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ABSTRACTS

of contributions to the

17th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys16

Institut für Theoretische Physik, Universität Leipzig, Germany

24 – 26 November 2016

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Preface

Welcome to the 17th International NTZ-Workshop *CompPhys16* on *New Developments in Computational Physics*. As in previous years, also this year's Workshop will cover a broad spectrum of different fields ranging from general aspects of computational and statistical physics over computer simulation studies in condensed and soft matter physics, including applications to biological systems, and random networks to the intriguing properties of quantum systems and high-energy physics. Following the traditional setup of the Workshop, it is also this year 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 24 – 25 November 2016 in the Theory Lecture Hall ("Hörsaal für Theoretische Physik") 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 location or date. and in particular to Ms. Antje Heydecke who coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Gabriele Menge, Ms. Susan Hussack, and Ms. Lea Voigt, for their invaluable help with all administrative matters.

As in previous years, the Saturday, 26 November 2016, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that a few years ago the Institute for Theoretical Physics has moved from the old location "Vor dem Hospitaltore 1" to the *new* office building in "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Research Academy Leipzig (RALeipzig), Deutsch-Französische Hochschule (DFH-UFA), EU Marie Curie IRSES Network DIONICOS: Dynamics of and in Complex Systems, DFG Collaborative Research Centre SFB/TRR 102, Alexander von Humboldt Foundation (AvH), and Graduate School "BuildMoNa".

Leipzig,
November 2016

Wolfhard Janke

Abstracts

SAMC simulation of Alanine and Glutamine oligomers (P)

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Thermodynamics and structure of single Poly-Alanine (polyA) and Poly-Glutamine (polyQ) peptides are investigated by the Stochastic Approximation Monte Carlo (SAMC) method. polyQ has been found to aggregate in a beta-sheet configuration while polyA tends to form alpha-helical structures. Both structure types are confirmed for this model and can be analyzed further.

Coarsening and aging of lattice polymers (P)

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The nonequilibrium properties of homopolymeric collapse were investigated using Monte Carlo simulations of the interacting self-avoiding walk (ISAW) in three dimension with short nearest neighbor (NN) and longer range next-nearest neighbor (NNN) interactions. Recently, the scaling behavior of the average cluster size as well as aging was investigated using a off-lattice polymer model by applying methods from domain coarsening phenomenons to polymers. We extend this work to lattice polymer models in order to be able to simulate longer polymers and define properties that are dependent on the underlying structure, like the equal-time two point correlation function. We found a power-law growth of ordered structures (or clusters) during the collapse of lattice polymers. The found exponent α ($= 0.38$ in the NN model and $= 1/3$ in the NNN model) was considerably smaller than the growth exponent previously reported ($\alpha = 1$) for off-lattice models. In addition we investigated aging and found the same dynamic aging exponent as in the off-lattice model for both interaction ranges ($\lambda_c = 1.25$).

Fluctuation-induced forces in confined He and Bose gases

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When condensed-matter systems in which low-energy thermal fluctuations occur are confined by a pair of parallel planes or walls to a film geometry, effective forces between the planes are generated by these fluctuations. Familiar examples are He4 near the lambda transition and Bose gases near the condensation transition. The cases of He or Bose gases in a 3D film geometry are particularly challenging since nontrivial dimensional crossovers of 3D bulk systems exhibiting long-range order at low temper- atures to effective 2D systems without long-range order must be handled in addition to bulk, boundary, and finite-size critical behaviors. We show that exact results can be obtained for analogous n-component ϕ^4 models in the limit $n \to \infty$ via inverse-scattering theory and other methods, and show that these results apply directly to the so-called imperfect Bose gas.

Improving causal Gaussian Bayesian network inference using parallel tempering (P)

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Gene regulatory networks describe molecules and their interactions within biological processes, e.g. signal transduction or disease mechanisms. While relationships in gene expressions can be studied experimentally, looking at a complex network of interactions would call for a massive amount of experiments. Thus, a considerable interest exists in supporting the experimental work by developing computational methods to infer gene regulatory networks from available gene expression data. To infer causality within those networks as opposed to mere correlations, we make use of causal orderings, where in a given ordering each gene only has a causal effect on subsequent, not on preceding genes. Gaussian Bayesian networks can be utilized to infer networks from mixed, observational and intervention, data. In this framework, for a given causal ordering, the likelihood of the model network can be maximized analytically. The difficulty arises of how to explore the space of causal orderings which grows an n! for n genes. This has been done previously via a simple Markov Chain Monte Carlo algorithm. The approach proofed reliable for small networks ($10 - 20$ genes) only, but unsatisfactory for larger networks (¿50 genes). We show that parallel tempering improves the reliability of the algorithm for large networks. By simulating multiple sets of Markov Chains at different temperatures and exchanging the systems regularly, systems are less likely to get stuck in local maxima of the "likelihood landscape". Parallel tempering helps in finding the orderings with highest maximum likelihood estimators as well as in exploring the set of alternative orderings with comparable maximum likelihood estimators. Thus, the chances of obtaining a reliable model of or even the actual underlying gene regulatory network are significantly increased.

Asymptotic scaling behavior of self-avoiding walks on critical percolation clusters (P)

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We study self-avoiding walks on three-dimensional critical percolation clusters using a new exact enumeration method. It overcomes the exponential increase in computation time by exploiting the clusters' fractal nature. We enumerate all $\simeq 10^{1200}$ conformations of walks with over 10^4 steps, far more than has ever been possible in previous studies (that is over 200 times more steps – over 10^{1000} times more conformations). The scaling exponent ν for the end-to-end distance turns out to be smaller than previously thought and appears to be the same on the backbones as on full clusters. We find strong evidence against the widely assumed scaling law for the number of conformations and propose an alternative, which perfectly fits our data.

[1] N. Fricke and W. Janke, Phys. Rev. Lett. **113** (2014) 255701.
[2] N. Fricke and W. Janke, *Exact enumeration of self-avoiding walks on critical percolation clusters in* 2–7 *dimensions*, Leipzig preprint (October 2016), submitted to J. Phys. **A**.

Phase transitions in disordered systems: The example of the random-field Ising model in four dimensions

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By performing a high-statistics simulation of the four-dimensional random-field Ising model at zero temperature for different shapes of the random-field distribution, we show that the model is ruled by a single universality class. We compute to a high accuracy the complete set of critical exponents for this class, including the correction-to-scaling exponent. Our results indicate that in four dimensions (i) dimensional reduction as predicted by the

perturbative renormalization group does not hold and (ii) three independent critical exponents are needed to describe the transition.

Massively parallel multicanonical simulations on GPUs

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Generalized-ensemble Monte Carlo simulations such as the multicanonical method and similar techniques are among the most efficient approaches for simulations of systems undergoing discontinuous phase transitions or with rugged free-energy landscapes. As Markov chain techniques, they are inherently sequential. It was demonstrated recently, however, that a combination of independent simulations that communicate weight updates at irregular intervals allows for the efficient utilization of parallel computational resources for such simulations. Implementing this approach for the many-thread architecture provided by current generations of graphics processing units (GPUs), we show how it can be efficiently employed with of the order of 104 parallel walkers and beyond, thus constituting a versatile tool for Monte Carlo simulations in the era of massively parallel computing. We applied our algorithm to the paradigmatic example of the two-dimensional Ising model as starting point and reference for practitioners in the field.

Large-scale molecular dynamics simulations are presented for a coarse-grained model of polymer melts in equilibrium

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Large-scale molecular dynamics simulations are presented for a coarse-grained model of polymer melts in equilibrium. From detailed Rouse mode analysis we show that the time-dependent relaxation of the autocorrelation function (ACF) of modes p can be well described by the effective stretched exponential function due to the crossover from Rouse to reptation regime. The ACF is independent of chain sizes N for $N/p < N_e$ (N_e is the entanglement length), and there exits a minimum of the stretching exponent as $N/p \to N_e$. As N/p increases, we verify the crossover scaling behavior of the effective relaxation time $\tau_{\mathrm{eff},p}$ from the Rouse regime to the reptation regime. We have also provided an evidence that the incoherent dynamic scattering function follows the same crossover scaling behavior of the mean square displacement of monomers at the corresponding characteristic time scales. The decay of the coherent dynamic scattering function is slowed down and a plateau is developed as chain sizes increase at the intermediate time and wave length scales. The tube diameter extracted from the coherent dynamic scattering function is equivalent to the previous estimate from the mean square displacement of monomers.

Random quantum systems with long-range interactions

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We consider the random transverse-field Ising model in $d = 1, 2$ and 3 dimensions with long-range ferromagnetic interactions which decay as a power $\alpha > d$ with the distance. Using a variant of the strong disorder renormalization group method we study numerically the phase-transition point from the paramagnetic side. We find that the fixed-point controlling the transition is of the strong disorder type, and based on the experience with other similar systems, we expect the results to be qualitatively correct, but probably not asymptotically exact. The distribution of the (sample dependent) pseudo-critical points is found to scale with $1/\ln L$, L being the linear size of the sample. Similarly, the critical magnetization scales with $(\ln L)^{\chi}/L^{d}$ and the excitation energy behaves

as $L^{-\alpha}$. Using extreme-value statistics we argue that extrapolating from the ferromagnetic side the magnetization approaches a finite limiting value and thus the transition is of mixed-order.

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[2] R. Juhász, I. A. Kovács, and F. Iglói, Phys. Rev. E **91** (2015) 032815.
[3] I. A. Kovács, R. Juhász, and F. Iglói, Phys. Rev. B **93** (2016) 184203.

Social simulation with exascale computer

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Simulations of social phenomena have been becoming a challenging field of supercomputers now. Typical applications are, for example, traffic control, economic risk management, interception of disease propagation and disaster evacuation. Such simulation models usually have many parameters, and they show various phases and regimes. For example, when we make traffic simulation, each car has unique origin and destination, and available route is not unique in most case. Control of each traffic light introduces some parameters. Capacity computing with modern supercomputer help to tame such complex social models.

Critical Ising model with a defect line: Exact solution

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The Ising model in two dimensions with the peculiar toroidal boundary conditions is analysed. This boundary condition, which we call the duality twisted boundary conditions, may be interpreted as inserting specific defect line ("seam") in the system, along non contractible circles of the cylinder, before closing it into a torus. We derive [1] exact expressions for the eigenvalues of the transfer matrix for the critical ferromagnetic Ising model on the $M \times N$ square lattice wrap on torus with specific defect line ("seam"). As result we have obtain analytically the partition function for the Ising model with such boundary condition. In the limit $N \to \infty$ we obtain the asymptotic expansion of the free energy and the inverse correlation lengths for infinitely long cylinder of circumference M with duality twisted boundary conditions.

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Towards the QCD phase diagram using complex Langevin

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Complex Langevin methods have been successfully applied in theories that suffer from a sign problem such as QCD with a chemical potential. We present and illustrate a novel method (dynamic stabilization) that ensures that Complex Langevin simulations stay close to the SU(3) manifold, which lead to correct and improved results in the framework of pure gauge simulations and QCD in the limit of heavy quarks.

Melting in 2D and a fresh perspective on Monte Carlo

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Recent progress in global-balance Monte Carlo algorithms has allowed to confirm the essentials of the Halperin-Nelson-Young theory (KTHNY) for the 2D Melting problem with short-range interactions [1]. A key challenge in these simulations are large correlation lengths which could be overcome by a new class of Monte Carlo algorithms [2]. In this talk, I will show that the new Monte Carlo paradigm can be extended to include long-range forces (including periodic images) rigorously, without any truncation effects. The resulting algorithm improves on the scaling of Ewald summation and opens a new perspective on large-scale simulation of charged or polar systems [3]. In addition, I will present first results on the 2D Melting problem with long-range forces.

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The axial nucleon charge g_A and its renormalization constant Z_A using the point-split axial vector current operator on the lattice

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We study the point-split axial vector current operator on the lattice. We calculate the axial charge g_A of the nucleon using this operator for $\beta = 5.50$ and $\beta = 5.80$. We compare the summation method and the global fit method for including the excited states contribution into the estimation of the axial charge. We take a look at the bare mass dependence of the axial charge. Finally we obtain the renormalization factor Z_A for the point-split axial current operator for $\beta = 5.50$ in the $\overline{MS}$ scheme. We compare the renormalized axial charge to that obtained with the local axial current operator and get a result which is significantly closer to the experimental value.

On the uniform sampling of ground states in the 2D $\pm J$ Ising spin-glass model

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It is well known that the Edwards-Anderson Ising spin glass with $\pm J$ bond distribution in two dimensions has a huge number of degenerate ground states, the number of which growths exponentially with increasing system size L. Except for very small system sizes it is not possible to enumerate all ground states explicitly. It is hence necessary to develop techniques for sampling the ground-state manifold uniformly. We present a new efficient algorithm serving this purpose. It is based on an exact analysis of clusters of free spins in a disorder configuration and a subsequent sampling step based on parallel tempering Monte Carlo. The algorithm allows us to find all ground states for systems with $L \leq 20$ as well as to pick ground states uniformly from the ground-state manifold for larger systems.

Approximate ground states of the random-field Potts model from a graph-cut method and parallel tempering (P)

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While the ground-state problem for the random-field Ising model is polynomial, and can be solved using a number of well known algorithms for maximum flow, the analogue random-field Potts model corresponds to a multi-terminal flow problem that is known to be NP hard. Hence an efficient exact algorithm is extremely unlikely to exist. Still, it is possible to employ embedding of binary degrees of freedom into the Potts spins to use graph-cut methods to solve the corresponding ground-state problem approximately with polynomial methods. It is shown here that this works relatively well. We compare results produced by this heuristic algorithm to energy minima found by an appropriately tuned parallel tempering method that is configured to find ground states for the considered system sizes with high probability. The method based on graph cuts finds the same states in a fraction of the time. The new method is used for a first exploratory study of the random-field Potts model in two dimensions.

Scaling laws in polymer collapse: Lattice vs off-lattice

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Collapse dynamics of a polymer after being quenched into the globular phase from an extended coil is studied via Monte Carlo simulation of a lattice model and a continuum model. Scaling laws related to the collapse time, cluster growth and aging dynamics have been compared. Primary results show that while the scaling related to the cluster growth are different in the concerned models, the aging exponent seems to be the same.

Exact solutions to plaquette Ising models with free and periodic boundaries

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An anisotropic limit of the 3d plaquette Ising model, in which the plaquette couplings in one direction were set to zero, was solved for free boundary conditions by Suzuki (Phys. Rev. Lett. 28 (1972) 507), who later dubbed it the fuki-nuke, or "no-ceiling", model. Defining new spin variables as the product of nearest-neighbour spins transforms the Hamiltonian into that of a stack of (standard) 2d Ising models and reveals the planar nature of the magnetic order, which is also present in the fully isotropic 3d plaquette model. More recently, the solution of the fuki-nuke model was discussed for periodic boundary conditions, which require a different approach to defining the product spin transformation, by Castelnovo et al. (Phys. Rev. B 81 (2010) 184303). We clarify the exact relation between partition functions with free and periodic boundary conditions expressed in terms of original and product spin variables for the 2d plaquette and 3d fuki-nuke models, noting that the differences are already present in the 1d Ising model. In addition, we solve the 2d plaquette Ising model with helical boundary conditions. The various exactly solved examples illustrate how correlations can be induced in finite systems as a consequence of the choice of boundary conditions.

Critical behavior in the presence of an order-parameter pinning field

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We apply a recently advocated simulation scheme that employs a local order-parameter pinning field to study quantum critical phenomena in the two-dimensional square-lattice bilayer quantum Heisenberg model. Using a world-line quantum Monte Carlo approach, we show that for this model, the pinning-field approach allows to locate the quantum critical point over a wide range of pinning-field strengths. However, the identification of the quantum critical scaling behavior is found to be hard since the pinning field introduces strong corrections to scaling. In order to further elucidate the scaling behavior in this situation, we also study an improved classical lattice model in the three-dimensional Ising universality class by means of Monte Carlo simulations on large lattice sizes, which allow us to employ refined finite-size scaling considerations. A renormalization group analysis exhibits the presence of an important crossover effect from the zero pinning-field to a critical adsorption fixed point. In line with field-theoretical results, we find that at the adsorption fixed point the short-distance expansion of the order-parameter profile exhibits a new universal critical exponent. This result also implies the presence of slowly-decaying scaling corrections, which we analyze in detail.

Quantum Hamilton equations: Derivation and application

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Non-relativistic quantum systems are analyzed theoretically or by numerical approaches using the Schrdinger equation. Compared to the options available to treat classical mechanical systems this is limited, both in methods and in scope. However, based on Nelson's stochastic mechanics, the mathematical structure of quantum mechanics has in some aspects been developed into a form analogous to classical analytical mechanics. We show here that finding the Nash equilibrium for a stochastic optimal control problem, which is the quantum equivalent to Hamilton's principle of least action, allows to derive two things: i) the Schrödinger equation as the Hamilton-Jacobi-Bellman equation of this optimal control problem and ii) a set of quantum dynamical equations which are the generalization of Hamilton's equations of motion to the quantum world. We derive their general form for the non-stationary and the stationary case. For the harmonic oscillator, the stationary equations lead to the coherent states, and we establish a numerical procedure to solve for the ground state properties without using the Schrödinger equation.

Spectrum and entropy of Anosov-Kolmogorov systems and MIXMAX generator

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We shall present the computation of the spectrum and of the entropy of hyperbolic systems of Anosov-Kolmogorov. These dynamical systems have strong stochastic properties and can be efficiently used to generate pseudorandom numbers for Monte Carlo simulations. These high entropy generators are able to generate random numbers with a high speed of 1 Gbps.

Convex hulls of self-avoiding random walks: A large-deviation study (P)

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We study the convex hulls of different types of random walks, i.e., the smallest convex polygon enclosing the trajectory of a random walk with T steps. While the convex hulls of normal random walks are decently studied [1, 2], very little is known about the convex hulls of other important types of random walks as the Self-Avoiding Random Walk (SAW) and the Loop-Erased Random Walk (LERW). Using Monte-Carlo sampling-techniques, we can study a large part of the support of the distributions [3] of the area A or perimeter L of the convex hulls. This enables us to reach probability densities below $p(A) = 10^{-800}$ and scrutinize large-deviation properties. Similar to normal random walks, the probability densities show a universal scaling behavior dependent on the inverse fractal dimension ν and the dimension of the observable (e.g., $d = 2$ for A). Further, we determined the rate function $\phi = -1/T \log P(.)$ which shows convergence to a limit shape for $T \to \infty$.

[1] G. Claussen, A. K. Hartmann, and S. N. Majumdar, *Convex hulls of random walks: Large-deviation properties*, Phys. Rev. E **91** (2015) 052104.
[2] Ronen Eldan, *Volumetric properties of the convex hull of an n-dimensional Brownian motion*, Electron. J. Probab. **19** (2014) 1.
[3] A.K. Hartmann, *Sampling rare events: Statistics of local sequence alignments*, Phys. Rev. E **65** (2002) 056102.

The microcanonical barrier and the ensemble tailoring framework

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In this work [1] we discover a principle difference between the canonical first-order phase transition and the corresponding microcanonical transition. We find that every system with a temperature-driven canonical first-order phase transition has an corresponding total-energy-driven transition with a lower transition barrier. The analytical reasoning that was used to obtain this assessment additionally suggests an approach to tailor artificial ensembles, with a desired barrier behavior.

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Local energy minima of the 3d Edwards-Anderson model

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It is well known that the unique thermodynamic behavior of spin glasses results from a rough energy-landscapes which is characterized by a multitude of valleys and barriers. However, for non-meanfield systems these properties are not well understood and the investigation by means of traditional Monte Carlo methods is challenging. We employ flat-histogram Monte Carlo methods in combination with a novel dynamic greedy algorithm in order to investigate the energy landscape of the three-dimensional Edwards Anderson model. We were able to determine the number and the spectrum of local energy minima.

Folding in small polyethylene systems: Single chains and few chains

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The phase behaviour of polyethylene has been under wide investigation during the last six decades. But investigation of single-chain crystallization is a technically difficult problem. One of the reasons for this is that in the case of molecular dynamics simulations as well as in experiments, it is not so easy to distinguish kinetic and thermodynamic effects on chain ordering folding. We present results of a Stochastic Approximation Monte Carlo (SAMC) study of ordering of relative short single polyethylene chains and on the aggregation of a few such chains. Our simulations are based on a chemically realistic united atom model [1].

[1] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. **103** (1995) 1702–1709.

Population annealing: Massively parallel simulations in statistical physics

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While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so *serial* code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. *Population annealing*, that was initially suggested by Hukushima and Iba and more recently was studied systematically by Machta, is a sequential Monte Carlo scheme that is potentially able to make use of such highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach. The relative performance with respect to such more traditional techniques, the appropriate choice of population sizes temperature protocols and other parameters, the estimation of statistical and systematic errors and many other features, however, are essentially uncharted territory. Here, we use a systematic comparison of population annealing to Metropolis as well as parallel tempering simulations for the Ising model to gauge the potential of this new approach, and we suggest a range of heuristics for its application in more general circumstances.

Canonical free-energy barrier of particle and polymer cluster formation

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We present a methodology to study temperature-driven cluster formation in the canonical ensemble for both particle and polymer systems [1]. In particular, this allows a shape-free determination of the free-energy barrier. Combined with rigorous results on equilibrium droplet formation, this enables a well-defined finite-size scaling analysis of the free-energy barrier at fixed density. We verify our theoretical predictions using parallel multi-canonical simulations [2] of a Lennard-Jones particle gas and generalize this approach to cluster formation in a dilute bead-spring polymer solution. Our results suggest an analogy between polymer aggregation and particle condensation, when the macromolecules are interpreted as extended particles. We will briefly comment on the role of kinetic energy on the free-energy barrier, which is commonly neglected in computer simulation studies.

[1] J. Zierenberg, P. Schierz, and W. Janke, arXiv:1607.08355.
[2] J. Zierenberg, M. Marenz, and W. Janke, Comput. Phys. Comm. **184** (2013) 1155.