November 27, 2012

# ABSTRACTS

**of contributions to the**

## 13th International NTZ-Workshop on

## *New Developments in Computational Physics*

# CompPhys12


**Institut für Theoretische Physik,**
**Universität Leipzig, Germany**


**29 November – 01 December 2012**

**http://www.physik.uni-leipzig.de/~janke/CompPhys12**


Supported by Research Academy Leipzig (RALeipzig), Top-level Research Area PbF2 (Mathematical Sciences), DFG Research Group FOR877, DFG SFB/TRR 102, Alexander von Humboldt Foundation, Deutsch-Französische Hochschule (DFH-UFA), DFG Graduate School of Excellence "BuildMoNa", and Centre for Theoretical Sciences (NTZ) of Universität Leipzig.

# Preface

As in previous years, also the 13th International NTZ-Workshop *CompPhys12* on *New Developments in Computational Physics* covers a broad spectrum of different fields ranging from general aspects of computational and statistical physics over applications in condensed and soft matter physics, including biological applications, and random networks to the intriguing properties of quantum systems and high-energy physics. And following the tradition, also this year's Workshop is designed to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig at the beginning of Christmas time.

The main part of the Workshop takes place from 29 – 30 November 2012 in the Lecture Hall "Theorie Hörsaal" and the "Aula" of the Experimental Physics building in Linnéstr. 5. We are very grateful to all colleagues who helped moving their regular lecture courses to another place or date, and in particular to Ms. Isabell Schulthoff who coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Susan Hussack, Ms. Gabriele Menge, and Ms. Lea Voigt, for their invaluable help with all administrative matters.

As in previous years, the Saturday, 01 December 2012, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that the Institute has moved this summer from "Vor dem Hospitaltore 1" to the *new* location "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Research Academy Leipzig (RALeipzig), Top-level Research Area PbF2 (Mathematical Sciences), DFG Research Group FOR877, DFG SFB/TRR 102, Alexander von Humboldt Foundation, Deutsch-Französische Hochschule (DFH-UFA), and DFG Graduate School of Excellence "BuildMoNa".

Leipzig, November 2012
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# Abstracts

## Thermodynamics of a polymer chain inside a spherical cage

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We performed multicanonical Monte Carlo simulations in order to determine the thermodynamical and structural properties of a semiflexible polymer chain inside an attractive, unstructured sphere. The main objective of this study is to present the influence of the attracting sphere in terms of thermodynamical and structural quantities when varying the attraction strength of the sphere. In this frame, the system under consideration exhibits a rich phase diagram ranging from highly ordered, compact to extended, random coil structures and from desorbed to partially or even completely adsorbed conformations. These findings are identified with different structural observables [1], in particular the ground-state conformations are detected [2] and all results are compared with flat substrates [3].

[1] H. Arkın and W. Janke, Phys. Rev. E **85** (2012) 051802.
[2] H. Arkın and W. Janke, J. Phys. Chem. B **116** (2012) 10379.
[3] H. Arkın and W. Janke, to appear in Eur. Phys. J. Special Topics (2012), in press.

## Parallel streams of pseudorandom numbers for Monte Carlo simulations: Using most reliable algorithms and applying parallelism of modern CPUs and GPUs

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1. The new library for pseudorandom number generation for modern CPUs and GPUs is presented. It contains both single-threaded and multithreaded realizations of a number of modern and most reliable generators and includes the ability to initialize up to $10^{19}$ independent streams. In particular, the library includes the pseudorandom number generators recently proposed and studied in [1] and the efficient SIMD realizations proposed in [2]. Using massive parallelism of modern GPUs and SIMD parallelism of modern CPUs allows to substantially improve performance of the generators.

2. The multi-GPU realization for multidimensional Monte Carlo integration algorithm is also presented. The widely used Monte Carlo integration algorithm VEGAS is parallelized for multi-GPU, using both CUDA and MPI technologies. The performance of numerical integration is substantially higher when using a single GPU compared to using a single CPU. Also, the performance of numerical integration substantially and linearly increases with increasing the number of CPU/GPU nodes involved in the calculation.

[1] L.Yu. Barash, Europhys. Lett. **95** (2011) 10003; F. Panneton, P. L'Ecuyer, and M. Matsumoto, ACM Trans. on Mathem. Softw. **32**, 1 (2006) 1–16; M. Matsumoto and T. Nishimura, ACM Trans. on Mod. and Comp. Sim. **8** (1998) 3; P. L'Ecuyer, Oper. Res. **47** (1999) 159.; Math. of Comp. **68** (1999) 261.
[2] L.Yu. Barash and L.N. Shchur, Comp. Phys. Commun. **182** (2011) 1518.
[3] L.Yu. Barash, unpublished.

# Wall-liquid and wall-crystal interfacial free energies via thermodynamic integration: A molecular dynamics simulation study

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A method is proposed to compute the interfacial free energy of a Lennard-Jones system in contact with a structured wall by molecular dynamics simulation. Both the bulk liquid and bulk face-centered-cubic crystal phase along the (111) orientation are considered. Our approach is based on a thermodynamic integration scheme where first the bulk Lennard-Jones system is reversibly transformed to a state where it interacts with a structureless flat wall. In a second step, the flat structureless wall is reversibly transformed into an atomistic wall with crystalline structure. The dependence of the interfacial free energy on various parameters such as the wall potential, the density and orientation of the wall is investigated. The conditions are indicated under which a Lennard-Jones crystal partially wets a flat wall.

# Contact angles, wetting transitions, and macroscopic interfacial fluctuations

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The study of wetting phenomena at surfaces by means of Monte Carlo simulations is reviewed, with emphasis on recently obtained progress. Macroscopically, the transition from partial wetting to complete wetting occurs when the contact angle of a (large) droplet, that is described by Young's equation, vanishes. However, simulations deal with systems of nanoscopic dimensions, and simulations of nanodroplets (or fluids confined in nanocapillaries) are impractical due to various reasons. But for systems exhibiting a symmetry between bulk coexisting phases the wall tensions appearing in Young's equation can be directly estimated, using thermodynamic integration methods. The wetting transition then is directly located, using Young's equation, with no need to simulate droplets. Recently this approach has been extended to systems lacking any symmetry, applying an "ensemble mixing" method (combining a system with periodic boundary conditions with a system with walls). As an example, an application to the Asakura-Oosawa model of colloid-polymer mixtures is given. It is shown that by varying the range of the wall-colloid repulsion one can vary the behavior of the system from "complete wetting" to "complete drying". For the case of critical wetting, a new finite-size scaling approach (with anisotropic correlations) is developed, and tested by the two-dimensional Ising model. Unlike bulk criticality, the order parameter at a second-order wetting transition fluctuates over a macroscopic range.

# Finite-size spectra and conformal operator content of a mixed quantum spin chain (P)

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Several low-lying energy levels of a mixed quantum spin with bond alternation and exchange anisotropy have been calculated using the Lanczos method for five different chain lengths up to $L = 20$. Extrapolated to the infinite-volume limit, the energy levels have been associated to the conformal operator content of a Gaussian critical theory that yields continuously varying critical exponents as the exchange anisotropy parameter is tuned from the isotropic antiferromagnetic point to values smaller than unity. The analysis is in excellent agreement with the Gaussian interpretation.

# Replica-exchange cluster algorithm (P)

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In finite-size scaling analyses of Monte Carlo simulations of second-order phase transitions one often needs an extended temperature range around the critical point. By combining the parallel tempering algorithm with cluster updates and an adaptive routine to find the temperature window of interest, we introduce a flexible and powerful method for systematic investigations of critical phenomena. As a result, we gain one to two orders of magnitude in the performance for 2D and 3D Ising models in comparison with the recently proposed Wang-Landau recursion for cluster algorithms based on the multibondic algorithm, which is already a great improvement over the standard multicanonical variant.

[1] E. Bittner and W. Janke, Phys. Rev. E **84** (2011) 036701.

# Conformational transitions in random heteropolymer models

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We study the conformational transitions in heteropolymers within the frames of a lattice model containing two types of monomers A and B. Such a model can describe in particular the sequences of hydrophobic and hydrophilic residues in proteins (K.F. Lau and K.A. Dill, Macromolecules **22** (1989) 3986) and polyampholytes with oppositely charged groups (Y. Kantor and M. Kardar, Europhys. Lett. **28** (1994) 169). We generalize this lattice model by introducing various types of short-range monomer-monomer interactions. Applying the pruned-enriched Rosenbluth chain-growth algorithm (PERM) we analyze numerically the peculiarities of transitions from extended into compact states as function of the fraction of A and B monomers along the heteropolymer chain.

# Identification of biological control networks from dynamics (P)

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An observation of a state transition provides partial information on the interactions constituting a high-dimensional deterministic system. Here we strive to quantify how the number of observed single state transitions and/or short trajectories reduces the number of interaction matrices consistent with the set of observations. As a test-bed, we use several established Boolean (threshold unit) models of cell cycle control in living organisms. The numerical study also uses ensembles of randomly reshuffled matrices as a null model. We find that the original interaction matrices are easier to reconstruct than the shuffled surrogates.

## Formation of condensates in pair-factorized steady states (P)

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We numerically survey predictions on the shapes and scaling laws of particle condensates that emerge as a result of spontaneous symmetry breaking in pair-factorized steady states of a stochastic transport process. The specific model consists of indistinguishable particles that stochastically hop between sites controlled by a tunable potential. We identify the different condensate shapes within their respective parameter regimes as well as determine precisely the condensate width scaling.

## Efficient implementation of Sweeny's algorithm for simulations of the random-cluster model

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The simulation of spin models close to points of continuous phase transitions is heavily impeded by the occurrence of critical slowing down. A number of cluster algorithms usually based on the Fortuin-Kasteleyn representation of the Potts model and suitable generalizations for continuous-spin models has been used to increase simulation efficiency. The first algorithm making use of this representation, suggested by Sweeny in 1983, has not found widespread adoption due to problems in its efficient implementation. It has been shown recently, however, that it is indeed more efficient in reducing critical slowing down than the more well-known variants due to Swendsen/Wang and Wolff. Here, we discuss efficient implementations of Sweeny's approach based on union-and-find algorithms and using recent algorithmic advances in dynamic connectivity algorithms, and show how these can be used for efficient simulations in the random-cluster model.

## Application of Hierarchic Genetic Strategy to 3D borehole resistivity inverse simulations (P)

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We present a twin adaptive strategy hp-HGS (Hierarchic Genetic Strategy) for solving inverse problems related to 3D direct current borehole resistivity measurement simulations. The term "simulation of measurements" is widely used by the geophysical community. A quantity of interest, voltage, is measured at a receiver electrode located in the logging instrument. We use the self-adaptive goal-oriented hp-Finite Element Method (hp-FEM) computer simulations of the process of measurements in deviated wells (when the angle between the borehole and formation layers are $< 90^{\circ}$). We employ HGS to solve the inverse problem. Each individual in the population represents a single configuration of the formation layers. The evaluation of the individual is performed by solving the direct problem by means of the hp-FEM algorithm and by comparison with measured logging curve.

## Stability in Boolean networks with distributed delays (P)

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In this paper, we investigate the effect of distributing delays on the stability of Boolean dynamics in order, disorder and critical regimes. To demonstrate this point, we study the time evolution of the cumulative Hamming distance. We show that ensembles of random Boolean networks updated synchronously according to the nodes' flat distributed delays could present higher dynamical robustness against flip perturbations in critical, chaotic and frozen networks with proper distributions of delays.

## Thermal behavior of the Lee-Yang zeros in the O(3) model

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We present a numerical study of the behavior of the Lee-Yang zeros in the O(3) model. The location of the first four zeros is obtained accurately using an iterative and quite fast method. In every case, we obtain the same scaling exponents using the modulus or the components of the magnetization vector. We focus on the differences of their scaling functions at and below the critical temperature. We obtain the expected scaling exponents at every simulated temperature. We also estimate the zeros density, obtaining the expected values for scaling exponents and order parameters.

## Structure optimization for the HP model of protein folding by means of "local heat pulse"-quench cycles (P)

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Protein folding is a very challenging task because its energy landscape exhibits a huge number of local minima. For such simulations, efficient heuristic algorithms are of high value. Our aim is to investigate, whether and how the "local heat pulse"-quench cycling (LHPQC) approach [1], which has proved to be very efficient for traveling salesman and Coulomb glass problems, can be applied to protein folding tasks. As a first approach, we consider the two-dimensional hydrophobic-polar (HP) model [2]. We compare the efficiencies of multi-start local search, simulated annealing, and LHPQC for S20, S64, and S100b [3, 4]. In this, we manipulate the protein states by means of pull moves [4].

[1] A. Möbius, A. Neklioudov, A. Díaz-Sánchez, K.H. Hoffmann, A. Fachat, and M. Schreiber, Phys. Rev. Lett. **79** (1997) 4297.
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[3] N. Lesh, M. Mitzenmacher, and S. Whitesides, Proceedings of the 7th Annual International Conference on *Research in Computational Molecular Biology* (2003), p. 188.
[4] R. Unger and J. Moult, J. Mol. Biol. **231** (1993) 75.

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

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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 $H$.

# Thermodynamic Casimir forces between a sphere and a plate: Monte Carlo simulation of a spin model

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We study the thermodynamic Casimir force between a spherical object and a plate. We consider the bulk universality class of the three-dimensional Ising model, which is relevant for experiments on binary mixtures. To this end, we simulate the improved Blume-Capel model. Following Hucht, we compute the force by integrating energy differences over the inverse temperature. We demonstrate that these energy differences can be computed efficiently by using a particular cluster algorithm. Our numerical results for strongly symmetry breaking boundary conditions are compared with the Derjaguin approximation for small distances and the small-sphere expansion for large distances between the sphere and the plate.

# Some exact results in systems of immobile interacting particles

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Two models of immobile particles, containing either a single species or else two distinct species, are considered. Each particle interacts at most once throughout its entire history. The resulting large number of stationary states leads to a non-vanishing configurational entropy. Exact results on particle-densities as well as correlators are found, for arbitrary initial conditions. The single-species model is the dual of the 1D zero-temperature kinetic Ising model with Kimball-Deker-Haake dynamics. Both infinite and semi-infinite chains are analysed.

# The size dependence of the vapour-liquid interfacial tension

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Following the Tolman approach, the surface tension of spherical vapour-liquid interfaces is analysed in terms of the pressure difference due to curvature. Thereby, the excess equimolar radius, which can be obtained directly from the density profile, is used instead of the Tolman length. By canonical molecular dynamics simulation of small droplets, the magnitude of the excess equimolar radius (as well as the Tolman length) is shown to be smaller than $0.5\sigma$ for the truncated-shifted Lennard-Jones fluid. Curvature-independent size effects are examined by simulating thin planar liquid slabs. For the Lennard-Jones fluid, it is found that the interfacial tension of such slabs decreases significantly as they become extremely thin, an effect which occurs on a characteristic length scale exceeding the Tolman length. On this basis, it is concluded that the size dependence of the surface tension of small liquid droplets cannot be discussed in terms of the curvature alone.

# Scattering function of semiflexible polymer chains under good solvent conditions

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Using the pruned-enriched Rosenbluth Monte Carlo algorithm, the scattering functions of semiflexible macromolecules in dilute solution under good solvent conditions are estimated both in $d = 2$ and $d = 3$ dimensions, considering also the effect of stretching forces. Using self-avoiding walks of up to $N = 25\,600$ steps on the square and simple cubic lattices, variable chain stiffness is modeled by introducing an energy penalty $\epsilon_b$ for chain bending; varying $q_b = \exp(-\epsilon_b/k_BT)$ from $q_b = 1$ (completely flexible chains) to $q_b = 0.005$, the persistence length can be varied over two orders of magnitude. For unstretched semiflexible chains we test the applicability of the Kratky-Porod worm-like chain model to describe the scattering function, and discuss methods for extracting persistence length estimates from scattering. While in $d = 2$ the direct crossover from rod-like chains to self-avoiding walks invalidates the Kratky-Porod description, it holds in $d = 3$ for stiff chains if the number of Kuhn segments $n_K$ does not exceed a limiting value $n_K^*$ (which depends on the persistence length). For stretched chains, the Pincus blob size enters as a further characteristic length scale. The anisotropy of the scattering is well described by the modified Debye function, if the actual observed chain extension $\langle X\rangle$ (end-to-end distance in the direction of the force) as well as the corresponding longitudinal and transverse linear dimensions $\langle X^2\rangle - \langle X\rangle^2$, $\langle R_{g,\perp}^2\rangle$ are used.

# Sheared Ising models in three dimensions

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The nonequilibrium phase transition in sheared three-dimensional Ising models is investigated using Monte Carlo simulations in two different geometries corresponding to different shear normals. We demonstrate that in the high-shear limit both systems undergo a strongly anisotropic phase transition at exactly known critical temperatures $T_c$ which depend on the direction of the shear normal. Using dimensional analysis, we determine the anisotropy exponent $\theta = 2$ as well as the correlation length exponents $\nu_{\text{parallel}} = 1$ and $\nu_{\text{perp}} = 1/2$. These results are verified by simulations, though considerable corrections to scaling are found. The correlation functions perpendicular to the shear direction can be calculated exactly and show Ornstein-Zernike behavior.

# Corner contribution to percolation cluster numbers

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We study the number of clusters in 2d critical percolation, $N_\Gamma$, which intersect a given subset of bonds, $\Gamma$. In the simplest case, when $\Gamma$ is a simple closed curve, $N_\Gamma$ is related to the entanglement entropy of the critical diluted quantum Ising model, in which $\Gamma$ represents the boundary between the subsystem and the environment. Due to corners in $\Gamma$ there are universal logarithmic corrections to $N_\Gamma$, which are calculated in the continuum limit through conformal invariance. The exact formulae are confirmed by large scale Monte Carlo simulations. These results are extended to anisotropic percolation where they confirm a result of discrete holomorphicity.

# The effect of boundary conditions on Schramm-Loewner evolution in the 2D Ising spin glass at zero temperature

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The domain wall of the two-dimensional Ising spin glasses has this symmetry that it is scale invariant. Domain wall length scales with the system size $L$ as $L^{d_f}$ where $d_f$ is known as the fractal dimension. Recent works indicate that $d_f \approx 1.27$ for Gaussian bond distribution and $1.09 \lesssim d_f \lesssim 1.39$ for bimodal one. This work is going to investigate whether the domain wall of such a system is also conformally invariant. Different boundary conditions are considered and for each case $d_f$ and the diffusion constant of the relative Brownian motion, $\kappa$, are calculated. The results show that changing the boundary conditions of the system does not change the fractal dimension. However, it has a strong influence on $\kappa$ and therefore SLE properties of the system.

# Correlated valence-bond states

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We study generalizations of the singlet-sector amplitude-product (AP) states in the valence-bond basis of $S = 1/2$ quantum spin systems. In the standard AP states, the weight of a tiling of the system into valence bonds (singlets of two spins) is a product of amplitudes depending on the length of the bonds. We here introduce correlated AP (CAP) states, in which the amplitude product is further multiplied by factors depending on two bonds connected to a pair of nearest-neighboring sites. In two dimensions the standard AP states can describe an antiferromagnetic (Neel) state or a spin liquid, but it cannot describe any valence-bond solid (VBS) order. With the CAP states, Neel-VBS transitions are realized as a function of some parameter describing the bond correlations. We here study such phase transitions of CAP wave-functions on the square lattice. We find examples of direct first-order Neel-VBS transitions, as well as cases where there is an extended U(1) spin liquid phase intervening between the Neel and VBS states. In the latter case the transitions are continuous and we extract critical exponents and address the issue of a possible emergent U(1) symmetry in the near-critical VBS.

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# Simple polymer in a sphercial cage (P)

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**(with Johannes Zierenberg**[1]**, Handan Arkın-Olgar**[1,2] **and Wolfhard Janke**[1]**)**

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We study the change of the pseudo phase transition of a simple homopolymer inside a spherical confinement. Of particular interest is the shift of the collapse and freezing transitions with shrinking radius of the sphere. The polymer is a simple bead-stick model, where the distance between neighboring monomers is fixed, between three monomers in a row acts a bending potential and all non neighboring monomers interact via a Lennard-Jones potential. We use modern Monte Carlo methods to investigate the phase space of this model. Most of the results are obtained by parallel tempering simulations followed by a multi-histogram reweighting method combining a direct and a recursive procedure. To crosscheck our results, especially near the pseudo phase transition, we used a parallelized kind of the multicanonical simulation. To characterize the pseudo phase transition we analyze fluctuations of energetic and conformational observables. As zero order case the spherical cage is modeled only as a geometrical constraint without any interaction with the polymer. In further simulations we switched on an interaction between the polymer and the surface of the sphere and looked for effects induced by this interaction.

# The universality class of the 2D "Touch-and-Stop" cluster growth percolation model (P)

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We consider the "Touch-and-Stop" cluster growth percolation (CGP) model on the two-dimensional square lattice. A key-parameter in the model is the fraction $p$ of occupied "seed" sites that act as nucleation centers from which a particular cluster growth procedure is started. We consider two growth-styles: rhombic and disk-shaped cluster growth. For intermediate values of $p$, the final state, attained by the growth procedure, exhibits a cluster of occupied sites that spans the entire lattice. Using numerical simulations we investigate the percolation probability and the order parameter and perform a finite-size scaling analysis for lattices of side length up to $L = 1024$ in order to carefully determine the critical exponents that govern the respective transition. In contrast to previous studies reported in [1], we find strong numerical evidence that the CGP model is in the standard percolation universality class.

[1] N. Tsakiris, M. Maragakis, K. Kosmidis, and P. Argyrakis, Phys. Rev. E **82** (2010) 041108.

# On parallelization of structure optimization via "local heat pulse"-quench cycles (P)

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Optimization problems with a large number of degrees of freedom often exhibit extremely many local minima. For such tasks, the heuristic strategy of optimization by "local heat pulse"-quench cycles (LHPQC) has proved to be very helpful, for combinatorial optimization tasks with discrete degrees of freedom [1] as well as for structure optimization with continuous variables [2]. Its basic idea is to cyclically disturb a few randomly chosen degrees of freedom of the current best local minimum and to quench the obtained state by a highly efficient local search code. As the optimization proceeds, the amplitude of the disturbance slowly decreases. The more cycles are performed for each of the considered amplitude values, the lower are the finally reached local minima on average. This approach is applied to a lattice structure prediction problem: We use the general utility lattice program (GULP) by J.D. Gale and co-workers [3] as local search code. As a test case, the energy landscape of the hypothetical periodic $Mg_{10}Al_4Ge_2Si_8O_{36}$ compound is investigated, where the interactions are modelled by Buckingham and three-body potentials [4], and where both the cell parameters and the atom positions are free to vary. When applied as a single thread algorithm, the LHPQC procedure is robust and far more efficient than the previous approaches to the same test problem in Ref. [4] by means of multi-start local search, simulated annealing, and evolutionary algorithms, compare Ref. [2]. Our contribution focuses to parallelization aspects of the LHPQC algorithm when applied to structure optimization tasks. First, we study spectra of local minima obtained for several amplitude decrease rates. Following Ref. [5], we demonstrate that it can be advantageous simply to divide up the available cpu time to some independent, "less careful" searches. In this, the lowest of the obtained local minima is considered as result of the composite algorithm. Second, we investigate which parallelization profit can be gained in simultaneously treating an ensemble of local minima. In this, a new local minimum, which is obtained in an individual cycle starting from a certain local minimum, A, and which is lower than A, is substituted for the highest local minimum of the ensemble instead of for A.

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[2] A. Möbius and J.C. Schön, talk at *CompPhys11*, in Electronic Proceedings [www.physik.uni-leipzig.de/~janke/CompPhys11/Folien/moebius.pdf].
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[5] B.A. Huberman, R.M. Lukose, and T. Hogg, Science **275** (1997) 51.

# Time dependent aspects of fluid adsorption in mesopores

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Adsorption of fluids in mesopores is often accompanied by the phenomenon of hysteresis, i.e., the amount adsorbed from the gas phase is not only controlled by the actual gas pressure, but may depend on the history. This is in distinct disagreement to the basic concept of thermodynamic states which are conceived to depend only on the actual boundary conditions. It is common practice to save the validity of thermodynamics in view of these experimental results by introducing metastable states [1, 2]. Neimark *et al.* [3] discuss the construction of a ground state that incorporates the microstates of both branches of the hysteresis loop. The underlying picture assumes that the system fluctuates between the two branches of the hysteresis loop under grand canonical boundary conditions. The present contribution constitutes the first attempt to give an estimate of the typical cycle time by determining the lifetimes of the states inside the hysteresis loop. It turns out that the shortest lived states have a lifetime that corresponds to several times the age of the universe. This finding endorses the concept of COS (Curves of States) that has been laid down in a previous paper [4]. The COS are associated with the notion that the adsorption hysteresis loop is best characterized by bistability rather than by metastability. In other fields of physics with an ambiguity of states under the same boundary conditions the lifetimes are found to be much shorter which makes the notion of metastability convincing. It is of interest to note that even in case of fluid adsorption in mesopores authors have demonstrated in simulation that systems may have lifetimes being so short that fluctuations could be shown in one run of a Monte Carlo calculation [3]. At the first glance this looks like a contradiction to our findings. However, careful inspection of the boundary conditions show that adsorption systems with comparetively short lived states may show up in simulation, but hardly in a real experiment.

[1] D. Wallacher, N. Künzer, D. Kovalev, N. Knorr, and K. Knorr, Phys. Rev. Lett. **92** (2004) 195704.
[2] R. Valiullin, S. Naumov, P. Galvosas, J. Kärger, H.J. Woo, F. Porcheron, and P. Monson, Nature **443** (2006) 965–968.
[3] A.V. Neimark and A. Visnyakov, J. Phys. Chem. B **110** (2006) 9403–9412.
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# Multicanonical analysis of the gonihedric Ising model (P)

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The gonihedric Ising model originates from catching basic properties of fluctuating random surfaces in a bosonic string theory. Formulated as a lattice model of interacting classical spins it can be investigated by means of the multicanonical Monte Carlo algorithm to resolve open questions on the first-order phase transition. The transition temperature has been determined for the model and a dual representation; also the interface tension has been measured for both models and appears to be quite strong.

# Simulated tempering and magnetizing simulations of a Potts model

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We applied the simulated tempering and magnetizing (STM) method to the two-dimensional three-state Potts model with different lattice sizes for further investigation of its applicability. In the method, the external (magnetic) field is also treated as a dynamical variable updated by Metropolis criteria, besides the temperature. The random walks in temperature and external field were realized during the STM simulations. The calculated density of states shows that the area sampled by STM is larger than that by ST. Thus, we can calculate various thermal averages under any combinations of temperature and external field by STM. We further study the

crossover behavior between Potts and Ising case. With the combination of large lattice size simulations, we show that under negative external field, the Potts model behaves like the Ising model as the lattice size increases, in agreement with theoretical implications.

## Stochastic description of a bistable frustrated unit (P)

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Oscillations are an essential feature of processes in biological systems. Biological oscillators can be found in a multitude of different realizations, such as the glycolytic regulator, circadian clocks or regulatory genetic circuits. In the current description of biological oscillators, two essential elements have been identified: an inhibitory feedback loop and a source of delay in that loop allowing the oscillating variables to overshoot a steady state. We study the effects of the inherent time scales on a simple regulatory system implemented as a stochastic process.

[1] D. Labavic, H. Nagel, W. Janke, and H. Meyer-Ortmanns, preprint arXiv:1209.0581 [physics.bio-ph].

## Spin correlations in the 3D Ising model on infinite cuboids

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We determine the zero momentum projected spin-spin correlation functions $\Gamma$ in the 3D Ising model with Monte Carlo (MC) simulations employing the worm algorithm on manifolds with hypercubic symmetry and without boundaries. We find the 3D Ising critical exponents $\nu = 0.6298(11)$ (correlation length), $\gamma = 1.2390(10)$ (magnetic susceptibility) and $\eta = 0.0314(35)$ (anomaleous dimension) without ever using finite-size scaling.

## Maximal-entropy random walk, centrality measures and communities

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Relationships between entities can be represented as a graph structure upon which a process takes place, be it information or opinion spread on social networks, including citation and collaboration networks, WWW or the Internet, or perhaps a physical process (molecule movement, disease transmission) on physical or biological networks. In such models, several questions arise naturally: 1) which entity in the network is the most important or influential, 2) can the network be divided into meaningful modules. Answers to the first question are contained in the notion of centrality measures, and to the second in community finding algorithms. Both of them extensively utilise concepts originating from graph theory and the theory of Markov chains. I compare the performance of two extremely different types of random walk in answering the questions above. One type is the commonly used diffusive random walk, and the other maximal-entropy random walk (MERW). I will argue that MERW can formally unify the distinct approaches of complex networks analysis, and I will strive to assess its suitability for the known community search algorithms that exploit random walks.

# Voter model with surface tension (P)

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We provide an alternative mechanism for the emergence of surface tension in the dynamic rules of the voter model. The stochastic process is analysed in square lattices with the use of Monte Carlo simulations.

# A stochastic mechanics simulation of a hard-boson gas

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We present a simulation study of the properties of the Tonks-Girardeau gas, a system of $N$ hard-core bosons confined in a one-dimensional harmonic trap. For this system the ground-state wave function is exactly known based on a Bose-Fermi mapping theorem. We employ Nelsons' interpretation of quantum mechanics in which this $N$-body wave function gives rise to a set of stochastic differential equations for the positions of the $N$ particles, which can be simulated by standard methods. Particularly, real space densities and momentum distributions can simply be determined by time averages along particle trajectories. Employing this approach we are able to significantly extend the range of particle numbers $N$ treated numerically compared to earlier approaches, while reproducing all exactly known results for this model. We also show that for the bosons in a harmonic trap, contrary to what has been assumed so far, the momentum distribution reflects the system size scaling of the occupation numbers of the natural orbitals, i.e., it can be used to decide on the presence of a Bose-Einstein condensate.

# Applying the repeated interaction process on quantum spin chains

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We study the dynamics of free fermionic quantum spin chains, submitted to the repeated interaction process. We show that when the system and the bath are prepared in Gaussian states, the system dynamics is fully characterized by the evolution of the two-point correlations. Considering the XX chain in interaction at its boundaries with two quantum reservoirs, we show that the steady state is completely characterized by the magnetization profile and the associated current.

# Numerical test of the Cardy-Jacobsen conjecture in the site-diluted Potts model in three dimensions

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We present a microcanonical Monte Carlo simulation of the site-diluted Potts model in three dimensions with eight internal states, partly carried out in the citizen supercomputer Ibercivis. Upon dilution, the pure model's first-order transition becomes of the second-order at a tricritical point. We compute accurately the critical exponents at the tricritical point. As expected from the Cardy-Jacobsen conjecture, they are compatible with their Random Field Ising Model counterpart. The conclusion is further reinforced by comparison with older data for the Potts model with four states.

# Broadscale examination of the influence of disorder on semiflexible polymers (P)

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We study the static properties of a semiflexible polymer exposed to a quenched random environment by means of computer simulations. The polymer is modeled as a two-dimensional Heisenberg chain. For the random environment we consider a hard-disk potential. We apply an off-lattice growth algorithm to investigate the influence of both disorder area fraction and polymer stiffness on the equilibrium properties of the polymer. We show that the additional length scale induced by the stiffness of the polymer extends the well-known phenomenology considerably. The polymer's response to the disorder is either contraction or extension depending on the ratio of polymer stiffness and void-space extension. Additionally, the structure of the potential is reflected in the observables that characterize the polymer.

# Structure and dynamics at polymer-solid interfaces: Atomistic molecular dynamics (MD) simulations of 1,4-polybutadiene at graphite surfaces (P)

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Polymer dynamics in confinement is both of fundamental interest concerning our understanding of the glass transition, as well as of high technological importance for the performance of composite materials. The results here presented are concerned with atomistic MD simulations of a chemically realistic model of a 1,4-polybutadiene melt (55% TRANS and 45% CIS content) confined between two walls of graphite. The focus of our study is to investigate the effects of confinement on the chain dynamics in the melt and to reveal to what extent the walls are influencing structure and dynamics of the melt. The physical properties here investigated are density profiles and collective dielectric relaxation. The results presented are key to a better understanding of the glass transition process in a confined polymer system.

# Estimate of the energy of vacuum fluctuations of non-Abelian gauge fields from the uncertainty relations (P)

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We derive the commutation relations for field strengths of non-Abelian gauge fields by requiring that the quantum mechanical equations of motion coincide with the classical field equations. The equations of motion with respect to time derivative coincide with the corresponding field equations, while those with respect to space derivatives agree with classical field equations if constraint equations are fulfilled. Using the uncertainty relations for field strengths at the same times, which follows from the commutation relations, we estimate the energy gap of vacuum fluctuations in the long wave limit as $\mathcal{E}_{0,k} \sim c\hbar\Lambda^{-2}V^{-1}(g^2/c\hbar)^{1/3}$ and the total energy $\mathcal{E}_0 \sim \Lambda c\hbar(g^2/\hbar c)^{1/3}$ with $\Lambda$ being a cutoff separating the weak- and strong-coupling regimes.

[1] S. Stepanow, preprint arXiv:1207.5199 [hep-th].

# Theoretical description of polymer crystallization

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We develop a description of polymer crystallization (trans-states-repulsion (TSR) mechanism) by considering the repulsion between the monomers caused by the frequent occupation of trans-states along the chains, which is efficient below a characteristic temperature $T_m$, as the driving force. The thickness of stems and bundles, which form due to these repulsive interactions, is determined by setting equal the emergence time of stems of the length $d_l$ with the Rouse time of a piece of polymer of the same length $d_l$. The increase of the scattering intensity at early times is considered to be due to the rigid property of fluctuational clusters, which are built up of contacting stems.

# Quantitative indicators for roles in online discussion groups

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A number of usenet groups have a long history where individual users are found to participate over long time ranges. These groups therefore offer the possibility to test hypotheses like, e.g., preferential attachment scenarios on such time scales. Our focus is in particular on developing quantitative indicators for the type of discussion (e.g., technical or philosophical) and the self-defined roles of the participants. Analysing technical discussions we identify time evolving network motives that describe *expert* members who answer many questions while in *philosophical* discussions some members occur who initiate a multitude of discussions. Developing indicators for these roles we observe quantitatively how they may evolve and may change with time.

# Spin glasses with many components

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We investigate zero and finite temperature properties of the one-dimensional spin-glass model for vector spins in the limit of an infinite number $m$ of spin components where the interactions decrease with a power, $\sigma$, of the distance. A diluted version of this model is also studied. At zero temperature, defect energies are determined from the difference in ground-state energies between systems with periodic and anti-periodic boundary conditions to determine the dependence on $\sigma$ of the defect energy exponent $\theta$. A good fit to this dependence is $\theta = \frac{3}{4} - \sigma$. This implies that the lower critical value of $\sigma$ is $3/4$ and corresponds to the lower critical dimension in the $d$-dimensional short-range version of the model. For finite temperatures the large $m$ saddle-point equations are solved self-consistently which gives access to the correlation function, the order parameter and the spin-glass susceptibility. Special attention is paid to the different forms of finite-size scaling scaling effects below and above the upper critical value, $\sigma = 5/8$, which corresponds to the upper critical dimension 8 of the short-range model.

# Finite-size scaling analysis of the distributions of pseudo-critical temperatures in spin glasses

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Using the results of large scale numerical simulations we study the probability distribution of the pseudo critical temperature for the three-dimensional Edwards-Anderson Ising spin glass and for the fully connected

Sherrington-Kirkpatrick model. We find that the behavior of our data is nicely described by straightforward finite-size scaling relations.

## Emergence of gene regulatory networks under functional constraints

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Gene regulatory networks allow the control of gene expression patterns in living cells. We ask here to what extent the network architecture is determined by the output patterns of gene regulatory networks. Given a framework for describing regulatory interactions and dynamics introduced by Burda *et al.* [1], we consider in the space of all regulatory networks those that have prescribed functional capabilities. Markov Chain Monte Carlo sampling is then used to determine how these functional constraints lead to specific structures of the interactions. Particularly, we generate ensemble of regulatory networks with baker's and fission yeast cell-cycle biological pathway imposed. As a result, we find that on average roughly 60% of interactions are well reproduced, and concerning the whole ensemble almost all networks have from 50% to 70% of links in common with yeast cell-cycle network.

[1] Z. Burda, A. Krzywicki, O.C. Martin, and M. Zagórski, Proc. Natl. Acad. Sci. U.S.A. **108** (2011) 17263–17268 [arXiv:1104.4511].

## Scaling properties of a parallel implementation of the multicanonical algorithm

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The multicanonical method has been proven powerful for statistical investigations of lattice and off-lattice systems throughout the last two decades. We discuss an intuitive but very efficient parallel implementation of this algorithm and analyze its scaling properties for discrete energy systems, namely the Ising model and the 8-state Potts model. The simple parallelization relies on independent equilibrium simulations in each iteration with identical weights, merging their statistics in order to obtain estimates for the successive weights. With good care, this allows faster investigations of large systems, because it distributes the time-consuming weight-iteration procedure and allows parallel production runs. We show that the parallel implementation scales very well for the simple Ising model, while the performance of the 8-state Potts model, which exhibits a first-order phase transition, is limited due to emerging barriers and the resulting large integrated autocorrelation times. The quality of estimates in parallel production runs remains of the same order at same statistical cost.