Workshop SimLab@KIT, November 29-30, 2010

Programme
for session “SimLab NanoMikro”

Date: November 29, 2010
Venue: Campus South, Main Auditorium (Audimax), Seminar Room: A, Building 30.95.

Session Chair: Florian Weigend, Department of Theoretical Chemistry, Karlsruhe Institute of Technology.

Time	Speaker	Affiliation	Title
14:45 – 15:30	Alexander Schug	Umeå University, Sweden	Trends in HPC biomolecular simulations of proteins and RNA
15:30 – 16:00	Andreas Dolfen	German Research School for Simulation Sciences, Jülich	Realistic Simulations of Strongly Correlated Systems
16:00 – 16:30	Timo Strunk	Karlsruhe Institute of Technology	Development and Evaluation of a GPU-optimized N-Body term for the simulation of biomolecules
16:30 – 16:45	Coffee break		
16:45 – 17:15	Soumya Bera	Karlsruhe Institute of Technology	Highly efficient numerical implementation of Chalker-Coddigton network model and applications
17:15 – 17:45	Simon Widmaier	Karlsruhe Institute of Technology	All-Atom Replica Exchange Simulations of Denaturant Induced Partial Unfolding of RNase H
17:45 – 18:15	Peter Schmitteckert	Karlsruhe Institute of Technology	Electronic Transport in and through Correlated Nanostructures

Further information you can find on the workshop’s website:
http://www.scc.kit.edu/veranstaltungen/

Trends in HPC biomolecular simulations of proteins and RNA

Alexander Schug, Umeå University, Sweden

Proteins and RNA form the biomolecular machinery in a cell. Valuable insight into the relationship between their structure and function has been gained from computer simulations like Molecular Dynamics, which have established themselves as a complementary tool to experimental observations. Many interesting biological processes like protein folding occur on the millisecond to second time scales while the feasible time scales even on large supercomputers is often limited to, at most, a few microseconds of simulation time. This limit is being steadily pushed by the exploration of novel computing platforms like GPU-computing or ANTON, advanced sampling techniques, the use of distributed computing, or coarse-graining the simulations and adjusting the level of detail to the biological question at hand. Another challenge is dealing with insufficient structural information, which is required as a basis for any simulation.

This limit can be overcome by integrating genomic information into molecular simulations in a mixed theory appraoch. The presentation will cover several specific examples from Protein complexes like those involved in Two Component Signal Transduction to RNA-systems like Riboswitches to show how simulations can help in understanding the structure/function relationship of biomolecules.

Realistic Simulations of Strongly Correlated Systems

Andreas Dolfen, German Research School for Simulation Sciences, Jülich

The physics of strongly correlated materials poses one of the most challenging problems in condensed-matter sciences. Standard approximations applicable to wide classes of materials such as the local density approximation fail, due to the importance of the Coulomb repulsion between localized electrons. Instead, we resort to non-perturbative many-body methods. The calculations are, however, only feasible for rather small model systems. The full Hamiltonian of a real material is approximated by a model Hamiltonian comprising only the most important electronic degrees of freedom, while the effect of all other electrons is included in an average way by renormalizing the parameters. Realistic calculations of strongly correlated materials need to include sufficiently many of these electronic degrees of freedom.

The new generation of massively parallel supercomputers allows for these realistic calculations. However, using their computational power requires newly devised algorithms. As a solver we use the Lanczos method, which needs the full many-body state of the correlated system. It is thus limited by the available main memory. The foremost problem for a distributed-memory implementation is that the multiplication of the Hamiltonian to the many-body state leads to highly non-local memory access patterns. Our solution to this problem relies on the efficient implementation of MPI collective communication on these systems. We show that the new algorithm scales very well on JUGENE, Jülich's Blue Gene/P. The idea is not only applicable to correlated electrons but is also used in simulating quantum spin systems. Moreover, it can also be generalized to exploit further levels of parallelization as provided, for instance, by new unconventional processing units such as the Cell Broadband Engine.

Development and Evaluation of a GPU-optimized N-Body term for the simulation of biomolecules

Timo Strunk, Institute of Nanotechnology (INT), Karlsruhe Institute of Technology

Advancements in the massively parallel sampling of the conformational space of biomolecules enables, for example, protein structure prediction, in-silico drug development and cell signalling. Despite the existence of highly distributed protein simulation architectures like POEM@HOME, there was no abundant computational resource both strong in serial strength and in parallel sampling.

In this study we investigate the optimization of our n-body Lennard Jones forcefield for the efficient Monte-Carlo sampling of small to medium-size biomolecules on massively parallel architectures, like modern GPUs. We benchmark both NVIDIA and AMD GPU chipsets in the OpenCL framework in comparison to CPU architectures. The N-Body interactions are broken down into small local grids, which fit into the local GPU caches to permit simultaneous evaluation.

Using the n-body term we accelerate the Lennard-Jones and Clash-Potential of the complete free-energy PFF02 [1] shown to fold a multitude of different protein-folds and implement a modified structure-based Lennard Jones forcefield.

We proof the applicability of our novel forcefield by reversible folding-simulations of a three-helix protein using this Go-potential from completely unfolded structures.

[1] Verma, A; Wenzel, W - A Free-Energy Approach for All-Atom Protein Simulation, Biophys. J. 96, 3483 – 3494 (2009).

Highly efficient numerical implementation of Chalker−Coddigton network model and applications

Soumya Bera, Institute of Nanotechnology (INT), Karlsruhe Institute of Technology

Formulation of quantum dynamics at the Anderson transition in terms of a network model was introduced by Chalker and Coddington in 1988 to describe the integer quantum Hall effect. Such network models have been systematically exploited in both analytical studies and numerical simulations and played a key role in advancing our understanding of quantum Hall critical points, including the conventional integer quantum Hall effect and systems with unconventional symmetries. On the other hand, highly efficient numerical routines for diagonalizing sparse matrices have been developed over the last decade. Combined with the increase in computer power and an improved understanding of finite-size effects, this development has recently paved the way for highly accurate numerical studies of critical behaviour for a variety of Anderson critical points.

Recently, we have developed a highly optimized numerical implementation of the Chalker−Coddington network model (CCNM) with intensive use of sparse matrix libraries ARPACK and MUMPS for diagonalization and solving linear equations. In particular, we have performed detailed profiling of the serial code and subsequently employed multilevel hybrid (shared memory and distributed memory) strategies for parallelization. The dimension of the matrices computed is of the order of 10 million x 10 million and 10^6 disorder realizations have been done. For the computations the parallel machine HP XC 3000 (HC3) at KIT has been used. The favourable scaling of the implementation allowed to investigate (1) the interaction effect at the integer quantum Hall transition (IQHT) and (2) relations between point contact conductance and multi-fractality in the numerical framework using the CCNM.

All-Atom Replica Exchange Simulations of Denaturant Induced Partial Unfolding of RNase H

Simon Widmaier, Institute of Nanotechnology (INT), Karlsruhe Institute of Technology

The unfolding of Ribonuclease H (RNaseH) in water/guanidinium chloride solvent at 300K can be analyzed by means of single-molecule fluorescence resonance energy transfer (FRET) experiments, from which a deduction on a stable, partially unfolded configuration is possible. Highly effective biomolecular simulation methods, like replica exchange, allow a fast sampling of the energy landscape of complex biomolecules and are applicable for the quest for partially unfolded configurations of RNaseH.

We here present the results of two comparative all-atom replica exchange simulations performed on *E. Coli* RNaseH (2RN2) using water as well as denaturant guanidinium chloride solvent. The combinatory influence of temperature and denaturant solvent reveal distinct unfolding mechanisms depending on the choice of the solvent type. GdmCl solvent based replica exchange simulations can amplify the induction of destbilizing effects in replica exchange simulations, particularly at moderate temperatures and therefore accelerate the search for representative structure ensembles.

Electronic Transport in and through Correlated Nanostructures

Peter Schmitteckert, Institute of Nanotechnology (INT), Karlsruhe Institute of Technology

The study of transport in out of equilibrium, strongly interacting systems, is of crucial importance for technological applications. It also addresses some of the most challenging fundamental questions, from the possibility of fluctuations theorems out of equilibrium, to the time evolution of quantum many body entanglement.

While experimental progress in this area has been swift and steady, the theory has been held back by considerable technical difficulties. The physics of interest occurs usually in non perturbative regimes, where analytical methods are few and limited. Numerical approaches require real time simulations which up to recently had been notoriously difficult.

In our project we apply the Density Matrix Renormalization Group (DMRG) to perform time dependent simulations for strongly interacting quantum systems. As an introduction to the approach and to a remarkable consequence of electron-electron interaction, we present our results concerning the spin-charge separation in one-dimensional wires.

We then continue with the main results of our project, namely the extraction of conductance and current correlations from time dependent simulations. We present results for the interacting resonant level model (IRLM) at the self dual point, where we were also able to obtain analytical results based on the thermodynamic Bethe ansatz. Both approaches lead to an excellent agreement and are by now already an established benchmark for other approximative approaches. Most strikingly we find a negative differential conductance regime for high voltages and the measurement of the shot noise allows us to determine the effective charge of the charge carriers. Finally we provide first results for the Kondo system and discuss our current approach to obtain higher order cumulants.

Our code is currently SMP parallelized within a master-worker approach using Posix threads, where the workload can be distributed on worker threads either running on CPUs or GPUs. The simulations for the IRLM are performed at the XC2 of the Steinbuch Centre of Computing (Karlsruhe) and the Kondo calculation are running on the Juropa cluster at the Jülich supercomputing centre.