are assumed to flow in the short connection length flux tubes and add additional magnetic perturbations which change the magnetic topology severely. The change in magnetic topology leads to the formation of new, much larger short connection length flux tubes that can conduct much larger currents through the plasma edge. The current density inside the flux tubes is assumed to be constant to calculate the total current. This self amplification process leads to the formation of patterns, known as footprints, on various segments of the inner wall throughout the vessel. The resulting footprints are discussed.

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From Hydrophobic to Super-Hydrophobic Behaviour: A Multiphase Molecular Dynamics Study of Water on Nano-Rough Surfaces

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Nature has developed and optimised some surfaces for self-cleaning and drag reduction purposes. Scientists and engineers try to develop and manufacture biomimetic surfaces with similar properties[1]. Some of the most known and extensively studied natural surfaces with the above mentioned properties are the lotus leaf and shark's skin, respectively. The hydrophobic nature of the surface materials in combination with micro-roughness lead to super-hydrophobic behaviour. In our research we study the effect of nano-roughness and whether this can produce similar enhancements. We perform a series of simulations, starting from smooth, pristine graphene surfaces[2] to rough surfaces with or without the presence of a nano-thick air layer. We used the TIP4P/2005 water model[3], while interaction potentials between the solid surfaces and water molecules were parametrised by empirically matching the water contact angle (WCA) on each surface.
Chemical etching, carbon nanotube (CNT) growth or other manufacturing processes can produce nano-rough surfaces. The existing nano-cavities on these surfaces can trap air molecules that increase the hydrophobicity of the surface and at the same time reduce the drag.
In general, vapor layer formation near the interface is likely to be enhanced in the vicinity of hydrophobic surfaces. This is primarily due to the structure of water molecules next to a hydrophobic surface which are less ordered than in bulk. Accordingly, cohesive strength of water may be significantly reduced. Once the nuclear barrier is exceeded, the thin vapor layer is formed on the solid surface[4]. Due to the presence of the gas filled sub nano-cavities, bubbles grow to cover the corrugate surface, and a dewetting transition leads to a super-hydrophobic state. Dewetting transition dependence of capillary number is also reported in the present study.

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Lattice Boltzmann Simulations on GPUs with ESPResSo

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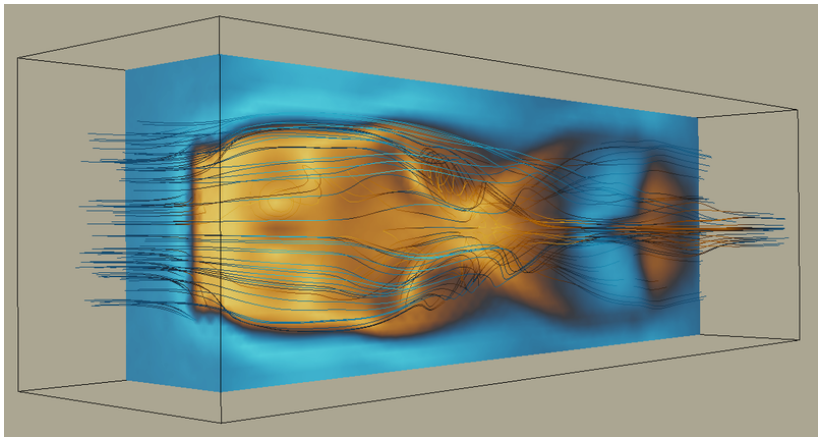

Visualization of the velocities of a turbulent flow field. Blue represents high and yellow low values.

In coarse-grained Molecular Dynamics (MD) simulations of large macromolecules, the number of solvent molecules is usually so large that most of the computation time is spent on the solvent. For this reason one is interested in replacing the solvent for example by a lattice fluid using the Lattice-Boltzmann (LB) method. The LB method is well established and is known to lead to a hydrodynamic flow field on large lengths and timescales, that satisfies the Navier-Stokes equation. If the lattice fluid is coupled to a conventional particle-based MD simulation, it mediates a hydrodynamic long range interaction between the particles. Coarse-grained simulations are usually performed in the isothermal ensemble, which in this case requires to thermalize both the particles and the fluid. While the MD particles are easily coupled via frictional terms to the fluid, the correct thermalization of the lattice fluid requires to switch into mode space, which makes thermalized LB more complex and computationally expensive[1].
Being a lattice method, LB is particularly well suited for the highly parallel architecture of graphics processors (GPUs). We present a fully thermalized GPU-LB implementation which is coupled to a MD that is running on a conventional CPU using the simulation package ESPResSo (http://www.espressomd.org). In our implementation, the LB update is largely independent of the MD propagation, which allows to arrange the parts calculated on the GPU to be calculated while the CPU code calculates the MD forces. Furthermore, the

memory is allocated such that it allows for coalesced access to fluid value structures. The MD core is parallelized via the Message Passing Interface (MPI), which allows to make use of recent multi core processors or parallel computers. Our LB implementation runs up to 50 times faster on a single NVIDIA Tesla C2050 than an equivalent CPU implementation on two recent Intel Xeon E5620 quadcore CPUs, therefore replacing a full compute rack by a single desktop PC with a high end graphics card.

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Anomalous Diffusion in Membranes

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Biological membranes are one of the basic constituents of cells which play an essential role in both isolating them from the environment and controlling the flux of particles between the interior and the exterior of the cell. They consist of a lipid bilayer, containing also abundant amounts of proteins, glycolipids, and cholesterol. Lateral diffusion of molecules in membranes plays an essential role in a variety of cellular processes, such as signaling, formation of lipid rafts, and apoptosis. The nature of these diffusion processes is still under debate. Fluorescence correlation spectroscopy, which is sensitive to motions of the lipid molecules on the millisecond time scale, reveals anomalous lateral diffusion[1], with a mean square displacement of the diffusing particles evolving as

$$\langle [\mathbf{x}(t) - \mathbf{x}(0)]^2 \rangle = 2D_\alpha t^\alpha$$

with $0 < \alpha < 1$ (subdiffusion). Molecular dynamics simulation and NMR relaxation spectroscopy following the lateral dynamics of the lipid molecules on the nanosecond time scale support, in contrast, the the picture of transient anomalous diffusion[2] or normal diffusion ($\alpha = 1$)[3]. In this work we present results from molecular dynamics simulations of a lipid bilayer consisting of 274 POPC molecules and 38 water molecules per lipid, which confirm the observation of anomalous lateral diffusion by fluorescence correlation spectroscopy in Ref.[1] as well as recent simulation results from a smaller system of a fully hydrated DOPC bilayer[4]. The results are interpreted within the framework of the generalized Langevin Langevin equation, taking into account appropriate conditions for anomalous diffusion[5].

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Enriched Finite Element Solution for the All-Electron Coulomb Problem in Solids

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The computation of the electrostatic potential and total energy of crystalline solids has been an ongoing problem in solid state physics. In quantum mechanical calculations, the electrostatic potential is constructed as a sum of nuclear and electronic terms. In an infinite crystal, each of these terms diverges and the sum is only conditionally convergent due to the long-range $1/r$ nature of the Coulomb interaction. A common approach to such all-electron Coulomb problems is to smear the nuclear point charges (distributed nucleus approximation) and solve the resulting smoothed but strongly inhomogeneous problem in a basis which can be concentrated in the vicinity of the nuclei. Accurate solutions require strongly localized nuclear charges and so highly refined basis sets in the vicinity of the nuclei. The most common approach in highaccuracy calculations employs a combined spherical-harmonic and Fourier representation and so has $\mathcal{O}\left(N \log N\right)$ complexity.
In this poster, I will present a systematically improvable, linear-scaling formulation for the all-electron Coulomb problem in periodic solids that avoids the need for distributed nucleus approximations, Ewald sums, and operations in reciprocal space[1]. Linear scaling is achieved by introducing smooth, strictly local neutralizing densities to render nuclear interactions strictly local and solving the remaining neutral Poisson problem for the electrons in real space. The resulting formulation is amenable to solution using basis sets that are in H^1. In the numerical computations, we employ finite element and enriched finite element methods (adaptive integration scheme is adopted) to demonstrate the accuracy and convergence of the approach by direct comparison to standard Ewald sums and application to all-electron diamond.

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Cascade of Vortex Tube Collisions at $Re_\Gamma = 10\,000$

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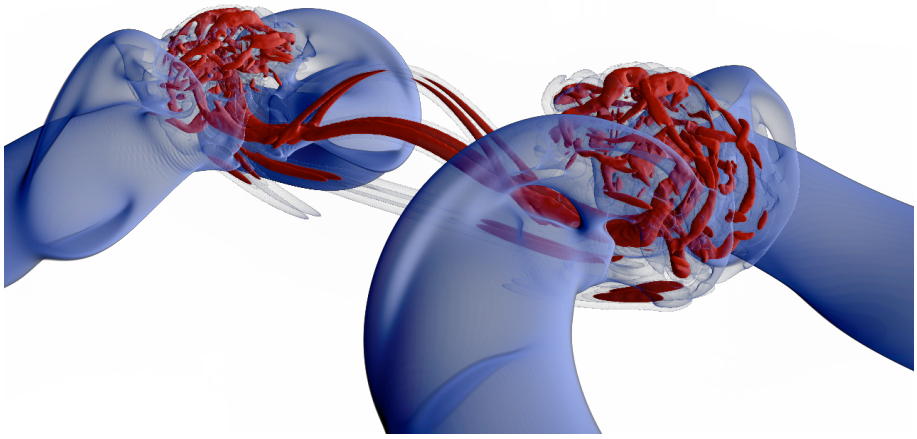
We present simulations of the collision of two anti-parallel vortex tubes, with and without axial flow in a periodic box at $Re_\Gamma = 10\,000$ using a remeshed vortex method[1]. In the non-axial flow case, after the first, well-known vortex reconnection of the tubes (Fig. 1), a quiescent period is followed by a second vortex collision of the remaining structures. The characteristics of this second collision are an increase of energy in the small scales of the flow; remnant vorticity left behind in thread-like structures; a persistent $-7/3$ slope in the three-dimensional energy spectrum; and a significant increase in enstrophy and helicity in the flow. Characteristics of the secondary collision are also observed during the first reconnection of the vortex tubes with axial flow.
The simulations indicate that vortical flows containing initially large-scale vortical structures can transfer energy from large scales to smaller scales through a cascade of vortex collisions.



Volume rendering of the vorticity field for the collision of two anti-parallel vortex tubes, after the first reconnection and before the quiescent period

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SWARM-ARRAY COMPUTING
Autonomic Approaches Towards Achieving Automated Fault Tolerance in HPC Systems

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The increasing number of faults that occur in large scale high-performance computing systems cannot be efficiently administered with existing and traditional fault tolerant techniques which are manual. In this research a framework is proposed that directly the problem of the reliance of conventional approaches for fault tolerance on human intervention and the large times required for reinstating execution once a fault has occurred. Development of a novel framework is the outcome; a framework for achieving automated fault tolerance in high-performance computing systems, which is referred to as 'Swarm-Array Computing'.

The swarm-array computing framework brings together the concepts of parallel computing, high-performance computing, autonomic computing and multi-agent systems. The framework rests, first, on the notion that the arrays of cores of a high-performance computing system represent a landscape on which a parallel computing task can be distributed. It takes the idea, second, that these parallel computing tasks can be carried onto the landscape aboard a set of mobile agents. Each agent set, equivalent to a robot swarm, and representing a specific parallel computing task, can move across the landscape to find a locale where it can thrive (i.e. execute its task amid an abundance of computing resources). Areas of available computing resources represent lower-lying areas in the landscape.

Three approaches, which are supported by experimental studies, as a means for achieving automated fault tolerance. In the first approach, software agents are able to make decisions about the expected failure of a computing core and relocate to a safe core[1]. In the second approach, this intelligence is located within the computing cores, which make decisions about their possible failure and push the software agents onto neighbouring cores[2]. In the third approach, these two forms of intelligence are combined in a hybrid system with an arbitration mechanism to select which intelligence type is given priority when the imminent failure of a core is detected[3]. The key result is that task can be relocated without manual intervention and with a time delay in the order of milliseconds.

The above concepts form one of the elements of the notion that brings self-management to the work from the field of Autonomic Computing[4]. A second element is in the intelligence embodied within both the cores and the mobile agents to sense and to act proactively when the imminent failure of a core is predicted. In order to support this, a cognitive architecture for the agents is offered[5].

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Optimizing Working Parameters of the Smooth Particle Mesh Ewald Algorithm in Terms of Accuracy and Efficiency

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The computation of long range interactions under periodic boundary conditions is frequently encountered in molecular simulations. However, the very slow decay of the interactions with respect to the distance introduces an essential computational difficulty. A group of commonly used methods to solve this problem are the mesh-based methods, for example, the Particle–Particle–Particle–Mesh method (P3M)[1,2], the Particle Mesh Ewald method (PME)[3] and the smooth Particle Mesh Ewald method (SPME)[4]. These techniques have been successfully employed in computer simulations, but their parameters cover a large space, which should be optimized for speed and accuracy. For SPME, we are going to tune 4 parameters, one of which is a 3 component vector, therefore there are 6 degrees of freedom. Without any knowledge of how accurate and fast the method is, it is nearly impossible to try out the optimal combination of parameters in such a high dimensional parameter space.

The parameter determination can be split into two steps. First, one has to obtain the desired accuracy. The best way is to have an analytical error estimate, that is to know how much error will be introduced as a function of parameters. Then among those sets of parameters satisfying the accuracy requirement, one can choose the most time-saving one. Error estimates exist for the PME[5], and for the P3M[6]. Also a parameter tuning algorithm for the P3M has been implemented in the simulation package ESPResSo[7], based on Ref.[6].

The main contribution of our work is to provide an, so far missing, error estimate for SPME of homogeneously charged systems. Furthermore a work flow optimizing the parameters in respect to speed and accuracy is proposed and tested. Two branches of SPME are considered, i.e. the *ik*– and *analytical* differentiation, that just differ in the method of the force calculation. Then results of various computational tests are discussed, that demonstrate the reliability of the automatically derived parameters. Finally we show the equivalence of *ik*– and *analytical* differentiation in terms of efficiency, and the parameter tuning according to a reference system.

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Collective Dynamics in Molten Alkali Halides

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We present classical molecular dynamics (MD) simulations with the Born- Huggins-Mayer-Tosi-Fumi potential that reproduce very well the dynamic structure factors of NaCl and KCl, and less well that of NaI, measured with inelastic X-ray scattering[1]. We show that phonon dispersion relations can be obtained from MD trajectories by analysing the appropriate time correlation functions[2]. The advantages with respect to
tting the spectra are that a physical model is not needed, phase information is not lost, and the same accuracy can be achieved with shorter MD runs. We automatized the data analysis using harmonic inversion[3].

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Structure of the Tip4p Water Model in the Ice I_h Phase

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Potential water models have been widely used throughout the last decades in a variety of computer simulations. Especially in the simulations of processes where water is used as a solvent, the influence of the model is easily underestimated and can provide a large source of error. We investigated the behavior of the Tip4p model[1] with different parameterizations[1–3] in the hexagonal, ordinary ice phase. The interactions included the 12-6 Lennard Jones and the Coulomb interaction, which is known for its long interaction range and requires careful attention. To this end, random spherical nano sized water clusters were arranged in the experimentally determined tetrahedral structure. These configurations were minimized in energy with a semi-dynamic technique, resulting in local energy minimum configurations of the specific water model. The mean bond length and bond angles were measured in the core regions of the local minimum configurations, characterizing the crystal structures. The results confirmed the stability of the hexagonal structure for all considered parameterizations.
In the ordinary ice phase, the water molecules may be arranged in $(3/2)^N$ degenerate ground states resulting in a residual entropy[4]. This residual entropy has been verified in experiment[5] and recently investigated in computer simulations[6]. We found that the degeneration was slightly lifted due to the geometry of the model.
In addition, we performed Monte Carlo simulations investigating the influence of the lattice constant and possible energy cutoffs on small systems with periodic boundary conditions. A study of these systems with statistical tools promises more insight into the behavior of water in and near the ice phase.

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