HPC-Workshop of the University Oldenburg

25 February 2013 – Room A14 0-030, Campus Haarentor/Uhlhornsweg

Agenda

9:00 – 9:10 **Opening**

9:10 – 9:30 **Quantum chemical calculations with the MOLCAS program package**
Jan Mitschker, Hendrik Spieker and Thorsten Klüner
Theoretical Chemistry, Institute of Pure and Applied Chemistry, University of Oldenburg

9:30 – 9:50 **Quantum chemical calculations with the GAUSSIAN program package**
Wilke Dononelli, Hendrik Spieker, Nils Burchardt, Florian Habecker, Jan Warfsmann and Thorsten Klüner
Theoretical Chemistry, Institute of Pure and Applied Chemistry, University of Oldenburg

9:50 – 10:10 **O2 activation by Ag impurities and CO oxidation on nanoporous gold. A computational study.**
Lyudmila V. Moskaleva[1], Volkmar Zielasek[1], Thorsten Klüner[1], Konstantin M. Neyman[3], Marcus Bäumer[1]
[1]Institut für Angewandte und Physikalische Chemie, Universität Bremen; [2]Institute of Pure and Applied Chemistry, University of Oldenburg; [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona and IQTCUB and Departament de Química Física, Universitat de Barcelona, Barcelona, Spain

10:10 – 10:30 **The Surrogate Hamiltonian approach to open quantum system: Implementation and applications**
Erik Asplund and Thorsten Klüner
Theoretical Chemistry, Institute of Pure and Applied Chemistry, University of Oldenburg

10:30 – 10:50 **Coffee break**

10:50 – 11:10 **Vulnerability of proximity graphs to failure and attacks**
Christoph Norrenbrock, Oliver Melchert and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

11:10 – 11:30 **Efficient simulation of fractional Brownian motion for several values of the Hurst exponent**
Alexander K. Hartmann[1], Alberto Rosso[2] and Satya Majumdar[2]
[1]Computational Theoretical Physics, Institute of Physics, University of Oldenburg; [2] Université Paris Sud, France

11:30 – 11:50 **Spin Glass simulations on Graphics Processing Units (GPUs)**
Markus Manssen and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

11:50 – 12:10 **Ground states of one-dimensional long-range random-field Ising magnets**
Timo Dewenter and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

12:10 – 13:00 **Lunch break**

13:00 – 13:30 | **X86-Technologie Update**
Heinz-Werner Cembrowski
IBM Deutschland

13:30 – 14:00 | **GPFS Server: Big Data und Fast Data für HPC- und Cloud-Umgebungen**
Oliver Kill
pro-com DATENSYSTEME GmbH, Eislingen

14:00 – 14:15 | **Coffee break**

14:15 – 14:35 | **Tide-induced fingering flow during submarine groundwater discharge**
Janek Greskowiak
Institut für Biologie und Umweltwissenschaften IBU, University of Oldenburg

14:35 – 14:55 | **OpenFoam in Wind Energy**
Wided Medjroubi
ForWind - Center for Wind Energy Research, Oldenburg

14:55 – 15:15 | **Parallel performance Investigations of OpenFOAM on FLOW cluster**
Cherif Mihoubi
Fraunhofer Institute for Wind Energy and Energy System Technology IWES, Oldenburg

15:15 – 15:35 | **Simulation of offshore wind farm wakes with the LES model PALM**
Björn Witha, Gerald Steinfeld and Martin Dörenkämper
ForWind - Center for Wind Energy Research, Oldenburg

15:35 – 15:55 | **Generation of a wind and stability atlas for the North Sea using the WRF model for mesoscale simulations on FLOW**
Robert Günther
ForWind - Center for Wind Energy Research, Oldenburg

15:55 – 16:15 | **Ocean Modelling using the parallel modeling system FCVCOM-SWAVE**
Karsten Lettmann and Jörg-Olaf Wolf
Institut für Chemie und Biologie des Meeres ICBM, University of Oldenburg

16:15 – 16:30 | **Coffee break**

16:30 – 16:50 | **Score statistics of multiple sequence alignments**
Pascal Fieth and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

16:50 – 17:10 | **Properties of Loop statistics in the Negative Weight Percolation (NWP) model**
Gunnar Claußen, Oliver Melchert and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

17:10 – 17:30 | **Mean-field behavior of the negative-weight percolation model on random regular graphs**
Oliver Melchert, Marc Mezard and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

17:30 – 18:10 | **Open discussion**

Available Abstracts

The Surrogate Hamiltonian approach to open quantum system: Implementation and applications

Erik Asplund and Thorsten Klüner
Theoretical Chemistry, Institute of Pure and Applied Chemistry, University of Oldenburg

In this talk the Surrogate Hamiltonian approach to open quantum system will be reviewed and its application the surface photochemistry will be briefly elucidated. The implementation of the method will be explained and an overview of the parallelization strategy is given. Furthermore, scaling, problems and experiences on HERO is shortly discussed.

Vulnerability of proximity graphs to failure and attacks

Christoph Norrenbrock, Oliver Melchert and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

We study numerically different proximity graphs (Delaunay-Triangulation, Gabriel graph, relative neighbourhood graph, minimum-radius graph) that are discussed as "backbones", e.g.,collections of radio-devices without fixed infrastructure. Typically, remote devices are seldom linked directly to each other, but connected indirectly via several paths composed of multiple nodes and edges. This motivates the question how structure and information-transmission efficiency of these graphs are affected by a failure of a given fraction of nodes. Therefore, we study and compare the influence of different node-removal strategies by considering systems up to $N = 4 \cdot 10^4$ and determine, using finite-size scaling techniques, the fraction of nodes (for each strategy) that yields a breakup of the respective graph in the thermodynamic limit.

Efficient simulation of fractional Brownian motion for several values of the Hurst exponent

Alexander K. Hartmann[1], Alberto Rosso[2] and Satya Majumdar[2]
[1]Computational Theoretical Physics, Institute of Physics, University of Oldenburg; [2] Université Paris Sud, France

We study fractional Brownian motion (fBm) characterized by the Hurst exponent H. Using a Monte Carlo sampling technique, we are able to numerically generate fBm processes with an absorbing boundary at the origin at discrete times for a large number of 10^7 time steps even for small values like $H = 1/4$. The results are compatible with previous analytical results that the distribution of (rescaled) endpoints y follow a power law $P(y) \sim y^{\phi}$ with $\phi = (1 - H)/H$, even for small values of H.

Spin Glass simulations on Graphics Processing Units (GPUs)

Markus Manssen and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

Graphics Processing Units (GPUs), though originally constructed for graphics calculations, are in essence just processors optimized for highly parallel computations. And with the release of general purpose programming frameworks like CUDA and OpenCL their processing power has become utilizable in a variety of fields. Spin glasses are named for their slow, glassy behavior, which makes simulating them so time consuming, that even special computers like JANUS have been constructed for this purpose. But as they offer several possibilities for parallelization, GPU programming can serve as an alternative for tackling this demanding problem. We give an introduction into the GPU programming paradigma and discuss our implementation of the Edwards-Anderson Model of spin glasses.

Ground states of one-dimensional long-range random-field Ising magnets

Timo Dewenter and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

In random-field Ising magnets (RFIMs) Ising spins interact ferromagnetically with each other. Disorder is introduced by local random fields which act on each spin and whose values are drawn from a Gaussian distribution. At zero temperature, at a critical random-field strength h_c the system undergoes a phase transition. Here, we consider an one-dimensional RFIM with long-range interactions that are only present between spins with a probability that decays like a power-law in the geometric distance between the interacting spins. The parameter σ in the power-law exponent enables us to tune the effective dimension of the model. Different values of σ are used to investigate numerically [1] the three parameter regions, which are the mean-field, non-mean-field region and the region without a phase transition ($h_c = 0$). Ground states are calculated [2] with graph theoretical algorithms by mapping the system to a

directed graph. The critical random-field strength h_c and the critical exponents are obtained by finite-size scaling and then compared to analytical predictions and to results of a hierarchical model [3].

[1] A.K. Hartmann, *Practical Guide to Computer Simulations, World-Scientific*, 2009
[2] A. K. Hartmann and H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2002
[3] C. Monthus and T. Garel, J. Stat. Mech., P07010, 2011

Score statistics of multiple sequence alignments

Pascal Fieth and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

Optimally aligned sequences of amino acids [1] can be studied numerically [2] in the biologically relevant high scoring region by means of parallel tempering simulations [3]. Preceding studies have shown that the scores of gapped pairwise sequence alignments of finite-length sequences follow a Gumbel extreme value distribution, modified by a Gaussian correction [4] rather than a simple Gumbel extreme value distribution as previously predicted for ungapped pairwise alignments. In this study these methods are applied to the case of multiple sequence alignment (MSA). Here the distributions of the sum-of-pair scores of the MSA of more than two sequences are studied. In particular the distribution of protein MSA-scores using different common substitution matrices (BLOSUM and PAM) are analysed for protein background frequencies of real sequences.

[1] R. Durbin et al., *Biological sequence analysis*, Cambridge University Press, 1998
[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, World Scientific, 2009
[3] A.K. Hartmann and Heiko Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, 2001
[4] S. Wolfsheimer et al., *Local Sequence Alignments Statistics: Deviations from the Gumbel Statistics in the Rare-Event Tail*, Algorithms for Molecular Biology, 2007

Properties of Loop statistics in the Negative Weight Percolation (NWP) model

Gunnar Claußen, Oliver Melchert and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

The NWP model is a non-standard bond percolation model, where edges of a lattice are associated with positive or negative numbers called weights. The purpose of this is to find out closed loops with total negative weight and further the configuration of loops which minimizes the total weight. In our numerical studies on this model, which were carried out on the GOLEM and HERO clusters, we investigate the distrubtion of loop lengths with the aim of determining critical exponents which can be used to describe the overall behaviour of the model.

Mean-field behavior of the negative-weight percolation model on random regular graphs

Oliver Melchert, Marc Mezard and Alexander K. Hartmann
Computational Theoretical Physics, Institute of Physics, University of Oldenburg

In the presented study, we investigate the critical properties of minimum-weight loops and paths in the negative-weight percolation (NWP) problem on 3-regular random graphs (RRGs), i.e. graphs where each node has exactly 3 neighbors and were there is no regular lattice structure [1]. By studying a particular model on RRGs, one has direct access to the mean-field exponents that govern the model for $d > d_u$. The presented study aims to support the previous conjecture $d_u = 6$ [2] by directly computing the mean field exponents for the NWP model with a bimodal weight distribution, and comparing them to those found for a regular hypercubic lattice with dimension $d = 6$. The presented results are obtained via computer simulations, using an appropriate mapping to a matching problem, as well as by analytic means, using the replica symmetric cavity method for a related polymer problem. We find that the numerical values for the critical exponents on RRGs agree with those found for $d = 6$-dimensional hypercubic lattice graphs within errorbars and hence support the conjectured upper critical dimension $d_u = 6$.

[1] OM, A.K. Hartmann, and M. Mezard, PRE 84, 041106 (2011)
[2] OM, L. Apolo, and A.K. Hartmann, PRE 81, 051108 (2010)