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Fast Methods for Long-Range Interactions in Complex Systems

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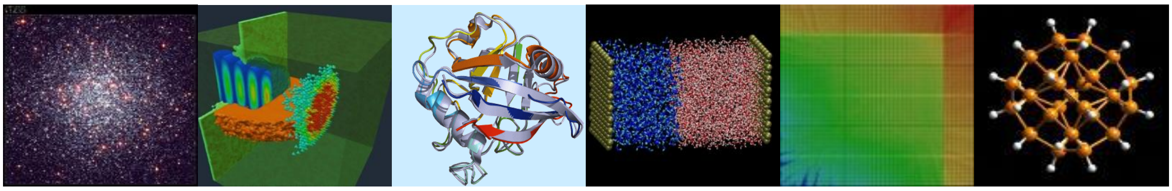

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Poster Presentations

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Preface

Computer simulations of complex particle systems have a still increasing impact in a broad field of physics, e.g. astrophysics, statistical physics, plasma physics, material sciences, physical chemistry or biophysics, to name a few. Along with the development of computer hardware, which today shows a performance in the range of PFlop/s, it is essential to develop efficient and scalable algorithms which solve the physical problem. Since with more powerful computer systems usually also the problem size is increased, it is important to implement optimally scaling algorithms, which increase the computational effort proportionally to the number of particles.

Especially in fields, where long-range interactions between particles have to be considered the numerical effort is usually very large. Since most of 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 are $O(N^2)$ for open systems or include infinite lattice sums in periodic systems, fast implementations rely on approximations. Although, in principle, various methods might be considered as *exact representations* of the problem, approximations with controllable 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 including inhomogeneous dielectric properties, require the implementation of different electrostatic methods. Furthermore, the interdisciplinary character of the problem led to the fact that either very similar methods or complementary methods were developed independently in parallel in different disciplines or were *discovered* in other research areas and adopted to other fields.

Therefore the present school does not only focus on one 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

In addition to the mathematical description of the methods, focus is given to the parallelization and implementation on parallel computers. Therefore, also a special session is devoted to an introduction to parallel programming and various parallelization paradigms (MPI, OpenMP, PThreads). Practical sessions complement the talks on theoretical foundations and implementation issues of different algorithms.

This first summer school 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), sponsored by the German Ministry for Science and Education (BMBF), which aims to build a publicly accessible parallel library.

Financial support of this school came from the Wilhelm and Else Heraeus Foundation, which is gratefully acknowledged. 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 lots of effort in the realization of the present poster abstracts, lecture notes, WEB pages and lots of plannings. We are also most grateful to Elke Bielitza who was indispensable for this school by taking care of logistical details, transports, registration, catering and a lot more. Further thanks are expressed to Johannes Grotendorst who gave valuable advice and expertise of organizational details and also to Oliver Bücker, René Halver, Thomas Plaga and Marga Vaeßen for technical and administrational support.

Jülich, September 2010

Paul Gibbon
Thomas Lippert
Godehard Sutmann

WE-Heraeus Summer School 2010

Fast Methods for Long-Range Interactions in Complex Systems

	Monday **6 September**	**Tuesday** **7 September**	**Wednesday** **8 September**	**Thursday** **9 September**	**Friday** **10 September**
9:00 – 9:30	**Registration**	*G. Sutmann* **Parallel Algorithms for Particle Simulations**	*M. Bolten* **Multigrid Methods for Longe-Range Interactions**	*P. Gibbon* **Parallel Tree Methods I**	*F. Gähler* **Local Cutoff-Methods for Long-Range Interactions I**
09:30 – 10:15	**Welcome**	*D. Potts* **Non-Equidistant Fast-Fourier Transforms**	*M. Bolten* **Parallel Multigrid**	*P. Gibbon* **Parallel Tree Methods II**	*F. Gähler* **Local Cutoff-Methods for Long-Range Interactions II**
10:15 – 10:45	*N. Attig* **Challenges in High Performance Computing**	**Coffee Break**			
10:45 – 11:30	**Coffee Break**	*D. Potts* **NFFT and Fast Summation**	*A. Arnold* **Fourier Transform-Based Methods I**	*I. Kabadshow* **The Fast Multipole Method**	*N. Eicker* **The Future of Cluster Computing**
11:30 – 12:15	*G.Sutmann* **Particle Simulation Methods**	*D. Potts / N. Pippig* **Parallel NFFT and Fast Algorithms**	*A. Arnold* **Fourier Transform-Based Methods II**	*I. Kabadshow* **Periodic FMM & Parallel FMM**	**Final Remarks** **Visit of JSC Facilities**
12:15 – 13:30	**Lunch Break**				
13:30 – 14:15	*L. Arnold / A. Schiller* **Introduction to MPI & Parallel Computing**	*M. Bolten* **The Multigrid Method**	*A. Arnold* **Optimal Methods: P^{3}M**	*R. Speck / M. Winkel* **Introduction to PEPC**	**Departure**
14:15 – 14:45	Practical Session **Parallel Computing**	*D. Potts / M. Pippig* **Introduction to Practical NFFT**	*O. Lenz / A. Arnold* **Introduction to Espresso**	Practical Session **Experiences with PEPC**	
14:45 – 15:45		Practical Session **Experiences with NFFT**	Practical Session **Experiences with Espresso**		
15:45 – 16:15				*I. Kabadshow / H. Dachsel* **Practical FMM**	
16:15 – 17:00				Practical Session **Experiences with FMM**	
17:00 – 17:30		**Poster Presentations**	**Social Programme** **Excursion to Aachen**		
17:30 – 19:00	**Get-Together**	**Poster Session**			

Contents

Molecular Dynamics of Metal Oxide Systems with Long-Range Interactions

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The simulation of oxide systems is less advanced compared to metals or covalent materials because of the occuring electrostatic interactions of both charges and dipoles which are long ranged. We use the Wolf[1] direct, pairwise r^{-1} summation method with spherical truncation for charges. With Wolf summation, the computational effort scales linearly in the system size. A convergence parameter κ according to the Ewald parameter of the well known Ewald[2] summation allows to perform only a direct summation in real space. Energy conservation is achieved by a suitable shift of the potential. Furthermore we extended the Wolf summation to dipolar interactions.

The polarizable oxigen atoms in a metal oxide are described with the Tangney-Scandalo[3] (TS) interaction force field where the dipole moments are determined by iteration to a self-consistent solution. The short range interactions are treated with a pair potential of Morse-stretch form.

As a first result simulations[4] of microstructural and thermodynamic properties in silica are shown, which agree with the TS results but reduce the simulation time by up to three orders in magnitude.

References

1. D. Wolf, P. Keblinski, S. R. Phillpot and J. Eggebrecht, J. Chem. Phys. **110**, 8254, 1999.
2. P. P. Ewald, Ann. Phys. **369**, 253, 1921.
3. P. Tangney and S. Scandalo, J. Chem. Phys. **117**, 8898, 2002.
4. P. Brommer, P. Beck, A. Chatzopoulos, F. Gähler, J. Roth and H.-R. Trebin, J. Chem. Phys. **132**, 194109, 2010.

Heme Transport in Gram Negative Bacteria

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Molecular Dynamics Simulation[5] plays an important role in protein science today. It has been successfully used to predict protein-ligand interactions on the atomic level and to calculate free-energies. MD can also be used to investigate the stability of protein-protein complexes and to determine the residues mainly involved in complex stability.

Using Newton's second law of motion the movements of every atom are computed as a function the position of the other atoms in the system. With this one arrives at a time resolved image of the behavior of a protein.

Unfortunately this method is computationally very demanding, so only short time frames of a few hundred nanoseconds (where a protein does not leave a given local minimum of its conformational space) can be calculated, whereas biologically relevant processes can take up to several milliseconds.

Upon binding of a ligand or other protein, large conformational changes can happen in a very short time. The protein will then find itself in a different minimum of its conformational space. To observe these rare events on a computer one has to artificially bias the system, encouraging the protein to perform the reaction of interest.

We recently reported crystal structures of a protein complex involved in the iron uptake system of gram-negative bacteria[4]. This system involves a small protein with a bound heme-molecule (HasA) binding to a transmembrane receptor (HasR) and transferring the heme in the process. The heme is then transported through the channel into the periplasmic space.

Using targeted MD[3] we were able to show the binding process of HasA to the receptor HasR and the conformational changes of HasA involved in the process. We were also capable of showing the heme transfer between the proteins and delivered an explanation why one of the reported mutations was unable to transfer the heme.

Using steered MD[2] we were able to simulate transport through the transmembrane pore of the receptor. We simulated the energy transfer of a helper protein (HasB, a TonB homolog) which results in an unfolding of the plug domain and subsequent transport of the heme bound to one residue of the plug[1].

References

1. Gumbart et al., Biophysical Journal **93**, 496, 2007.
2. Jensen et al., Proc.Natl. Acad. Sci. **99**, 6731, 2002.
3. Schlitter et al., J. Mol Graph. **12**, 2, 1994.
4. Krieg et al., PNAS **106**, 1045, 2009.
5. Case et al., University of California, San Francisco, 2004.

Ergodicity Breaking and Magnetism in Nanosystems

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We first discuss the occurrence of an ergodicity breaking energy threshold in anisotropic spin systems and we show that this threshold determines magnetic reversal times. We called this threshold Topological Non-connectivity Threshold (TNT). Below this threshold the system is non ergodic, which is: it cannot explore the available constant energy surface. This implies that in an isolated system the magnetization cannot reverse its sign below the TNT, while above the TNT we found a power law divergence of the magnetic reversal times at the TNT.

In case of long range interaction among the spins, the disconnected energy portion determined by the TNT remains finite, even in the large particle number limit. On the other hand for nanoscale structures, the TNT has important consequences both for short and long range interacting spins.

When the system is in contact with a heat bath, the magnetization can reverse its sign even below the TNT, but this threshold has still important consequences on magnetization reversal times: this threshold represents an effective energy barrier for magnetic reversal, so that for average thermal energy below the TNT, the reversal times depend exponentially on this energy barrier.

In order to understand whether the TNT can determine a ferromagnetic behaviour in nanoscale structures, due to long magnetic reversal times, we analyze realistic long range interactions, such as the dipole interaction and the RKKY interaction, which might be responsible for the ferromagnetic behaviour of diluted magnetic semiconductors, with a Curie temperature around $100K$ and for the room temperature ferromagnetic behaviour of diluted ferromagnetic oxides, having Curie temperatures far in excess of $300K$.

References

1. F. Borgonovi, G. L. Celardo, B. Goncalves, L. Spadafora, *Magnetic Reversal Time in Open Long Range Systems*, Phys. Rev. E **77**, 061119 (2008).
2. G. L. Celardo, J. Barre, F. Borgonovi, S. Ruffo, *Time Scale for Magnetic Reversal and The Topological Non–connectivity Threshold*, Phys. Rev. E **73**, 011108 (2006).
3. F. Borgonovi, G. L. Celardo, M. Maianti, E. Pedersoli, *Broken Ergodicity in classically chaotic spin systems*, Journal of Statistical Physics, Vol. **116**, Nos. 1435, September (2004).

Relaxation of Dynamical Systems with Long-Range Forces: A Numerical Investigation

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We study the dynamical relaxation of spherical systems governed by $r^{-\alpha}$ forces, by numerically integrating the equations of motion of N (pressureless) mass shells. The initial conditions are characterized by a very low virial ratio, i.e. they lead to a cold collapse. The code [2] generalizes to the case of arbitrary values of α Hénon's code (originally developed to study globular clusters in Newtonian gravity, i.e. $\alpha = 2$, [3]). We found that for all the explored values of α the relaxation process involves first a rapid Violent Relaxation phase [6] , followed by a longer and gentle relaxation phase due to Phase Mixing. For α increasing from 1.2 to 2.6, some dynamical characteristics (such as the relaxation time in units of dynamical time) increase or decrease steadily. In general, systems involving force laws with $\alpha < 2$ have longer mixing times compared to those of systems with $\alpha > 2$, that are by contrast characterized by faster evaporation that results in a fast core-halo segregation.The final relaxed states are very similar and well described by an exponential differential energy distribution. From an astrophysical point of view some of the results can be useful to our understanding of Modified Newtonian Gravity, where the relaxation mechanisms are not well understood (see, e.g. [7]).

References

1. P. H. Chavanis, *Dynamics and thermodynamics of systems with long-range interactions: interpretation of the different functionals*, Dynamic and Thermodynamics of systems with long-range interactions: Theory and Experiments. AIP Conference Proceedings, Volume 970, pp. 39-90, 2008.
2. P. Di Cintio, *Relaxation of dynamical systems with long-range interactions*, Bologna University, Master Thesis (Unpublished), 2009.
3. M. Hénon, *Evolution Initiale d'un Amas spherique*, Annales d'Astrophysique, 27, vol.2, pp. 83-8, 1964.
4. M. Joyce & T. Worrakitpoonpon, *Relaxation to thermal equilibrium in the self-gravitating sheet model*, arXiv1004.2266J.
5. H. E. Kandrup, *Violent Relaxation, Phase Mixing, and Gravitational Landau Damping*, ApJ, 500, pp 120-128, 1998.
6. D. Lynden-Bell, *Statistical mechanics of Violent Relaxation in stellar systems*, MNRAS, 136, pp 101-121, 1967.
7. C. Nipoti, P. Londrillo, L. Ciotti, *Dissipationless collapse in modified Newtonian dynamics*, ApJ, 660, pp 256-266, 2007.

8. I. V. Pogorelov & H. E. Kandrup, *Energy trapping in loaded string models with long- and short-range couplings*, Annals of the New York Academy of Sciences vol. 1045: Non linear dynamics in Physics and Astronomy, in memory of Henry Kandrup. ed Wiley InterSciences, 2005.

In Silico Titration of Biomolecules: Molecular Dynamics at Constant pH

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When addressing the structure-function relationship of proteins by means of molecular dynamics simulation, a recurring problem is the assignment of the protonation state of titratable residues, such as aspartatic acid, glutamic acids and histidines. Since these residues are frequently encountered inside the active site, it is essential to use the correct protonation states for such residues in the simulation. However, choosing these protonation states is not straightforward, as they depend strongly on the local environment. Furthermore, protonation is also strongly coupled to protein conformation. Thus, even if the overall protonation state of the protein is assigned correctly at the start of a simulation, it might no longer be correct at later stages.

To overcome this shortcoming of classical molecular dynamics simulations we have developed an approach that allows the protonation state of all titrating residues in the system to change during the simulation. These changes in protonation are governed by the interactions with the local environment and the pH of the solution, which is thus a parameter that can be set at the start of the simulation, just like temperature and pressure. In addition to performing simulations of systems under more realistic conditions, our method also allows one to efficiently locate protons in x-ray structures that usually do not reveal proton positions. In the poster we present the details of our method and show representative examples of molecular dyamics simulations at constant pH.

Diffusion Based Adaptive Load-Balancing for Domain Decomposition in Particle Simulations

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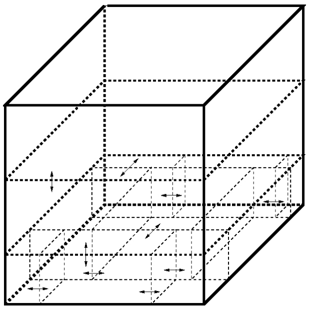
Parallel computing is a challenging topic in particle simulations, where the scaling up to a large number of processors strongly depend on the homogenous workload on the processors. According to Amdahl's law, only problems with nearly 100% parallelism will be scalable. The same applies to workload distribution.

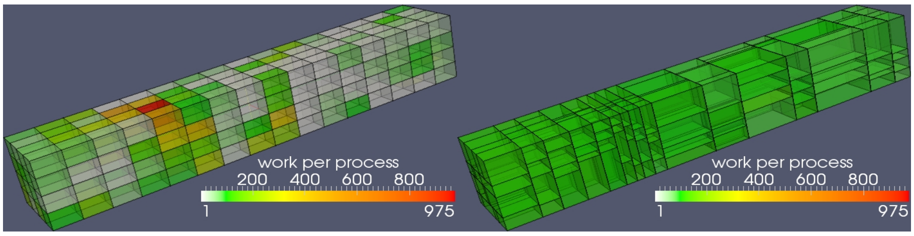
If, for inhomogenous particle distributions, e.g. when simulating clusters, self aggregation, phase seperation or supercritical systems, a uniform partitioning of geometrical domain decomposition with equal volumes is assumed, the work load $W(p) = \int_{\Omega_p} d^3r\ \rho_W(r)$ on different processors will be non-homogenous and the scaling of the underlying problem is determined by the slowest process. The work density $\rho_W(r)$ density might be differently defined, but a common measure would be the number of particles on each processor or the time, which is spent to calculate mutual interactions between particles.

In the present work we propose a diffusion based load-balancing scheme, which conserves surface normal vectors of domain boundaries but allows for compression or expansion of domain sizes. The scheme is based on local work exchanges between (i) neighbored domains in x-direction, (ii) neighbored domain columns (formed by domains in x-direction) and (iii) neighbored domain surfaces (formed by domains in x-y-layers). The problem corresponds to a time dependent global optimisation problem, which is solved in the present approach iteratively. The assumption which is made here is a quasi-static scenario, i.e. load-imbalance develops on a slower time scale than the convergence of the scheme. In each step, the work load is measured on each processor. If the work difference between neighbored domains $\delta W \neq 0$, the domain boundary is shifted towards the domain with larger work, according to



Schematic of domain boundary reorganization during the load-balancing scheme.

$$x_b^{(k+1)} = x_b^{(k)} - \frac{1}{\gamma} \frac{W_i^{(k)} - W_{i+1}^{(k)}}{W_i^{(k)} + W_{i+1}^{(k)}} \left(x_{i+1}^{(k)} - x_{i-1}^{(k)}\right)$$



Initial domain division (left) and after applying the load-balancing scheme (right).

where k is the iteration step of the scheme, $x_b^{(l)}$ are coordinates of domain boundaries, $W_j^{(l)}$ the work in domain j and γ is a weight which assures stability and convergence. As a stability criterion we find that $\gamma \geq 2\,(1 + d_{max}/d_{min})$, with $d_{min/max}$ the smaller and larger domains seperated by x_b. Best convergence is found for the minimum value of γ. It is found that the work load can be balanced even for strongly inhomogenous systems within tolerance intervals of $< 5\%$, which leads to a better scaling of factors > 2 for most cases studied. Furthermore a mathematical analysis of the stability and convergence of the scheme is given. Test cases are shown for strongly inhomogenous systems of semi-diluted polymer chains with $N_m = 250$ monomers under shear conditions. Appplying the load-balancing scheme, it is found that a scaling down to ≈ 50 particles/processor is achieved, from where scaling starts to saturate.

Prediction of Aqueous Acidities and Tautomer Ratios from Embedded Cluster Integral Equation Theory

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The embedded cluster reference interaction site model (EC-RISM) approach combines statistical-mechanical integral equation theory and quantum-chemical calculations in order to predict thermodynamic data for chemical reactions in solution[1]. The electronic structure of the solute is determined self-consistently with the structure of the solvent which is described by 3D RISM integral equation theory. The coupling is achieved by mapping the continuous solvent-site distribution onto a set of discrete background charges ("embedded cluster") and using it as an additional contribution to the molecular Hamiltonian. Recent progress in the understanding of conceptual and numerical features of the integral equation approximations[2] allows computations on hundreds of compounds in a reasonable time with good accuracy.

We report results from the application of the EC-RISM methodology to the prediction of aqueous $\mathrm{p}K_\mathrm{a}$ values and of tautomer ratios[3] for small organic molecules. We discuss critically important parameters that influence the accuracy of the approach, such as the adequate treatment of multiple conformations, the choice of the quantum-chemical level of theory, as well as the force field governing nonpolar solute-solvent interactions.

References

1. T. Kloss, J. Heil and S. M. Kast, J. Phys. Chem. B **112**, 4337, 2008.
2. T. Kloss and S. M. Kast, J. Chem. Phys. **129**, 236101, 2008.
3. S. M. Kast, J. Heil, S. Güssregen and K. F. Schmidt, J. Comput.-Aided Mol. Des. **24**, 343, 2010.

Adaptive Resolution Simulations of Water

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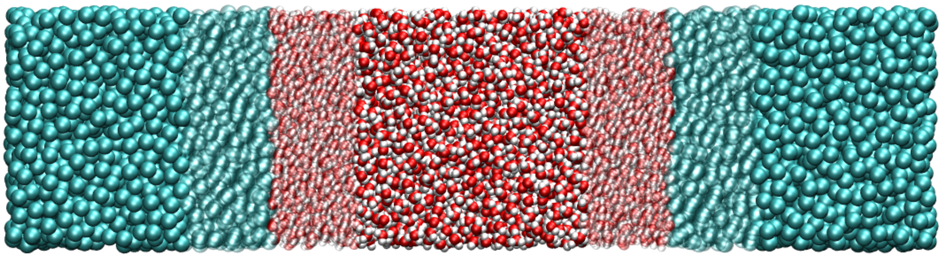
The Adaptive Resolution Scheme (AdResS)[1] allows molecular dynamics simulations of systems divided into two domains of different degree of resolution, the coarse-grained and the atomistic domain, through which particles can freely diffuse. We have used this scheme to study the SPC/E water model and its thermodynamic properties.
Two coarse-grained models[2], were developed from the all-atom SPC/E water model using structure based coarse-graining. The comparison of their thermodynamic properties showed that only either compressibility or pressure can be preserved using the present approach. Finally the coarse-grained models were used in an AdResS simulation to study the influence of coupling the atomistic and coarse-grained resolution.



References

1. M. Praprotnik, L. Delle Site and K. Kremer J. Chem. Phys. **12**, 224106, 2005.
2. H. Wang, C. Junghans, and K. Kremer Euro. Phys. J. E **28**, 221, 2009.

Dynamical Evolution of the Binary Population in Young Dense Star Clusters

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It's known for quite a while, that most stars do not form in isolation, but instead in star clusters consisting of up to several thousand stars. Additionally, observations of binaries in the solar neighborhood have shown, that binary systems can be found in such high numbers, that they cannot be purely explained by the formation through dynamical capture during the lifetimes of the stars.

Caused by the high density in the star clusters, the binary population in these clusters should be influenced significantly during the cluster evolution through stellar interactions. These can alter the orbital parameters of the binaries (in/decreasing the semi-major axis), exchange binary components or even lead to the destruction of binaries.

To investigate the effect of the natal environment on the binary population, N-body simulations with varying initial binary frequencies have been performed using the parallel, high precision code NBODY6++[1,2].

As has already been shown in previous studies, the simulations show that the main effect of the cluster evolution is to destroy wide binaries with semi-major axes exceeding 10^3 AU. However, our simulations show, that the effectiveness of this process depends on the mass of the stars: the more massive a star is, the less often it can be found with no companion after 1Myr. This could explain the observational findings, that the binary frequency of stars depends on the mass of the stars.

Additionally, the simulations show that, although the number of binaries varies significantly between simulations with different initial binary frequencies and with this the importance of binary-binary interactions, the overall evolution of the binary population is very similar for all simulations: about $8-10\%$ of all binaries are destroyed within the first Myr of cluster evolution independent of the initial binary fraction.

References

1. S. J. Aarseth, *Gravitational N-Body Simulations*, Nov. 2003.
2. R. Spurzem, *Direct N-body Simulations*, Journal of Computational and Applied Mathematics, **109**, 407–432, Sept. 1999.

Charged Colloids in a Narrow Slit Pore: Preliminary Studies

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Freezing effects in spatially confined fluids and colloidal dispersions receive strong scientific interest over the last several decades[1]. Confining surfaces can be found in many contexts like the inner pore walls of porous material, or in a blood cell. What one is interested in is for example the influence of confinement on the freezing and melting temperatures or the variety of lattice structures that occur in such systems[2]. In this contribution we present preliminary results from a study of heterogeneous nucleation in a charged system confined between two walls.

Our charged colloidal suspension is squeezed between two parallel planar walls along the z-axis and extends infinitely in the x-y plane. The system becomes quasi 2D when the wall separation gets comparable to the particle diameter. In our case we have a distance between the walls enough to fit 2 layers. The phase behavior in 2D systems is more complicated since no real long-range translational order exists. The theory predicts a hexatic phase with short-range translational and quasi-long orientational order between liquid and crystal phase[3].

The first steps of my work were molecular dynamics computer simulations of quasi 2D charged colloidal systems to see what kind of phase transition we have to deal with. The simulation showed there was a hysteresis in the system with 2 layers indicating a first-order phase transition. We will continue with studying nucleation in the system using the Forward Flux Sampling method[4,5] for rare events.

References

1. R. Messina, J. Phys.: Condens. Matter **21**, 113102, 2009.
2. J. Liu and J. Schöppe and T. Palberg, J. Chem. Phys **116**, 5901, 2002.
3. K. J. Strandburg, Rev. Mod. Phys. **60**, 161, 1988.
4. R. J. Allen and P. B. Warren and P. R. ten Wolde, Phys. Rev. Lett. **94**, 018104, 2005.
5. R. J. Allen and D. Frenkel and P. R. ten Wolde, J. Chem. Phys. **124**, 024102, 2006.

Performance Tuning of Molecular Dynamics Simulations Using PME

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Parallel molecular dynamics simulations with PME[1,2] electrostatics enjoy a considerable performance increase in Gromacs 4[3] compared to older versions. Part of that increase results from the fact that a subgroup of the processes is assigned exclusively for the reciprocal part of the PME calculation in a multiple-data, multiple-program (MPMD) approach. The reciprocal part requires a Fourier transformation of the charge grid and thus needs all-to-all communication among the participating processors. This communication pattern is a major scaling bottleneck for PME calculations in parallel[4] since on N processors, N*N messages have to be delivered. With separate PME processors, N is typically reduced by a factor of 2-4.

For optimum parallel performance, it is essential that every processor gets assigned an equal amount of work. Most critical for the MPMD approach is that the reciprocal processors complete their time step simultaneously with the real space processors such that waiting time is minimized. This is achieved by carefully balancing the ratio of real to reciprocal space processors and workload.

Gromacs predicts this ratio based upon hard-wired reference numbers. However, it does not know about the underlying network or processor clock rates, facts that influence the optimum ratio. Consequently, we directly seek the actual optimum with the help of short test runs. For a given number of processors, the adjustable parameters are the number of reciprocal processors and also the workload distribution between real and reciprocal space part of the Ewald sum. At high parallelization, the scaling usually benefits from shifting work to real space such that the fraction of reciprocal processors can be kept between a quarter and a half of the total available processors.

References

1. T. Darden, D. York, L. Pedersen, 1993. *Particle mesh Ewald: An N*log(N) method for Ewald sums in large systems*, J. Chem. Phys. **98 (12)**, 10089-10092
2. U. Essmann, L. Perera, M.L. Berkowitz, T. Darden, H. Lee, G. Pedersen, 1995. *A smooth particle mesh Ewald method*, J. Chem. Phys. **103 (19)**, 8577-8593
3. B. Hess, C. Kutzner, D. van der Spoel, E. Lindahl, 2008. *GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation.* JCTC **4 (3)**, 435-447
4. C. Kutzner, D. van der Spoel, M. Fechner, E. Lindahl, U. Schmitt, B. de Groot and H. Grubmüller, 2007. *Speeding up parallel GROMACS on high-latency networks*. J. Comp. Chem. **28 (12)**, 2075-2084

Torque Transmission in Magneto-Rheological Clutches

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Typical magneto-rheological fluids (MRF) consist of micron-sized magnetically permeable particles (mostly iron) dispersed in carrier oil. MRF are increasingly being considered in variety of devices such as dampers, vibration insulators, brakes or clutches. The activation of an external magnetic field causes a fast and dramatic change in the apparent viscosity of the MRF contained in the clutch. Chains of magnetized particles are formed between the two inner surfaces of the clutch within a few milliseconds. The flow properties of the MRF change from liquid to solid and, thus, render large torque transmission possible.[1]

In this study, numerical simulations based on the discrete element method (DEM) are used to model magneto-rheological fluids for application in automotive clutches. Calculations of the local magnetic field in the MRF show significant deviations from the applied external field. Taking this into account, an appropriate magnetization model[2,3] for the ferromagnetic particles as well as mechanical interactions among particles and between the particles and the surface of the clutch are implemented.

The influence of volume fraction of the suspension and applied magnetic field on the torque transmission is investigated and the results are compared with experiments.

References

1. R. G. Larson, *The Structure and Rheology of Complex Fluids*, New York: Oxford University Press, 360-387, 1999.
2. A. Raghunathan, Y. Melikhov, J, E. Snyder and D. C. Jiles, Appl. Phys. Lett. **95**, 172510, 2009.
3. F. Liorzou, B. Phelps and D. L. Atherton, IEEE Trans. Magn. **36**, 418, 2000.

Counterion Effects on Biomolecule Conformation and Complex Formation in Water

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Many biomolecules have ionisable groups and the importance of the effects of counterion interactions with these groups on structural and thermodynamic properties of biomolecules is now widely recognised (see e.g.[1–3]). Here we report our recent studies on molecular mechanisms of specific counterion effects on structural and thermodynamic properties of different biomolecules with charged groups. We consider a diverse set of molecules varying in size and chemical composition: from bile acids to polypeptides. We study the specific effects of counterion binding by molecular simulations and various experimental techniques (NMR, different calorimetric methods). Such combination of experimental and theoretical techniques provides detailed insights into the molecular mechanisms of ion effects on the molecular charged groups.

We find that the competition between charged species for water molecules controls the conformational an association preferences of the biomolecules under study. The net effect of counterions on the biomolecules is determined by the strength of local interactions of the ions with the charged groups. Water plays a very important role in the mechanism of ion interactions with these groups because the strength of these interactions depends on the balance between group-water and group-ion interactions.

The results are discussed in the context of other experimental and theoretical studies on the effects of salts on biomolecules.

References

1. N. Vlachy, B. Jagoda-Cwiklik, R. Vacha, D. Touraud, P. Jungwirth and W. Kunz, Advances in Colloid And Interface Science **146**, 2009, 42.
2. M.V. Fedorov, J. M. Goodman and S. Schumm, Chem. Comm. **8**, 896, 2009.
3. M.V. Fedorov, J. M. Goodman and S. Schumm, J. Am. Chem. Soc. **131**, 10854, 2009.

Multiparticle Collision Dynamics on Cell Broadband Engine Using CellSs

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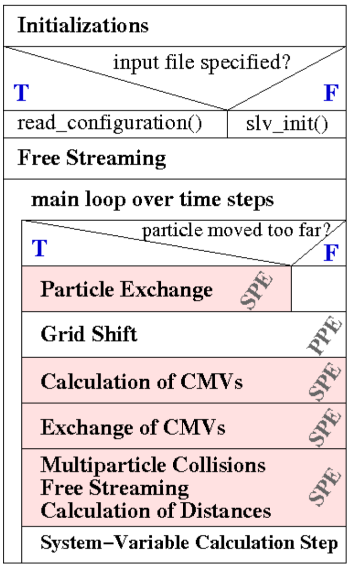
Multiparticle Collision Dynamics (MPC)[1] is a technique to simulate the hydrodynamic properties of fluid and flow phenomena at the mesoscale. It is a particle-based approach which bases on a free streaming of the particles and a stochastic rotation of the relative particle velocities. To accelerate the MPC algorithm, the Cell Broadband Engine (Cell/BE) is considered as target platform for a parallel implementation. The Cell/BE is a single-chip multi-processor with nine heterogeneous processor cores. The processors are grouped into two types: one PowerPC element (PPE) and eight so-called synergistic processing elements (SPEs). The PPE runs the operating system and manages system resources, whereas the SPEs are optimized for running compute-intensive applications.



Redesigned MPC algorithm

In the era of fast evolving new architectures particularly in the field of multicore design patterns, portability and ease of programming are important aspects. Hence, the purpose of this work is to use a programming model that is more general than the native programming API, so that the code can be executed also on other architectures with only minor changes. Therefore, the high-level programming model Cell Superscalar (CellSs)[2] is used to port the application to Cell/BE. CellSs allows the programmer to write sequential code based on which CellSs is able to exploit the existing concurrency and to use the different components of the Cell/BE (PPE and SPEs) by means of an automatic parallelization at execution time. Previous attempts[3] to develop a Cell/BE implementation based on the original MPC algorithm suffered from the limited amount of parallelizable program parts. The parallelized routines corresponded to less than 50% of the whole application which significantly limits the performance and scalability. By redesigning the MPC algorithm to a domain decomposition approach which considers the Cell/BE and CellSs specific requirements (see Fig. 1) the parallelism could be increased significantly and all program parts could finally be parallelized.

References

1. A. Malevanets and R. Kapral, Mesoscopic model for solvent dynamics, J. Chem. Phys. **110**, 8605, 1999.
2. P. Bellens, J. M. Perez, R. M. Badia and J. Labarta, CellSs: a programming model for the cell BE architecture, In *SC ’06: Proceedings of the 2006 ACM/IEEE conference on Supercomputing*, 2006.
3. A. Schiller and G. Sutmann, Mesoscopic Simulations of Hydrodynamic Interactions Using a Particle-Based Model on Cell Broadband Engine, In *Mitteilungen – Gesellschaft für Informatik e. V., Parallel-Algorithmen und Rechnerstrukturen*, volume 26, pages 17–26, December 2009.

Ewald-Summation for the Rotne-Prager Tensor: Error Analysis and Parameter Optimization

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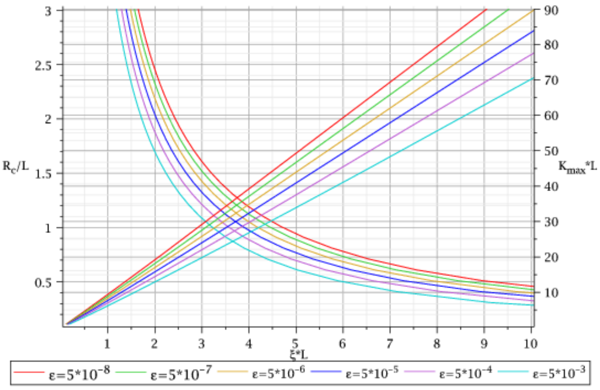
The calculation of hydrodynamic interactions between solvated particles is a computationally involved procedure, due to the missing superposition principle of these interactions. Only for diluted systems, many-body interactions may be neglected and closed form expressions may be formulated, which rely on interactions between particles, which can simply be summed over all particle pairs in the system.

Considering periodic boundary conditions, this problem is analogous to the lattice summation of Coulombic interactions. For hydrodynamic interactions an analog of the Ewald summation was formulated by Beenaker[1] and lateron by Smith et al.[2] on the level of the Rotne-Prager approximation[3].

In the present work the approximation errors of Ewald sum implementations are investigated under the condition that errors are equally distributed over real- and reciprocal space sums. The figure displays the values for the cutoff values K_c in reciprocal space and R_c in real space as function of the splitting parameter ξ for different prescribed error thresholds. The prescribed error bound is verified by computing the sums with appropriate



Real space cutoff radius R_c and reciprocal cutoff wavenumber K_c as function of the velocity field splitting parameter ξ for different error thresholds.

parameters for the tolerated errors and comparing with results which were computed close to numerical precision. An analytical model is proposed, which allows to predict the runtime behavior of real- and reciprocal sums as a function of the splitting parameter ξ, which allows to determine a set of parameters (R_c, K_c, ξ), which minimizes the CPU time. The model is validated by runtime measurements of an Ewald sum implementation.

References

1. C.W.J. Beenakker. Ewald sum of the Rotne-Prager tensor. *J. Chem. Phys.*, 85:1581–1582, 1986.
2. E.R. Smith, I.K. Snook, and W. van Megen. Hydrodynamic interactions in brownian dynamics. *Physica A*, 143:441–467, 1987.
3. J. Rotne and S. Prager. Variational treatment of hydrodynamic interaction on polymers. *J. Chem. Phys.*, 50:4831, 1969.

Simulations of Dimeron Ensembles in Pure Yang-Mills Theory

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Confinement of quarks is one of the most striking phenomena of the standard model, which has its origin in quantum chromodynamics (QCD). Until now attempts to solve QCD analytically have not been successful and, therefore, the mechanism of confinement is not understood in detail. The aim of this work is to study confinement in Yang-Mills theory, which is a toy model for QCD.

This is done by simulating so-called path integrals, which have a similar structure as partition functions in statistical physics. To compute physical observables, one has to average over all possible gluonic field configurations, where each field configuration is weighted exponentially by its negative classical Yang-Mills action. The basic idea of simulating dimeron ensembles is to restrict the above mentioned average to those field configurations, which represent linear superpositions of dimerons. Dimerons are solutions of the Yang-Mills equations of motion and, therefore, local minima of the action. Consequently, the weight factor of such field configurations is rather large and they are expected to approximate the full path integral quite well. Furthermore, merons, which are localized in space as well as in time and hence referred to as pseudoparticles. However, they exhibit long range tails, which fall off only like $1/distance$ inevitably giving rise to long range interactions between merons and/or dimerons.

Treating these long range interactions in an appropriate way amounts to getting rid of finite volume effects and is from a technical point of view rather difficult. One possibility to reduce the strength of the long range interactions is to gauge transform dimerons to a specific so-called singular gauge; in this gauge their tails fall off like $1/distance^3$. Another technique we have successfully applied is based on multi grids: we enclose the spacetime region of interest by a low resolution grid to evaluate the action of a dimeron field configuration. By doing this we prevent dimerons to be preferentially located on the boundary of our spacetime volume. Therefore, finite volume effects are significantly reduced.

References

1. F. Lenz, J. W. Negele and M. Thies, Confinement from merons Phys. Rev. **D 19**, 1826, 1979.

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