10

Computational Quantum Field Theory

10.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with focus on fluctuating paths and interfaces, biologically motivated problems such as protein folding, aggregation and adsorption as well as related properties of homopolymers, and the intriguing physics of low-dimensional quantum spin systems.

The methodology is a combination of numerical and analytical techniques. The numerical tools are mainly Monte Carlo and Molecular Dynamics computer simulations as well as exact enumeration techniques. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and is likely to become the third cornerstone of physics besides experiment and analytical theory as sketched in Fig. 10.1. Already now it often helps to bridge the gap between experiments and the often necessarily approximate calculations in analytic approaches. To achieve the desired high efficiency of the numerical studies we develop new algorithms and, to guarantee the flexibility required by basic research, all computer codes are implemented by ourselves. The technical tools are Fortran, C, C++, and Python programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Currently we are also exploring the possibilities of the rapidly developing graphics card computing, that is computer simulations on graphics processing units (GPUs) with many cores. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the Saxon computing centre in Dresden, and, upon successful grant application, at the national supercomputing centres in Jülich, Stuttgart and München on parallel high-capability computers. This hierarchy of various platforms gives good training and qualification opportunities for the students, which offers promising job perspectives in many different fields for their future careers.

Our research activities are closely integrated into the Graduate School “Build-

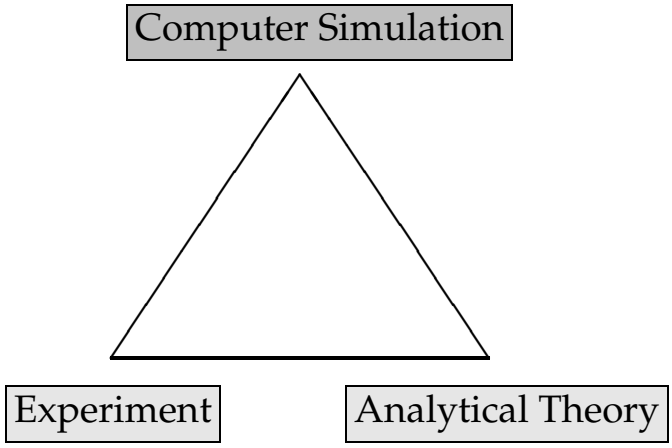


Figure 10.1: Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

MoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects*, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*, and the International Doctoral College *Statistical Physics of Complex Systems* with Université de Lorraine in Nancy, France, supported by the Deutsch-Französische Hochschule (DFH-UFA). In the second funding period 2011–2013, Coventry University in England has been integrated as an associated partner, and in the third funding period 2014–2016, also the National Academy of Sciences of Ukraine in Lviv has joined as another associated partner institution, offering our PhD students now several interesting options for secondments. For instance, in 2014, one PhD student started a "co-tutelle de thèse" jointly supervised with a colleague from Coventry University. Currently the DFH-UFA Doctoral College under the acronym "$\mathbb{L}^4$" is in its fourth funding period 2017–2020. The three Graduate Schools are all "Classes" of the Research Academy Leipzig (RALeipzig), providing the organizational frame for hosting visiting students and senior scientists, offering language courses, organizing childcare and for many other practical matters.

At a more post-graduate level our research projects are embedded into the Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* together with Halle University. Our group also actively contributes to two of the top level research areas ("Profillinien") and the Centre for Theoretical Sciences (NTZ) of the University. Beside "BuildMoNa" the latter structures are particularly instrumental for our cooperations with research groups in experimental physics and biochemistry on the one hand and with mathematics and computer science on the other.

On an international scale, our research projects are carried out in a wide net of collaborations which are currently mainly funded by the Alexander von Humboldt Foundation through an Institute Partnership with the National Academy of Sciences in Lviv, Ukraine, on *Polymers in Porous Environments and on Disordered Substrates* and the EU IRSES Network DIONICOS: *Dynamics of and in Complex Systems*, a consortium of 6 European and 12 non-European partners, including sites in England, France and Germany as well as in Armenia, Russia, Ukraine, India, the United States and

Venezuela, which commenced work in 2014. Further close contacts and collaborations are established with research groups in Armenia, Austria, China, France, Great Britain, India, Israel, Italy, Japan, Poland, Russia, Spain, Sweden, Taiwan, Turkey, Ukraine, and the United States. These contacts are refreshed and furthered through topical Workshops, Advanced Training Modules and Tutorials, and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

Wolfhard Janke

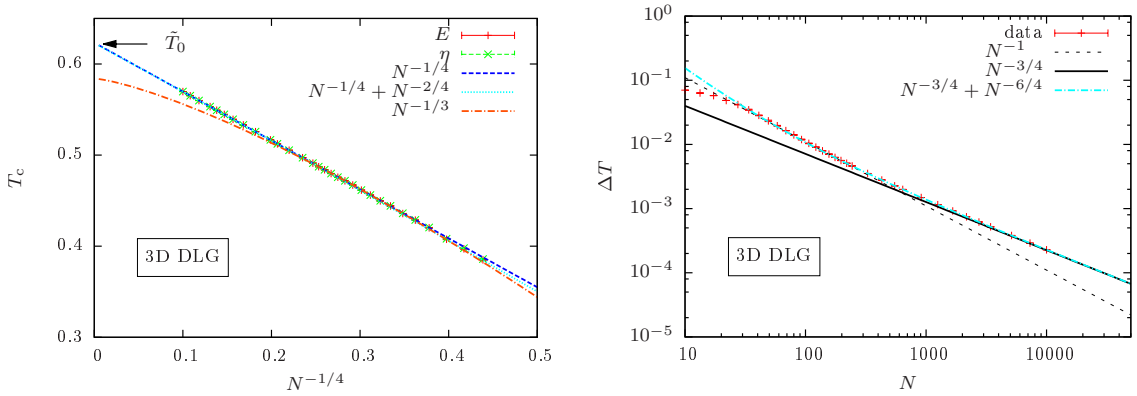


Figure 10.2: Finite-size scaling of (a) the transition temperature and (b) the transition rounding of a three-dimensional lattice gas at fixed density $\rho = 10^{-2}$.

10.2 Finite-size scaling predictions for the droplet condensation-evaporation transition

J. Zierenberg, A. Nußbaumer*, E. Bittner†, W. Janke

*Institut für Physik, Johannes Gutenberg Universität Mainz, Germany
†Institut für Theoretische Physik, Universität Heidelberg, Germany

We investigated the finite-size scaling behaviour of the droplet condensation-evaporation transition for the two- and three-dimensional Ising lattice gas as well as the three-dimensional Lennard-Jones gas [1, 2]. The lattice models allow to exploit the equivalence to the Ising model, comparing to exact results in two dimensions and low-temperature series expansions in three dimensions. The Lennard-Jones model ensured the generality of our results. Opposed to the consideration at fixed temperature [3], for which leading-order predictions exist [4], we considered here an orthogonal setup at fixed density. The relation of the two approaches was recently reviewed in Ref. [5].

Applying in the fixed density approach Taylor expansions around the infinite-system limit, we obtain the same leading-order scaling behaviour as in the fixed temperature case for the finite-size transition temperature $T_c(N)$ and rounding ΔT of a D-dimensional system with N particles:

$$T_c(N) - T_0 \propto N^{-1/(D+1)}, \tag{10.1}$$

$$\Delta T \propto N^{-d/(D+1)}. \tag{10.2}$$

This is not the standard $1/N$ finite-size scaling of a first-order phase transition, because droplet condensation-evaporation describes a transition between a homogenous gas phase and an inhomogeneous or mixed phase where a single droplet is in equilibrium with surrounding vapor. A comparison with our numerical results from parallel multicanonical simulations [6] is shown in Fig. 10.2 for the case of the three-dimensional lattice gas.

For intermediate system sizes, we observe a non-expected scaling regime where the system behaves as for homogeneous phase transitions, i.e., $T_c(N) - T_0 \propto N^{-1/d}$ and $\Delta T \propto N^{-1}$. For the three-dimensional lattice gas we can compare to low-temperature series expansion estimates of the transition temperature $\tilde{T}_0(\rho)$ and the agreement is very

good. With our approach, we were able to reach up to $N = 10\,000$ lattice particles and the finite-size scaling analysis suggests that we are in fact quite close to the asymptotic scaling regime.

[1] J. Zierenberg, W. Janke: Phys. Rev. E **92**, 012134 (2015)
[2] J. Zierenberg, W. Janke: in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012017 (2016)
[3] J. Zierenberg et al.: J. Phys: Conf. Ser. **510**, 012017 (2014)
[4] M. Biskup et al.: Europhys. Lett. **60**, 21 (2002); Commun. Math. Phys. **242**, 137 (2003)
[5] A. Nußbaumer et al.: J. Phys.: Conf. Ser. **759**, 012009 (2016)
[6] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)

10.3 Free-energy barriers of particle and polymer condensation

J. Zierenberg, P. Schierz, W. Janke

A common approach to study nucleation rates is the estimation of free-energy barriers. This usually requires knowledge about the shape of the forming droplet, a task that becomes notoriously difficult in macromolecular setups starting with a proper definition of the cluster boundary or a proper ensemble choice. Here, we demonstrate that a shape-free determination of temperature-driven cluster formation is directly accessible in the canonical ensemble for particle as well as polymer systems. Combined with rigorous results on canonical equilibrium droplet formation, this allows for a well-defined finite-size scaling analysis of the effective interfacial free energy at fixed density as illustrated in Fig. 10.3. We first verified the theoretical predictions for the formation of a liquid droplet in a supersaturated particle gas by (parallelized) generalized-ensemble Monte Carlo simulations [1–3] of a Lennard-Jones system [4–6]. Going one step further, we then generalized this approach to the aggregation process in a dilute polymer solution [6], cf. Fig. 10.4. Our results suggest an analogy between particle condensation and polymer aggregation, when the macromolecules are interpreted as extended particles.

Because the standard approach in Monte Carlo simulations is to work in the conformational ensemble governed by potential energy only, we show that excluding the kinetic energy from the partition function leads to finite-size differences in the free energy compared to the full ensemble [7, 8] but retains intensive parameters in the thermodynamic limit [6]. Our study of nucleation rates at fixed density corresponds to a heating-cooling framework where simulation and experiment may meet at the nanometer scale.

[1] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
[2] W. Janke: Int. J. Mod. Phys. C **03**, 1137 (1992); Physica A **254**, 164 (1998)
[3] J. Zierenberg et al.: Comput. Phys. Commun. **184**, 1155 (2013)
[4] J. Zierenberg, W. Janke: Phys. Rev. E **92**, 012134 (2015)

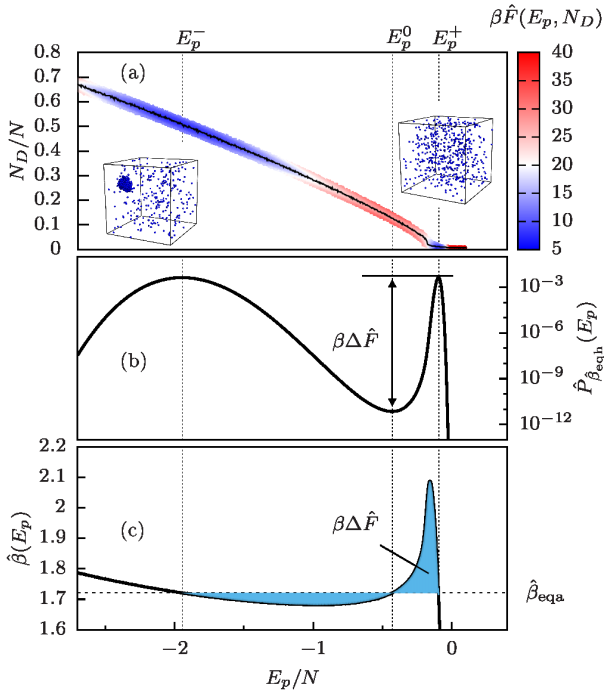


Figure 10.3: (a) Illustration of the free-energy landscape $\beta\hat{F}(E_p, N_D)$ (color map) as a function of potential energy E_p and droplet size N_D for $N = 512$ Lennard-Jones particles. The minimal free-energy path (black solid line) connects a droplet ($E_p \approx E_p^-$) and a gaseous ($E_p \approx E_p^+$) phase, visualized by the snapshots at $E_p^\pm$. The projection onto the reaction-coordinate E_p yields the canonical potential-energy probability distribution $\hat{P}_\beta(E_p)$, where the free-energy barrier $\beta\Delta\hat{F}$ is encoded in the ratio between maximum and minimum at $\hat{\beta}_{\rm eqh}$. (c) Equivalently, $\beta\Delta\hat{F}$ is the (equal) area size enclosed between the microcanonical inverse temperature $\hat{\beta}(E_p)$ and the accordingly defined transition temperature $\hat{\beta}_{\rm eqa}$, where $\hat{\beta}_{\rm eqa} = \hat{\beta}_{\rm eqh} = 1.72099(3)$.

[5] J. Zierenberg, W. Janke: in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012017 (2016)
[6] J. Zierenberg et al.: Nat. Commun. **8**, 14546 (2017)
[7] P. Schierz et al.: Phys. Rev. E **94**, 021301(R) (2016)
[8] W. Janke et al.: *Transition barrier at a first-order phase transition in the canonical and microcanonical ensemble*, Leipzig preprint (2017), to appear in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2017), in print

10.4 Binding transition of two grafted polymers

K. Tholen, J. Zierenberg, W. Janke

In this project we studied the binding of two flexible polymers grafted closeby to a steric surface. More specifically, we fixed one of their end points to a steric surface covering the $x - y$ plane at $z = 0$. No monomer was allowed to cross this geometric constraint,

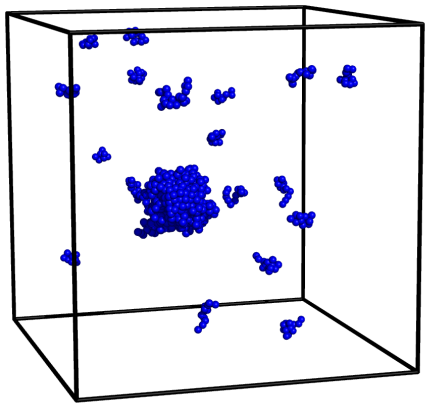
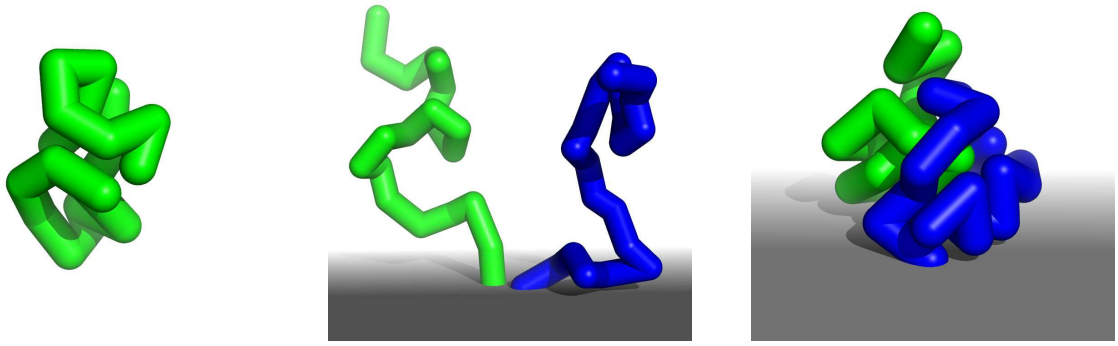


Figure 10.4: Illustration of an aggregate of polymers in a dilute solution ($N = 64$ bead-spring polymers with 13 monomers each; monomer density $\rho = 10^{-2}$). The snapshot stems from the droplet phase ($E_p \approx E_p^-$).

i.e., monomer coordinates with $z_i < 0$ were forbidden. No further interactions with the (inert) surface are assumed. The end points are grafted with distance $d = r_0$ (the equilibrium bond length of a FENE spring connecting the monomers) and are immobilized. If the polymers are not grafted, we enclose them in a cubic box of side length L with steric walls. For an illustration see Fig. 10.5.

As "binding" we refer to the process where two polymers attach to each other, in our case flexible polymers. If specific inter-polymer interactions are considered this may quickly lead to effects also characterized as zipping. Even more interesting is the equivalence between two-polymer binding of directed polymers and adsorption [1]. This should qualitatively remain valid also for flexible polymers, especially if one imagines the crossover scenario of a flexible polymer adsorbed to a nanowire, equivalent to the stiff limit of a polymer chain [2, 3], or a flexible polymer adsorbing to a flexible surface [4]. In fact, it was shown that grafting alters the first-order-like adsorption transition to a second-order-like transition [5].

From our Monte Carlo simulation data we conclude [6] that when grafting two polymers to a steric surface at a close distance an analogous scenario holds true, i.e., we observe a second-order-like binding transition, which is in contrast to the first-order-like finite-size binding transition for free polymers in a steric box. This is relevant for an experimental study of polymer binding, where in vitro polymers would be commonly grafted. In this case, one will neither observe a latent heat nor hysteresis effects associated with first-order-like transitions, which would be expected to occur in vivo. Still, grafted polymers may be studied with respect to aggregate properties and their dynamics which are expected to sufficiently coincide for observables which are not directly influenced by the geometric constraint. One exception is the average end-to-end distance and subsequently (no longer isotropic) geometric properties. Interesting effects may be anticipated for interacting surfaces, where the binding of polymers would



(a) (b) (c)

Figure 10.5: Snapshots of (a) a single polymer of length $N = 20$ in the globular phase below the collapse transition ($T = 0.7$) and two polymers of length $N = 20$ grafted to a steric surface (b) above (T = 4) and (c) below ($T = 0.7$) the binding transition.

compete with the surface attraction. Connecting to experimental setups, the surfaces may be considered both flat or curved, e.g., when grafting polymers to nanoparticles.

[1] J. Kierfeld, R. Lipowsky: Europhys. Lett. **62**, 285 (2003)
[2] T. Vogel et al.: J. Chem. Phys. **142**, 104901 (2015)
[3] J. Gross et al.: Phys. Chem. Chem. Phys. **17**, 30702 (2015)
[4] S. Karalus et al.: Phys. Rev. E **84**, 031803 (2011)
[5] M. Möddel et al.: Macromolecules **44**, 9013 (2011)
[6] J. Zierenberg et al.: Eur. Phys. J. – Special Topics **226**, 683 (2017)

10.5 Polymer adsorption to a nano-sphere

H. Arkın*, W. Janke

*Department of Physics Engineering, Faculty of Engineering, Ankara University, Tandogan, 06100 Ankara, Turkey

The interaction of macromolecules with differently shaped substrates is particularly important for interdisciplinary research and nano-technological applications including, e.g., the fabrication of biosensors and peptide adhesion to metals or semiconductors. The knowledge of structure formation for a variety of interfaces has therefore been a challenging subject of numerous experimental and computational studies.

Recently we have investigated the purely steric confinement effect of a spherical cage enclosing a simple flexible polymer chain to determine its influence on the location of the collapse and freezing transitions [1]. Another hybrid system under consideration was a polymer chain inside an attractive spherical cage for which we have constructed the finite-temperature phase diagram depending on the attraction strength of the sphere inner wall and the temperature [2, 3] and investigated the ground-state properties [4]. We have also compared the results with the attractive flat surface [5, 6]. These systems exhibit a rich phase behaviour ranging from highly ordered, compact to extended, random coil structures.

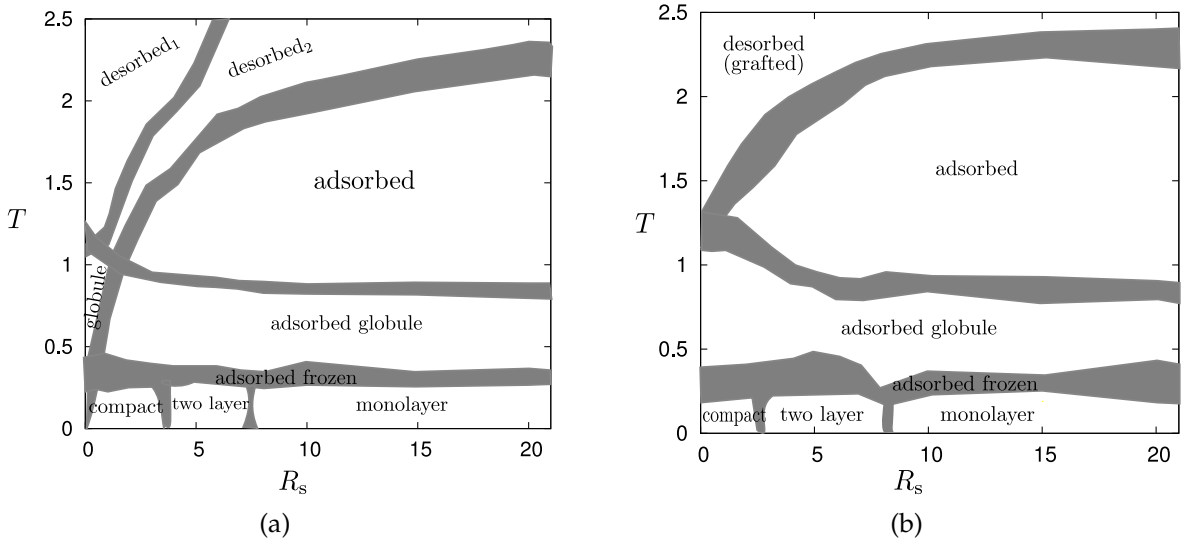


Figure 10.6: The phase diagram of a homopolymer interacting with an attractive spherical surface of radius R_s for (a) a non-grafted and (b) an end-grafted 20mer.

Here, we consider the opposite situation: A nano-sphere whose attractive outer spherical surface is the target for the adsorbing polymer. This problem could have practical implications for a broad variety of applications ranging from protein-ligand binding, designing smart sensors to molecular pattern recognition and for the discovery of new drugs that bind to specific receptors. Therefore it is interesting to study the adsorption of macromolecules on different types of substrates and identify the conformational changes that a polymer can experience at the interface.

In this project we investigate a simple coarse-grained polymer model interacting with a spherical surface of varying radius (and consequently curvature) by means of extensive generalized-ensemble Monte Carlo computer simulations [7]. The employed multicanonical method enables us to describe the different phases of the finite chain over a wide range of sphere radius and temperature. In a comparative study, we determined how the structural phase diagram changes with the sphere radius and temperature, both for non-grafted and end-grafted polymer chains. The band widths of the boundaries separating the individual conformational phases in Fig. 10.6 indicate the variation of the peak locations of temperature derivatives of different structural observables which we have analyzed simultaneously [7]. Typical conformation for the case of a non-grafted polymer are shown in Fig. 10.7.

[1] M. Marenz et al.: Condens. Matter Phys. **15**, 43008 (2012)
[2] H. Arkın, W. Janke: Phys. Rev. E **85**, 051802 (2012)
[3] H. Arkın, W. Janke: J. Chem. Phys. **138**, 054904 (2013)
[4] H. Arkın, W. Janke: J. Phys. Chem. B **116**, 10379 (2012)
[5] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010); Macromolecules **44**, 9013 (2011)
[6] H. Arkın, W. Janke: Eur. Phys. J. – Special Topics **216**, 181 (2013)
[7] H. Arkın, W. Janke: *Polymer adsorption on curved surfaces*, Ankara/Leipzig preprint (2017), to be submitted

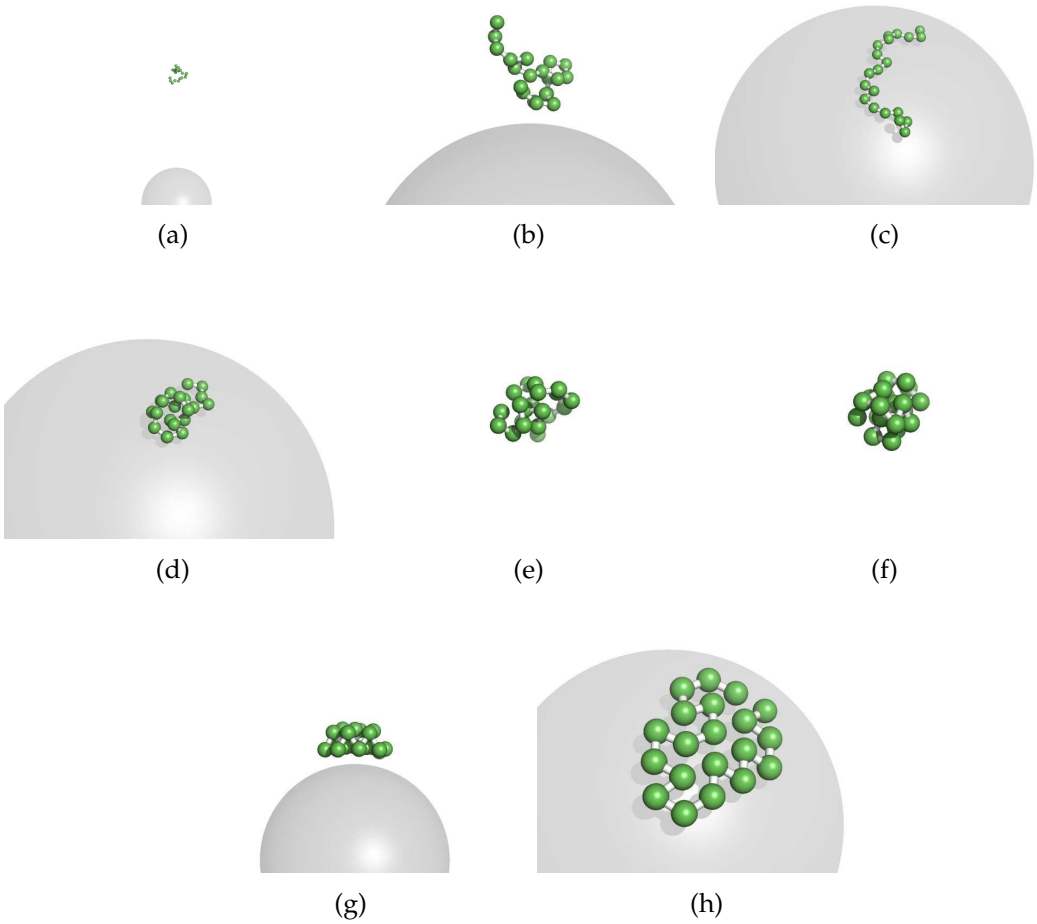


Figure 10.7: Typical conformations for the regions (a) desorbed$_1$, (b) desorbed$_2$, (c) adsorbed, (d) adsorbed globule, (e) globule, (f) compact, (g) two layer, and (h) monolayer in the phase diagram of a non-grafted polymer.

10.6 Polymer knots as a topological order parameter

M. Marenz, W. Janke

For the investigation of the generic behaviour of polymers and proteins with computer simulations, it is common to use minimalistic, coarse-grained models since this is the only possibility to investigate large time scales, length scales or parameter ranges. In this study we used a bead-stick model for a semiflexible polymer defined by the Hamiltonian

$$H = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right) + \kappa \sum_{i} (1 - \cos \theta_i) \ , \tag{10.3}$$

where r_{ij} is the distance between non-adjacent monomers, and θ_i is the angle of two adjacent bonds. The parameter κ allows to vary the bending stiffness of the polymer from flexible over semiflexible to stiff [1].

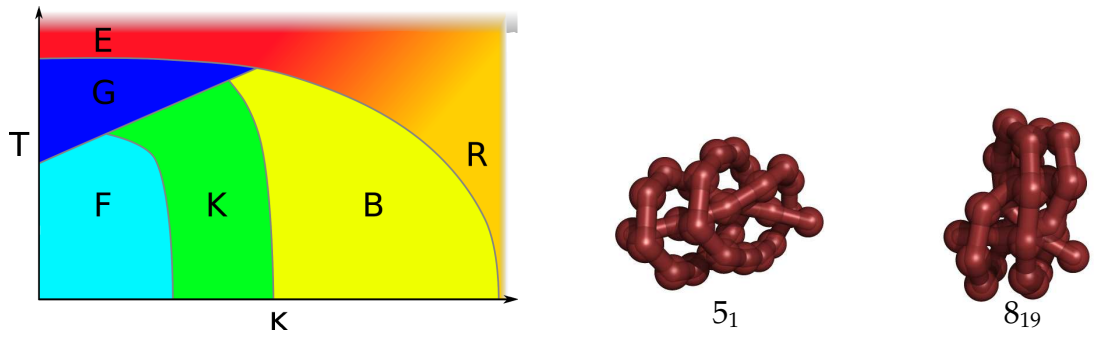


Figure 10.8: Sketch of the phase diagram for a semiflexible bead-stick model exhibiting several phases: E – elongated, R – rod-like, G – globular, F – frozen, K – knotted, B – bent. Next to the phase diagram two typical knots of types 5_1 and 8_{19} for a 28mer are shown.

To simulate the system in the complete (T, κ)-plane we used two advanced Monte Carlo algorithms. A parallel multicanonical algorithm [2] combined with a one-dimensional replica exchange in the κ direction and a two-dimensional replica-exchange method, which simulates the system in parallel in the T and κ direction. Employing both algorithms, we calculated surface plots of various observables (energy, end-to-end distance, radius of gyration, eigenvalues of gyration tensor) to construct the full pseudo-phase diagram for several polymer lengths ($N = 14, 28, 42$) [3, 4].

Despite the simplicity of the model, the phase diagram sketched in Fig. 10.8 is remarkably rich. Compared to former work simulating similar coarse-grained models [5], we observed a novel type of phases labeled by "K", which are characterized by thermodynamically stable knots [6], which may be considered as topological order parameters. The transitions into these knot phases exhibit some intriguing characteristics. Although we observed clear signals of a first-order transition between the knotted and unknotted phases, the transition apparently shows no latent heat [3, 4]. Instead the two sub-energies, the Lennard-Jones energy and the bending energy, are transformed into each other while the polymer knots itself, see Fig. 10.9.

[1] J. Zierenberg et al.: Polymers **8**, 333 (2016)
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] M. Marenz, W. Janke: Phys. Rev. Lett. **116**, 128301 (2016)
[4] M. Marenz, W. Janke: In *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012006 (2016)
[5] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)
[6] L.H. Kauffman: *Knots and Physics*, 2nd ed. (World Scientific, Singapore, 1991)

10.7 Comparative simulations of poly(3-hexylthiophene) models

J. Gross, M. Ivanov, W. Janke

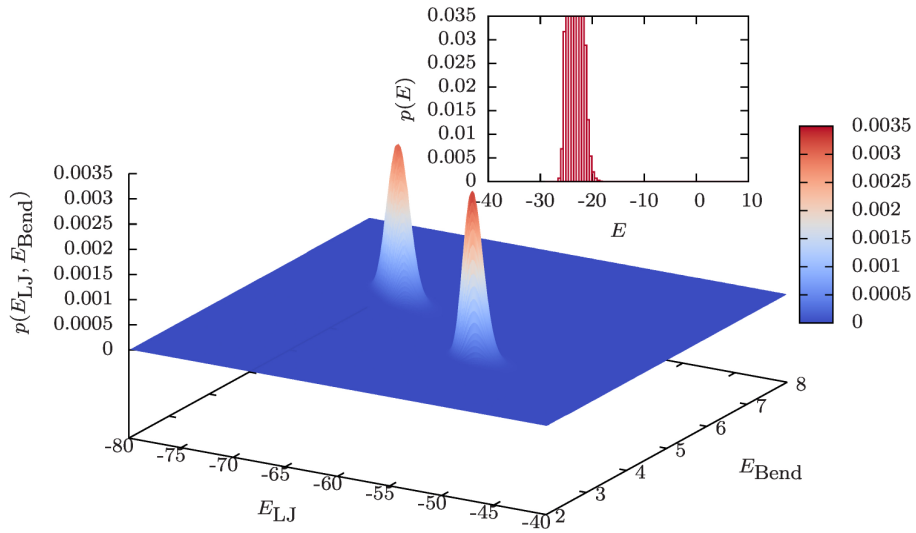
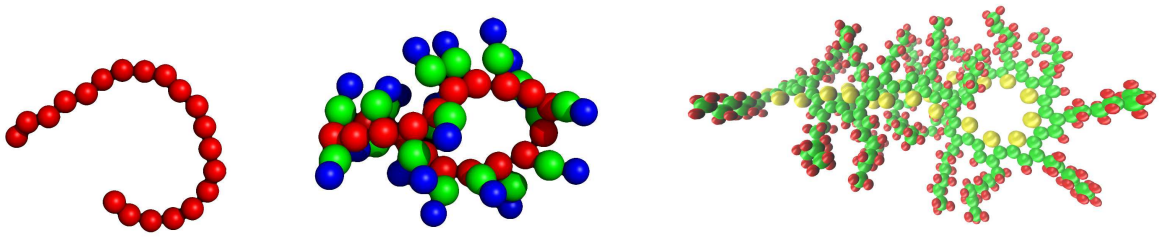


Figure 10.9: Two-dimensional energy histogram $p(E_{\mathrm{LJ}}, E_{\mathrm{Bend}})$ of a 28mer at the transition into the knot phase signaling clear phase coexistence. The inset shows the one-dimensional energy histogram $p(E)$ of the total energy $E = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}}$, which corresponds to a projection along the diagonal of the two-dimensional histogram. In this projection, the two peaks fall on top of each other, so only a single peak is visible in $p(E)$.

Regioregular Poly(3-hexylthiophene) (P3HT) is a very interesting conjugated polymer due to its electronic and optical properties [1]. One of its applications is the use as semiconducting layer in organic photovoltaics [2–4]. Studies of P3HT on the microscopic level are of great importance for a fundamental understanding of the tuneability of electronic properties and their dependence on external constraints, e.g. the adsorption on electrode surfaces. Hence a number of experimental studies addressed for example the influence of structure formation by polymer self-assembly on ideal surfaces on the electronic properties of oligo- and polythiophenes [5]. Due to the complexity of these macromolecules many of the experimental findings have not been supported with simulations so far, which in contrast is well-established for studies of small organic molecules. Our pervious study [6] reported on an collaborative effort within the DFG SFB/TRR 102 project to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with Monte Carlo simulations of a coarse-grained P3HT model developed by Huang *et al.* [7]. Based on our previous work on a three beads per monomer coarse-grained model, we expanded our studies in two directions. We focused our interest on the polymer itself and, firstly, investigated an even coarser model with one bead per monomer [8] using Monte Carlo simulations. Secondly, we simulated a fully atomistic representation of P3HT using molecular dynamics. We pursue these two routes to gauge the level of detail that is necessary to reproduce experimental findings more accurately. Another interest is the development of our own simplified model by systematically performing the coarse-grain procedure ourselves. For this we looked at the iterative Boltzmann inversion method [9]. The comparative analysis of all three models regarding structural observables, but also computational effort are discussed in Refs. [10, 11].



(a) (b) (c)

Figure 10.10: Hairpin conformations of Poly(3-hexylthiophene) for a degree of polymerization $DP_n = 20$ in three different models. (a) One-particle coarse-grained model (one bead per monomer), (b) three-particle coarse-grained model, and (c) fully atomistic model.

[1] X. Bai, S. Holdcroft: Macromolecules **26**, 4457 (1993); Z. Bao et al.: Appl. Phys. Lett. **69**, 4108 (1996); M.R. Andersson et al.: J. Mater. Chem. **9**, 1933 (1999); B.W. Boudouris et al.: Macromolecules **44**, 6653 (2011)
[2] J.M. Frost et al.: Nano Letters **6**, 1674 (2006)
[3] M. Campoy-Quiles et al.: Nat. Mater. **7**, 158 (2008)
[4] A.M. Ballantyne et al.: Adv. Funct. Mater. **18**, 2373 (2008)
[5] Z.Y. Yang et al.: ACS Nano **2**, 743 (2008); Y.F. Liu et al.: Nanoscale **5**, 7936 (2013)
[6] S. Förster et al.: J. Chem. Phys. **141**, 164701 (2014)
[7] D.M. Huang et al.: J. Chem. Theory Comput. **6**, 526 (2010)
[8] C.K. Lee et al.: Energy Environ. Sci. **4**, 4124 (2011)
[9] D. Reith et al.: J. Comput. Phys. **24**, 1624 (2003); Macromolecules **36**, 5406 (2003)
[10] J. Gross et al.: J. Phys.: Conf. Ser. **750**, 012009 (2016)
[11] J. Gross et al.: Eur. Phys. J. – Special Topics **226**, 667 (2017)

10.8 Effect of temperature on the scaling laws governing the kinetics of collapse of a homopolymer

S. Majumder, J. Zierenberg, W. Janke

The collapse transition of a polymer upon transfer from a good solvent (high temperature) to a poor solvent (low temperature) bears significant connection to the folding process of a proteins and other biomolecules. Thus understanding the kinetics of a homopolymer in that respect may provide useful primary information on the underlying mechanism of more realistic problems [1, 2]. On the other hand, if one considers the usual "pear-necklace" like picture of the collpase [3] as shown in Fig. 10.11 (a), it also resembles coarsening phenomena popular in spin and particle systems [4]. Over the last two years we have been exploiting this connection to understand the kinetics of collapse of a homopolymer [5, 6].

In this work, from the state of the art Monte Carlo simulations of an off-lattice polymer model, we understand the effect of the quench temperature (T_q) on the various scaling laws related to the collapse viz., scaling of the cluster growth and the dynamical

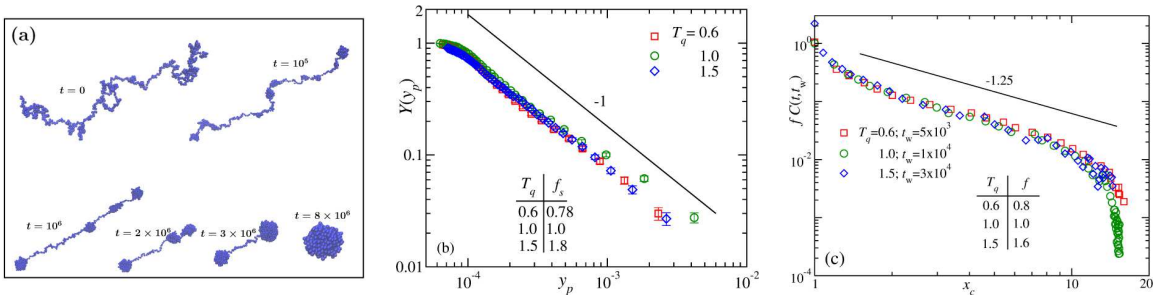


Figure 10.11: (a) Snapshots [1] showing the sequence of events occurring during the collapse of a polymer upon being quenched from an expanded state (at high temperature) into the globular phase (at low temperatures). (b) Universal finite-size scaling function $Y(y_p)$ with a non-universal metric factor (f_p) in the scaling variable y_p describing the scaling in the cluster growth during the collapse [2]. (c) Temperature-independent scaling plot for the aging and related dynamical scaling, probed by the behavior of a suitable density-density autocorrelation function $C(t, t_w)$ against $x_c = C_s(t)/C_s(t_w)$, the ratio of cluster sizes $C_s(t)$ at the observation time (t) and the waiting time (t_w) [2].

scaling related to the aging. Our results in conjunction with the nonequilibrium finite-size scaling analysis [7] show that the cluster growth is rather universal in nature and can be described by a universal finite-size scaling function with a non-universal metric factor that depends on the amplitudes of the growth [2]. Furthermore, the scaling related to the aging (which is probed by a suitable two-time density-density autocorrelation function) is also found to be independent of the quench temperature T_q, shown in Fig. 10.11 (c).

[1] S. Majumder, W. Janke: J. Phys.: Conf. Ser. **750**, 012020 (2016)
[2] S. Majumder et al.: Soft Matter **13**, 1276 (2017)
[3] A. Halperin, P. Goldbart: Phys. Rev. E **61**, 565 (2000)
[4] A.J. Bray: Adv. Phys. **51**, 481 (2002)
[5] S. Majumder, W. Janke: Europhys. Lett. **110**, 58001 (2015)
[6] S. Majumder, W. Janke: Phys. Rev. E **93**, 032506 (2016)
[7] S. Majumder, S.K. Das: Phys. Rev. E **81**, 050102(R) (2010); Phys. Rev. E **84**, 021110 (2011)

10.9 Kinetics of the collapse transition in lattice polymers

H. Christiansen, S. Majumder, W. Janke

The nonequilibrium properties of homopolymer collapse were investigated using Monte Carlo simulations of the interacting self-avoiding walk on a simple cubic lattice with short nearest neighbor [1] and longer range next-nearest neighbor interactions. We were able to reproduce the phenomenological picture of pearl necklace polymer collapse [2] (see Fig. 10.12), in which a polymer, when transferred from a good solvent to a bad solvent, undergoes a collapse transition from an expanded coil by forming clusters at locally higher densities which then subsequently coalesce with each other until only a single globular cluster is left. Recently, the scaling behavior of the average cluster size

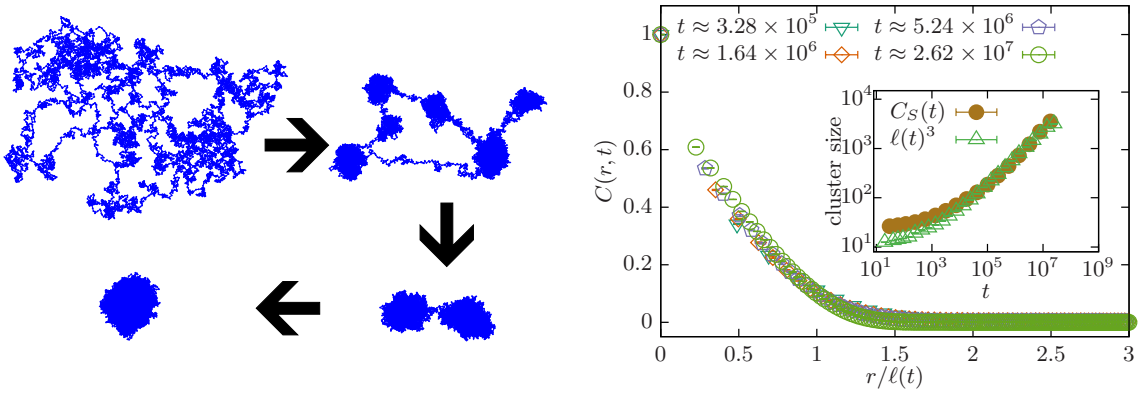


Figure 10.12: (a) Collapse of a polymer with length $N = 8192$ showing the formation and subsequent coarsening of clusters. (b) Scaling of the two point equal-time correlation function $C(r,t)$ at different times as a function of $r/\ell(t)$. The inset shows the comparison of $\ell(t)^3$ extracted from the correlation function and the cluster size $C_s(t)$ determined using the same method as in off-lattice simulations.

as well as aging was investigated using an off-lattice polymer model [3–5] by applying methods from domain coarsening investigations used in spin and particle systems to polymers. We extend this work to an investigation of lattice polymer collapse in order to be able to simulate one order of magnitude longer polymer chains (when compared to the off-lattice investigations) and define properties that are dependent on the underlying structure, like the equal-time two-point correlation function (see Fig. 10.12). The power-law growth exponent of the clusters of monomers was observed to be similar for both interaction ranges, however significantly smaller than in the off-lattice case ($\alpha \approx 0.6$ vs. $\alpha = 1$). In addition we investigated aging during the coarsening and found the same dynamic aging exponent with respect to the growing characteristic length of clusters as in the off-lattice model for both interaction ranges ($\lambda_c = 1.25$).

[1] H. Christiansen et al.: *Coarsening and aging of lattice polymers: Influence of bond fluctuations*, Leipzig preprint (2017), submitted
[2] A. Halperin, P.M. Goldbart: Phys. Rev. E **61**, 565 (2000)
[3] S. Majumder, W. Janke: Phys. Rev. E **93**, 032506 (2016)
[4] S. Majumder, W. Janke: Europhys. Lett. **110**, 58001 (2015)
[5] S. Majumder et al.: Soft Matter **13**, 1276 (2017)

10.10 Periodically driven DNA: A comparative study of Langevin and Brownian dynamics

R. Kumar, S. Kumar*, W. Janke

*Department of Physics, Banaras Hindu University, Varanasi 221 005, India

DNA replication is one of the most important biological processes in living organisms. Under the influence of special enzymes, two strands of the DNA double helix can separate themselves like a zip. The first step in the process of DNA replication is to

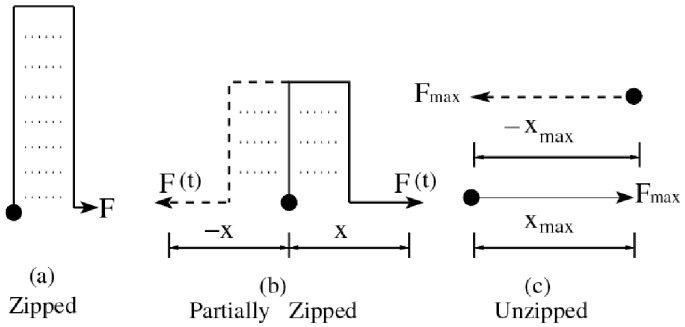


Figure 10.13: Schematic representations of DNA: (a) zipped, (b) partially zipped, and (c) unzipped state. One end is kept fixed (indicated by solid circles), while the other end may move.

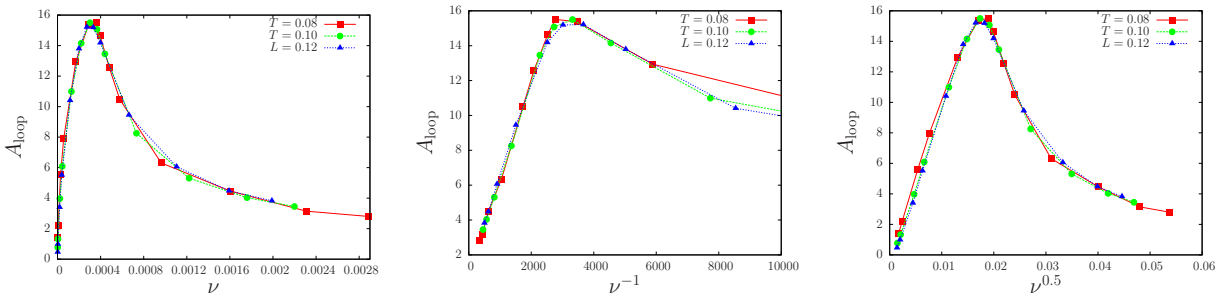


Figure 10.14: Effect of temperature on the area of the hysteresis loop for the model with parameters $L = 32$, $F = 1.0$, and $\gamma = 0.4$ for (a) A_{loop} vs. ν, (b) area vs. ν^{-1} in the higher frequency regime, and (c) area vs. $\nu^{0.5}$ in the lower frequency regime. Here the x-axis is rescaled in order to show the data collapse for all temperatures.

unzip the double-helix structure of the DNA molecule. Therefore, it is very important to study the unzipping of DNA. There has been some experimental studies at a constant force or loading rate used in SMFS experiments to unzip the DNA *in vitro*. In these experiments one end of the DNA was fixed and a constant force was applied on its other end. However, such processes are driven by different types of molecular motors *in vivo* [1].

A constant force or loading rate used in SMFS experiments provides a limited picture of these processes *in vitro*. Hence, the picture provided by constant force unzipping is not complete. This has been highlighted in recent studies, where it was suggested that by varying the frequency and amplitude of the applied force new aspects of a force-driven transition can be introduced [2–5], which otherwise would not be possible in the case of a steady force.

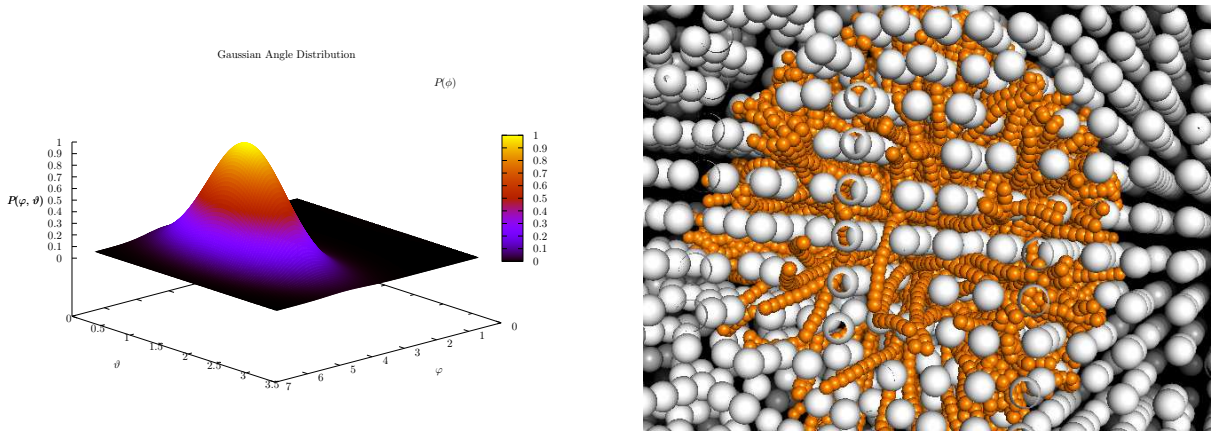
This model was further simplified in [6, 7] by reducing the degrees of freedom and studying the overdamped limit using Brownian dynamics. This simplified model was investigated only at zero temperature. Therefore, it became crucial to further investigate how the temperature effects the dynamics of such system using the detailed model described in [3]. Emphasis was placed on the effect of different temperatures on the scaling properties. Moreover, we compared results of the Langevin dynamics for the detailed model and Brownian dynamics for the simplified model. We observed that

the temperature and over-damped limit does not effect the scaling exponents. Hence, the model proposed by us is good enough to study the scaling properties and provides a possibility of analytic studies within certain limits. Moreover, currently we are trying to understand the effect of the over-damped limit in the detailed model proposed in [3].

[1] B. Alberts et al.: *Molecular Biology of the Cell* (Garland Publishing, New York, 1994)
[2] S. Kumar, M. S. Li: Phys. Rep. **486**, 1 (2010)
[3] S. Kumar, G. Mishra: Phys. Rev. Lett. **110**, 258102 (2013)
[4] G. Mishra et al.: Phys. Rev. E **87**, 022718 (2013)
[5] R.K. Mishra et al.: J. Chem. Phys. **138**, 244905 (2013)
[6] S. Kumar et al.: Phys. Rev. E **93**, 010402(R) (2016)
[7] R. Kumar et al.: *Comparative study of Brownian and Langevin dynamics for periodically driven DNA* , Leipzig/Varanasi preprint (2017), to be published

10.11 Computer simulations of semiflexible polymers in disordered environments

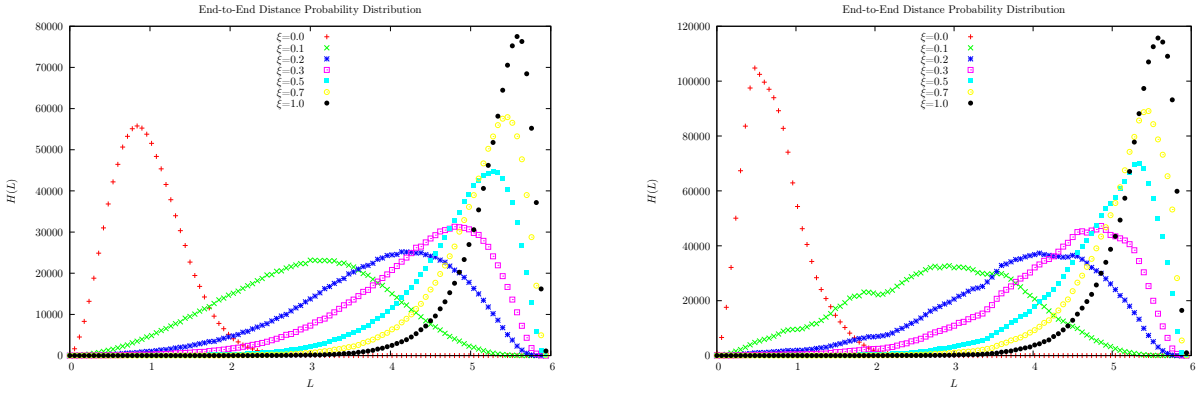
J. Bock, W. Janke



(a) Weighting histogram (b) Semiflexible polymer in 3D disorder

Figure 10.15: (a) Histogram used for the guiding field in 3D and (b) an examplary configuration of a polymer with $N = 30$ and $\xi = 1$.

Single-molecule experiments have established the wormlike chain (WLC) as a standard model for semiflexible polymers [1]. Exploiting the analogy of the WLC with a one-dimensional Heisenberg ferromagnet, it can be shown that the equilibrium tangent-tangent correlation function decays exponentially. The decay rate defines the thermal persistence length l_p. When the same polymer is embedded in a quenched, disordered environment in three dimensions, this property may change quantitatively or even qualitatively. We addressed this problem by performing extensive numerical simulations of



(a) Free polymers (b) Polymers in disorder

Figure 10.16: End-to-end distance distributions for (a) free polymers and (b) polymers in gaseous disorder, both in 3D.

semiflexible polymers in a simple lattice disorder and in a gaseous disorder constructed by microcanonical Lennard-Jones gas simulation which represents the disordered environment. Further plans are to simulate the polymers in algebraically correlated disorder. Only the space between the spheres is accessible to the polymer. The extreme strength and density of the environmental constraints are a great challenge to conventional Monte Carlo simulation schemes, which we found hard to overcome even with a sophisticated multicanonical histogram reweighting procedure [2]. We have therefore adopted a breadth-first chain-growth algorithm [3] that resolves this difficulty by circumventing energy barriers instead of trying to cross them [2, 4], see examples in Fig. 10.15. Therefore the already existing procedures were expanded to the third dimension to investigate the behaviour of the tangent-tangent correlation length, the mean square end-to-end distance and the end-to-end probability distribution function, see Fig. 10.16. A difference in behaviour is clear and the task now is to check wether the differences scale similarly as in two dimensions, where the disorder renormalization is stated to be [5]:

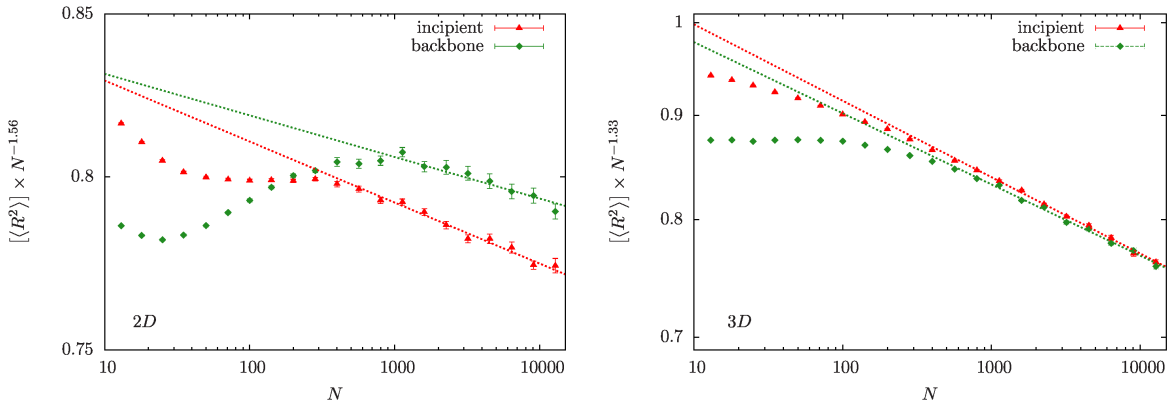
$$\frac{1}{l_p^*} = \frac{1}{l_p} + \frac{1}{l_p^D},$$

with l_p^* the renormalized persistence length, l_p the persistence length given as simulation parameter and l_p^D the measured disorder persistence length.

[1] O. Otto et al.: Nat. Commun. **4**, 1780 (2013)
[2] S. Schöbl et al.: Phys. Rev. E **84**, 051805 (2011)
[3] T. Garel, H. Orland: J. Phys. A: Math. Gen. **23**, L621 (1999)
[4] S. Schöbl et al.: J. Phys. A: Math. Theor. **45**, 475002 (2012)
[5] S. Schöbl et al.: Phys. Rev. Lett. **113**, 238302 (2014)

10.12 Self-avoiding walks on critical percolation clusters in 2 – 7 dimensions

N. Fricke, W. Janke



(a) (b)

Figure 10.17: Scaled disorder averages of the mean squared end-to-end distance as a function of the number of SAW steps on critical clusters and cluster backbones in (a) 2D and (b) 3D on a double-logarithmic scale. The values have been divided by $\approx N^{2\nu_{pc}}$ for better visibility. Straight lines show least-squares power-law fits to the data in the range $N = 800 - 12\,800$ for 2D and 3D incipient clusters and $N = 1131 - 12\,800$ for 3D backbones.

Self-avoiding walks (SAWs) on critical percolation clusters are a simple model for polymers in highly disordered environments such as porous rocks or a biological cell [1, 2]. The system is also appealing from a theoretical perspective as it combines two of the most ubiquitous models from statistical physics. It has therefore been studied intensely in the past both analytically and numerically. However, despite its conceptual simplicity, the problem proved extremely challenging. Few reliable predictions exist for the SAWs' scaling exponents, and our qualitative understanding of the model is also still limited. In particular, it is unclear how the disorder and the medium's fractal structure, characterized by its various fractal dimensions, impacts the SAWs' asymptotic scaling behavior. This understanding is crucial when we want to generalize from the results and make predictions for real-world systems.

The main difficulty for numerical investigation of the problem can be overcome by making use of the self-similar geometry of critical percolation clusters to factorize the problem, in an approach that we called scale-free enumeration (SFE) [3, 4]. In two preceding studies, we had used this method to investigate SAWs on critical percolation clusters in 2D [5] and 3D [6]. Recently we have expanded this perspective and looked at systems in up to 7D [7], above the supposed upper critical dimension of $D_{\text{uc}} = 6$.

We mainly focused on the scaling of the increase of the mean squared end-to-end distance with the number of steps,

$$[\langle R^2 \rangle] \sim N^{2\nu} \tag{10.4}$$

where ν is a universal scaling exponent. The reduced time complexity of our recently introduced SFE method allows us to exactly enumerate SAWs of over $N = 10^4$ steps, easily amounting to 10^{2000} conformations. Previously, only up to $N = 45$ steps on 2D clusters and 40 steps on 3D clusters could be handled by the standard "brute-force" enumeration method.

In 2D and 3D we studied walk lengths increasing in multiplicative steps of $\sqrt{2}$ from $N = 13$ up to $N = 12\,800$ ($= 100 \times 2^7$). For each length we took independent samples of at least 5×10^4 randomly generated percolating clusters and backbones. The results for the mean squared end-to-end distance as a function of N and least-squares fits of Eq. (10.4) to the data are shown in Fig. 10.17 on a double-logarithmic scale. The y-axes have been rescaled by $\approx N^{-2\nu_{p_c}}$, so that the slopes are close to zero and more details are visible. Note that while the conformational averages are evaluated exactly, we still have statistical fluctuations of the disorder averages reflected by the error bars.

Repeating this procedure in 4D – 7D, we finally arrive at Fig. 10.18, where we have also included a comparison with analytical predictions from various sources.

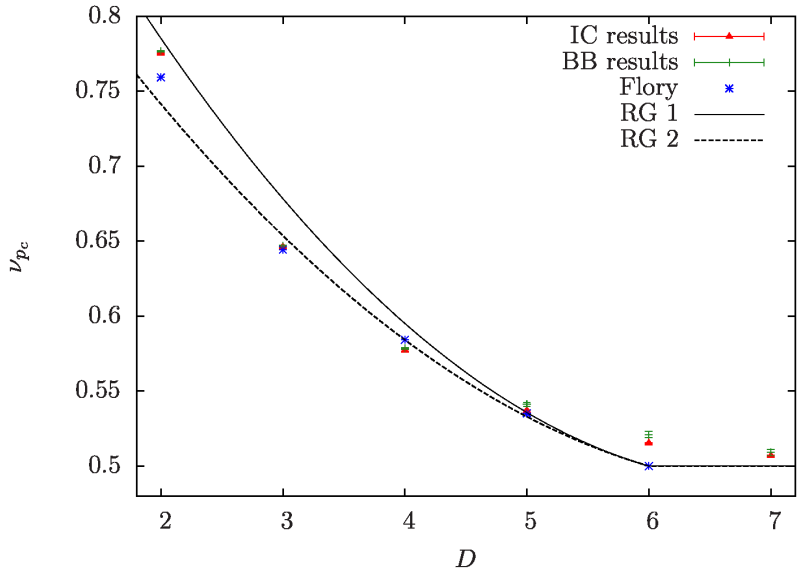


Figure 10.18: Results for ν_{p_c} on incipient clusters (IC, red) and backbones (BB, green) as a function of dimension compared to various analytical predictions. The blue asterisks correspond to Flory estimates [7]. The lines represent the field-theory estimates from [8] (RG1, solid) and [9] (RG2, dashed).

[1] D. Ben-Avraham, S. Havlin: *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge University Press, Cambridge, 2000)
[2] B.K. Chakrabarti (ed.): *Statistics of Linear Polymers in Disordered Media* (Elsevier, Amsterdam, 2005)
[3] N. Fricke, W. Janke: Eur. Phys. J. – Special Topics **216**, 175 (2013)
[4] N. Fricke, W. Janke: *How to enumerate* 10^{1000} *self-avoiding walk conformations on a critical percolation cluster*, Leipzig preprint (2017), to be published
[5] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)

[6] N. Fricke, W. Janke: Phys. Rev. Lett. **113**, 255701 (2014); Phys. Rev. Lett. **115**, 149902 (Erratum)
[7] N. Fricke, W. Janke: J. Phys. A: Math. Theor. **50**, 264002 (2017)
[8] C. von Ferber et al.: Phys. Rev. E **70**, 035104 (2004)
[9] H.K. Janssen, O. Stenull: Phys. Rev. E **75**, 020801 (2007); Phys. Rev. E **85**, 051126 (2012)

10.13 Dynamical greedy algorithm for the Edwards-Anderson model

S. Schnabel, W. Janke

One of the most intuitive and natural approaches to optimization problems is realized by so-called greedy algorithms. These methods create trajectories in the space of possible solution by always choosing the next step such that the energy is maximally reduced (or a fitness function maximally increased). Naturally, this will usually not find the global optimum, just as starting at a random spot and always walking uphill will usually not lead a wanderer to the summit of Mt. Everest. Therefore, in practice many attempts with randomly created starting points are made and if the problem is not too difficult the global optimum may be found this way.

On the other hand, there is practically no chance of success if the energy landscape is as complicated and possesses as many local minima as in the case of the Edwards-Anderson spin-glass model [1], whose Hamiltonian is given by

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j,$$

where the spins can take two values $S_i \in \{-1, 1\}$ and adjacent spins interact via normally distributed random couplings J_{ij}. If such a model on a three-dimensional cubic lattice of 1000 spins is considered, about 10^{30} attempts would be necessary in order to find the ground state this way.

However, the greedy algorithm can still be a very helpful tool, since it is a comparatively simple and reliable method to reach states of low energy. We devised a method to efficiently update the greedy algorithm, i.e., to reuse the data created during a minimization from a configuration $\mathbf{S}$ to the configuration $\mathbf{S}_{\min}$ to obtain the result $\mathbf{S}'_{\min}$ of the minimization from a configuration $\mathbf{S}'$ which differs from $\mathbf{S}$ only in the values of one or very few spins [2]. If furthermore, both, the terminal configuration, delivered by the greedy algorithm, and its energy are understood as attributes of the starting configuration, it is possible to use the energy of the minimized configurations $\mathbf{S}_{\min,t}$ to steer a path in the space of starting configurations $\mathbf{S}_t$.

A simple application is to apply the greedy algorithm again: It is tested which alteration (e.g., which single spin flip) of the starting configuration will reduce the energy of the *minimized* configuration by the largest amount and this locally optimal step is performed. Repeating this simple procedure as long as viable as a "second order greedy algorithm" will lead to much lower energies albeit not the ground state.

Alternatively, the energy of the minimized configuration can be used as argument for the occupation probability for a generalized ensemble [3]:

$$P(\mathbf{S}) = P(\mathbf{S}_{\min}),$$

which can then be sampled using Monte Carlo techniques. All states in the same "valley" in the energy landscape, i.e., all configuration which minimize to the same local energy minimum, now occur with the same probability and the barriers of high energy which greatly hamper standard Monte Carlo simulations simply vanish. In consequence, the configuration space is sampled much more easily and the performance of ground-state search is greatly improved.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
[2] S. Schnabel, W. Janke: *Dynamic greedy algorithms for the Edwards-Anderson model*, Leipzig preprint (2017), to appear in Comput. Phys. Commun. (2017), in print
[3] D.J. Wales: J. Phys. Chem. A **101**, 5111 (1997)

10.14 Distribution of local minima for the Edwards-Anderson model

S. Schnabel, W. Janke

In statistical physics the term "complex behaviour" is usually used to characterize systems that posses a rough free-energy landscape with many metastable states. This can be the result of competing interactions on different scales like in the case of protein folding or it may arise from quenched disorder as for spin glasses. A conceptually simple model for such a system is the Edwards-Anderson model [1], whose Hamiltonian is given by

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j,$$

where the spins sit on the sites of a cubic lattice, can take two values $S_i \in \{-1, 1\}$, and adjacent spins interact via normally distributed random couplings J_{ij}. Since these interactions can be both ferromagnetic and antiferromagnetic, there is no clear order established at low temperatures. Instead, many very different pure states might coexist, each one of them corresponding to a minimum in free energy.

Albeit not identical, minima of the energy, i.e., spin configurations that are stable against single spin flips are closely related to these states. It is thought that minima in energy form the end points of hierarchical tree-like structures with the branches corresponding to different states. Understanding the properties of these minima might, therefore, improve our understanding of the behaviour of the system. However, they have proven to be a very demanding subject of inquery.

We have developed an advanced Monte Carlo method that allows to sample the local energy minima with uniform distribution, i.e., each minimum configuration is occupied with equal probability. This is achieved by establishing within the simulation

the combination of a spin configuration together with a random minimization thereof. I.e., the repeated flipping of spins with positive energy until a local minimum is reached. If one now alters the spin configuration and the parameters of the minimization in a suitable way it is possible to ensure that all local minima are equally likely found this way.

A basic application of this method is the measurement of the distribution of the energy minima. Since existing algorithms are unable to perform such a task, there is no numerical data for comparison. However, we can use our results to test analytical predictions [2] that are based on the expansion of mean-field solutions.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
[2] A.J. Bray, M.A. Moore: J. Phys. C **14**, 1313 (1981)

10.15 Spin glasses with variable frustration

R. Kumar, M. Weigel*, W. Janke

*Applied Mathematics Research Centre, Coventry University, England, UK

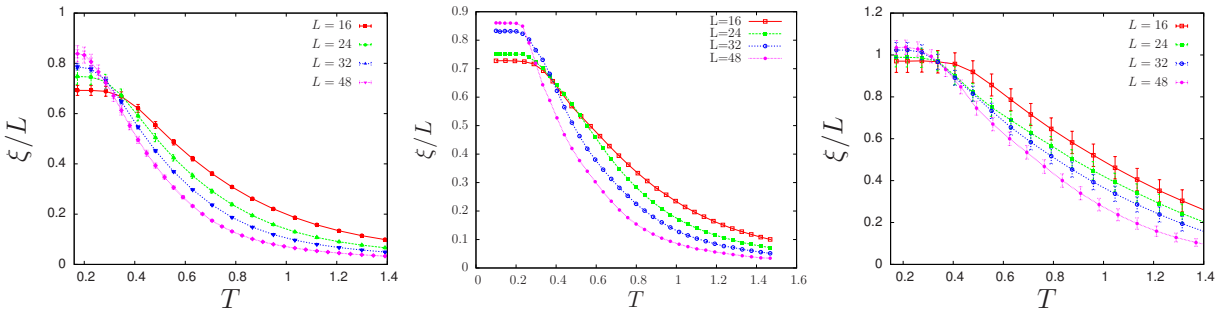


Figure 10.19: Correlation length as a function of temperature for (a) stochastically frustrated system, (b) a system with 46% frustration, and (c) a system with 20% frustration.

Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behaviour in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure [1]. We use a cluster algorithm proposed in [2] in order to reduce the equilibration time. The phase transition studies are done by looking at the divergence of the correlation length, see Fig. 10.19. The results are benchmarked by comparing to the stochastic case described in [3]. We also study the freezing temperature of such a system and observe a different behaviour compared to the stochastically frustrated case. Studies on larger system sizes are very crucial to confirm these differences.

We find that the divergence of the correlation length occurs at non-zero finite temperature for the 2D Ising spin glass. This gives hints of a phase transition, but such transitions have to be studied carefully in order to fully understand the phases [4].

[1] E. Ilker, A.N. Berker: Phys. Rev. E **89**, 042139 (2014)
[2] J. Houdayer: Eur. Phys. J. B **22**, 479 (2001)
[3] H.G. Katzgraber, L.W. Lee: Phys. Rev. B **71**, 134404 (2005)
[4] A. Hartmann: Phys. Rev. B **67**, 214404 (2003)

10.16 Ground-state and low-energy excitations of the random field q-state Potts model

R. Kumar[*], M. Kumar[†‡], M. Weigel[§], V. Banerjee[‡], S. Puri[†], W. Janke

[*]Doctoral College for the Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry ($\mathbb{L}^4$)
[†]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India
[‡]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi – 110016, India
[§]Applied Mathematics Research Centre, Coventry University, England, UK

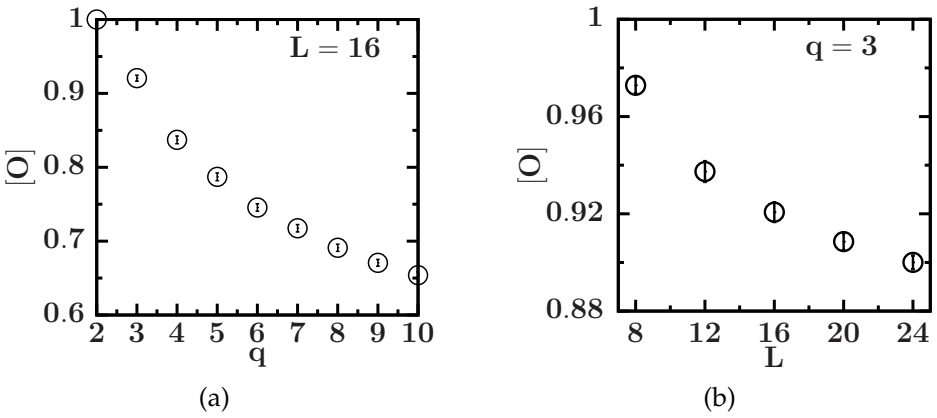


Figure 10.20: Overlap between the lowest states found by graph-cut methods (GCM) and the putative ground state (a) as a function of the number of Potts states q and (b) as a function of system size L.

While the ground-state (GS) problem for the random-field Ising model is polynomial, and can be solved using a number of well-known algorithms for maximum flow [1–4], the analogue random-field q-state Potts model with $q \geq 3$ corresponds to a multi-terminal flow problem that is known to be NP hard. Hence an efficient exact algorithm is extremely unlikely to exist [5]. Still, it is possible to employ an embedding of binary degrees of freedom into the Potts spins to use graph-cut methods (GCMs) 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 $d = 2, 3$.

We observe that the probability of finding a ground state decreases exponentially with q for GCM, but for parallel tempering this decay is linear. Hence, GCM is more suitable for lower q studies. We also find that the lower energies found by GCM are very close to the ground state and the excess energy is very small. The probability of finding the ground state falls exponentially with the system size, whereas for GCM it falls linearly. Therefore, GCM is better suited for studying larger system sizes. This is one very good feature of GCM as for the smaller system sizes we have larger finite-size effects. The overlap between the states found by GCM and the ground state is observed to be very large. Hence, we conclude that GCM produces the approximate GS which can be treated as an exact GS for sufficiently small q ($q = 3, 4$) for studying the critical behaviour and ground-state morphologies.

[1] G.P. Shrivastav et al.: Europhys. Lett. **96**, 36003 (2011)
[2] G.P. Shrivastav et al.: Phys. Rev. E **90**, 032140 (2014)
[3] G.P. Shrivastav et al.: Eur. Phys. J. E **37**, 98 (2014)
[4] V. Banerjee et al.: Ind. J. Phys. **88**, 1005 (2014)
[5] J.C. Angles d'Auriac et al.: J. Physique Lett. **46**, L173 (1985)

10.17 Boundary drive induced phase transitions in stochastic transport condensation models

H. Nagel, H. Christiansen, W. Janke

Stochastic mass transport processes such as the asymmetric simple exclusion process (ASEP) or the zero-range process (ZRP) are simple transport models for particle hopping aiming to improve the understanding of basic phenomena in the dynamics of particles in driven diffusive systems. An important class of such phenomena that can be studied and understood on an abstract level is the emergence of generic condensates. In this project we considered such a transport processes under driven particle exchange through open boundaries and systematically studied the emerging phase diagrams. While boundary drive induced phase transitions are known since long for the ASEP, the research for the ZRP with condensation dynamics is more recent [1].

More precisely we investigated transport processes with tunable weights [2] as well as various types of interactions at the boundaries to study these effects on a much broader scale. The tunable model allowed us to effectively interpolate between ZRP-type as well as strong short-range interactions. At the boundaries we considered the existence of fixed versus loose couplings as well as different approaches to particle injection and removal rates. For the generated cases we produced the phase diagrams under differing strengths of the driven particle exchange at the boundaries for symmetric and totally asymmetric dynamics [3–5]. The main phases, as shown in Fig. 10.21, are:

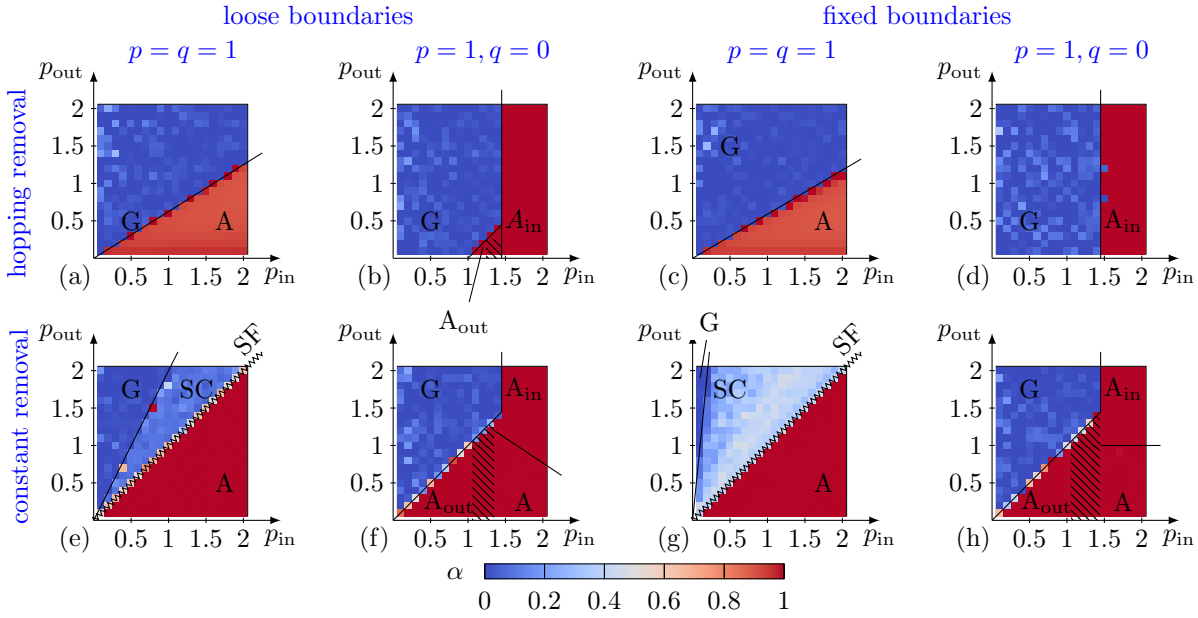


Figure 10.21: Phases induced by driven particle exchange through open boundary conditions of the system [5]. With respect to the specific implementation of the interaction at the boundary, different phase diagrams are observed.

a thin particle gas (G), formation of aggregate condensates (A) and the spanning bulk condensate (SC). While the phase diagrams with vanishing as well as stronger short-range interactions are very similar except for the SC phase, we observed a qualitatively different mechanism for aggregate condensate formation with short-range interactions.

[1] E. Levine et al.: J. Stat. Phys. **120**, 759 (2005)
[2] B. Wacław et al.: Phys. Rev. Lett. **103**, 080602 (2009)
[3] H. Nagel et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. H.-B. Schüttler, S. Lewis, M. Bachmann, D.P. Landau, Physics Procedia **57**, 77 (2014)
[4] H. Nagel et al.: Europhys. Lett. **111**, 30001 (2015)
[5] H. Nagel, W. Janke: J. Stat. Mech.: Theor. Exp., 013207 (2016)

10.18 Gate Opening, Diffusion, and Adsorption of CO_2 and N_2 Mixtures in ZIF-8

T. Chokbunpiam*, S. Fritzsche, C. Chmelik†, J. Caro‡, W. Janke, S. Hannongbua§

*Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand
†Institute for Experimental Physics I
‡Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Germany
§Computational Chemistry Unit Cell (CCUC), Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

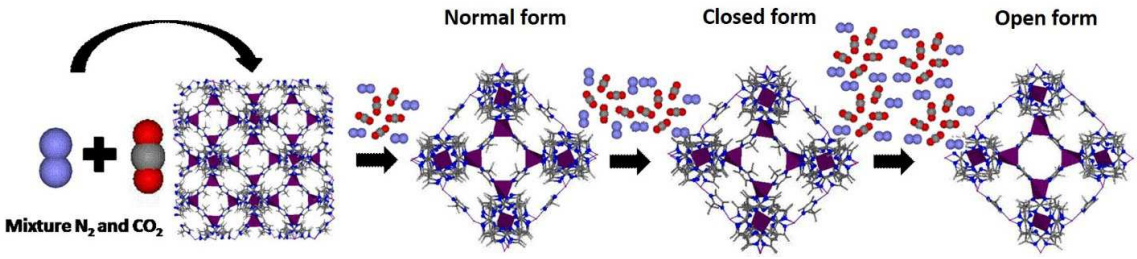


Figure 10.22: The change of the window sizes, i.e., 4-membered (normal lines, foreground) and 6-membered rings (strong lines) of ZIF-8 from normal to closed and to open forms.

Porous materials play an increasingly important role in research and industry. Particularly, during the past decade metal-organic frameworks (MOFs) [1] came into the focus of interest because of their great diversity, the big pores, and the possibility of custom-made design. Some of them have the highest internal surface areas per gram of all porous materials known to date. They consist of metal ions or metal oxide clusters that are connected by organic linkers forming porous frameworks. Replacing the organic linkers, new structures can be created and also exchange of the metal ions or metal ion clusters can change the properties of MOFs thus giving the possibility of tailoring the MOFs to specific applications. Zeolitic Imidazolate Frameworks (ZIFs) belong to the most promisings among the recently developed MOFs because of their extraordinary thermal and chemical stability and the huge variety of structures that can be designed [2]. In some of them, structural changes under increased loadings with guest molecules have been observed, e.g., the separation of an ethane/ethylene mixture could be drastically enhanced in ZIF-7 since only for ethane a gate opening effect took place. This gate opening leads to wider apertures (windows) between adjacent cavities that allow larger molecules to pass these bottlenecks or to enhance their diffusion inside the MOF framework.

In this project we investigate the possibility of gate opening for CO_2 or CO_2 and N_2 mixtures in ZIF-8 by Molecular Dynamics (MD) simulations with a flexible lattice and Gibbs ensemble Monte Carlo (GEMC) simulations with a rigid lattice. We define "gate opening" as the transition of a closed to an open window by conformational changes of the linker molecules, cf. Fig. 10.22. Gate-opening effects could be observed for both single-component gas adsorption [3] and in a CO_2/N_2 mixture [4]. In the mixture, the start of gate opening of ZIF-8 is more sensitive to N_2 because of its higher fugacity compared to CO_2. Evaluation of the self-diffusion coefficient and diffusion selectivity from MD and adsorption selectivity from GEMC made it possible to calculate membrane selectivities that agree satisfactorily with experiments.

[1] K.K. Gangu et al.: Inorg. Chim. Acta **446**, 61 (2016)
[2] K.S. Park et al.: Proc. Natl. Acad. Sci. USA **103**, 10186 (2006)
[3] T. Chokbunpiam et al.: Chem. Phys. Lett. **648**, 178 (2016)
[4] T. Chokbunpiam et al.: J. Phys. Chem. C **120**, 23458 (2016)

10.19 Boundary conditions and non-local constraints in plaquette models

M. Müller, W. Janke, D.A. Johnston*

*Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, UK

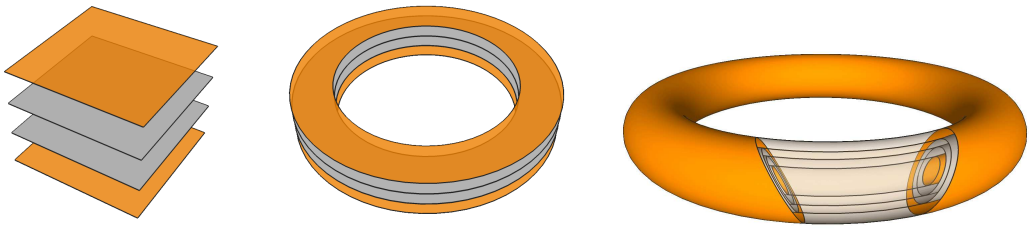


Figure 10.23: Fuki-Nuke models with free boundary conditions in one direction permit different topology of the lattice. We sketch the layers of independent layers of spins: (a) free boundary conditions in *all* directions, (b) periodic boundary conditions are set in one, and only one direction, and (c) periodic boundary conditions are set in both other directions.

An anisotropic limit of the 3*d* plaquette Ising model, in which the plaquette couplings in one direction were set to zero, was solved for free boundary conditions by Suzuki [1], 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) 2*d* Ising models and reveals the planar nature of the magnetic order, which is also present in the fully isotropic 3*d* plaquette model [2]. More recently, the solution of the fuki-nuke model was discussed for periodic boundary conditions applied to the spin lattice, which require a slightly different approach to defining the product spin transformation, by Castelnovo et al. [3].

We find that the essential features of the differences between free and periodic boundary conditions when using a product spin transformation are already present in the 1*d* Ising model [4], which thus provides an illuminating test case for its use in solving plaquette spin models and an alternative method for solving the 1*d* Ising model with periodic boundary conditions.

We clarify the exact relation between partition functions expressed in terms of the original and product spin variables for the 1*d* Ising model, 2*d* plaquette and 3*d* fuki-nuke models with free and periodic boundary conditions. Representing graphically the combinatorial factors that contribute to the partition function, we are able to solve the 2*d* plaquette model with free, periodic and helical boundary conditions and various combination of these in x- and y-directions, see Fig. 10.23. The various exactly solved examples illustrate how correlations can be induced in finite systems as a consequence of the choice of boundary conditions.

For the three-dimensional fuki-nuke model the exact finite-size partition function may be written as a product of 2*d* Ising partition functions in the case of free boundary conditions using the product variable transformation. A similar decoupling is not manifest with periodic boundary conditions, where all n-point 2*d* Ising spin-spin correlations also contribute to the expression for the 3*d* fuki-nuke partition function. As illustrated

in Fig. 10.24, this can be most easily understood in a pictorial way by employing the high-temperature expansion/dimer approach. It is perhaps worth remarking that the discussion of the fuki-nuke model in [3] conflates the discussion of free and periodic boundary conditions, although the overall picture of a $2d$ Ising-like transition in the thermodynamic limit of the $3d$ fuki-nuke model remains, of course, correct in both cases.

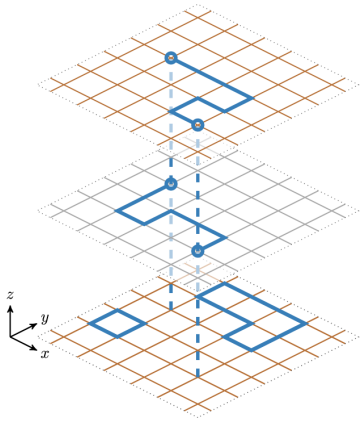


Figure 10.24: A dimer configuration of the Fuki-Nuke model with $L_z = 3$ that can contribute to the partition function, although the mid and top layer have dangling ends (symbolised by open circles). These are connected through the constraints (dashed vertical lines) and contribute to the two-point function in each of the two upper layers. Notice that additional, standard $2d$ Ising loops may appear, as those shown in the bottom layer, which are the standard contributions to the partition function of each layer.

A further consequence of the planar flip symmetry is found in a Hamiltonian related to the quantum dual of the plaquette model. This fits into the general framework developed in [5, 6] in which novel fracton topological phases are constructed by gauging symmetries acting on subsystems of dimension $2 \leq d_s < d$. Since the spin-flip symmetry in the $3d$ plaquette model acts on $2d$ planes it has precisely this property. The procedure for constructing the fracton Hamiltonian follows closely that of the Kitaev toric code, giving commuting electric and magnetic operators. We outline the role played by the spin-flip symmetry in enabling the appearance of fracton topological defects in a Hamiltonian related to the dual of the quantum version of the model [7].

[1] M. Suzuki: Phys. Rev. Lett. **28**, 507 (1972)
[2] M. Mueller et al.: Nucl. Phys. B **894**, 1 (2015); D.A. Johnston et al.: Mod. Phys. Lett. **B29**, 1550109 (2015)
[3] C. Castelnovo et al.: Phys. Rev. B **81**, 184303 (2010)
[4] M. Mueller et al.: Nucl. Phys. B **914**, 388 (2017)
[5] S. Vijay et al.: Phys. Rev. B **94**, 235157 (2016)
[6] D.J. Williamson: Phys. Rev. B **94**, 155128 (2016)
[7] D.A. Johnston et al.: Eur. Phys. J. – Special Topics **226**, 749 (2017)

10.20 The two-dimensional Blume-Capel model: Scaling and universality

J. Zierenberg, N.G. Fytas*, M. Weigel*, W. Janke, A. Malakis†

*Applied Mathematics Research Centre, Coventry University, England, UK
†Department of Physics, University of Athens, Greece

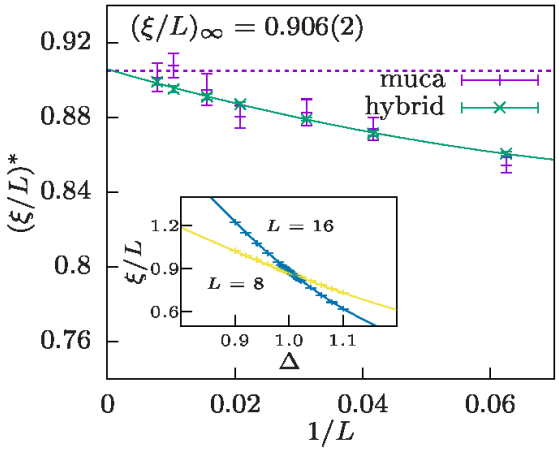


Figure 10.25: Finite-size scaling at $T = 1.398$ of the correlation length crossings $(\xi/L)^*$. The dashed horizontal shows the asymptotic value for the square-lattice Ising model with periodic boundaries. Compared are data from the multicanonical ("muca") and hybrid methods. The line shows a quadratic fit in $1/L$ to the data from the hybrid method. The inset demonstrates the crossing point of $L = 8$ and $L = 16$ obtained from both the muca (lines) and hybrid (data points) method.

The Blume-Capel model [1, 2] is a perfect test model for studies of phase transitions. We consider this spin-one Ising model in a crystal field on a square lattice in two dimension (2D), described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2 = E_J + \Delta E_\Delta \,. \tag{10.5}$$

We investigate the behaviour in the vicinity of the first-order and second-order regimes of the ferromagnet-paramagnet phase boundary, respectively [3]. To achieve high-precision results, we utilize a combination of (i) a parallel version of the multicanonical algorithm and (ii) a hybrid updating scheme combining Metropolis and generalized Wolff cluster moves. These techniques are combined to study for the first time the correlation length ξ of the model, using its scaling with system size L in the regime of second-order transitions to illustrate universality through the observed identity of the limiting value of ξ/L with the exactly known result for the Ising universality class, see Fig. 10.25.

In contrast to most previous work, we focused on crossing the phase boundary at constant temperature by varying the crystal field Δ [4]. Employing a multicanonical scheme in Δ allowed us to get results as continuous functions of Δ and to overcome

the free-energy barrier in the first-order regime of the transitions. A finite-size scaling analysis based on a specific-heat-like quantity and the magnetic susceptibility provided us with precise estimates for the transition points in both regimes of the phase diagram that compare very well to the most accurate estimates of the current literature. In the first-order regime, we found a somewhat surprising $1/L$ correction in the scaling of the conventionally defined magnetic susceptibility χ. As it turns out, this is due to the explicit symmetry breaking by using the absolute value of the magnetisation (i.e., $|M|$ instead of M) in the definition of χ. For a modified symmetry breaking prescription that leaves the disordered peak invariant, this correction disappears. It would be interesting to see whether similar corrections are found in other systems with first-order transitions, such as the Potts model.

[1] M. Blume: Phys. Rev. **141**, 517 (1966)
[2] H.W. Capel: Physica (Utr.) **32**, 966 (1966)
[3] J. Zierenberg et al.: Eur. Phys. J. – Special Topics **226**, 789 (2017)
[4] J. Zierenberg et al.: Phys. Rev. E **91**, 032126 (2015)

10.21 Finite-size scaling properties of the real microcanonical ensemble

P. Schierz, J. Zierenberg, W. Janke

The definition of the microcanonical ensemble can be found in any standard text book on statistical physics. Usually this ensemble is quickly dismissed in favor of the canonical ensemble since it is quite unrealistic for most physical systems in a laboratory. In the literature on phase transitions, however, this ensemble gained some interest also due to the development of the generalized ensemble methods MUCA [1, 2] and Wang-Landau [3]. Here, however, one refers to the microcanonical ensemble at constant *potential* energy while the "real" microcanonical ensemble was originally defined at constant *total* energy.

We previously investigated the behaviour of molecular dynamics and Monte Carlo simulations within this ensemble and made the interesting observation that a Monte Carlo simulation in this ensemble sampled the first-order aggregation transition in a very efficient way [4]. We found that this behaviour was previously described by Martin-Mayor [5] for the temperature-driven first-order phase transition in the Potts lattice model. We further investigated this simulation technique in the real microcanonical ensemble for a continuous Lennard-Jones system and found the same sampling advantage. We reached the same amount of particles with these simulations as with the sophisticated MUCA simulation technique.

In Ref. [6] we were able to develop a framework based on the generalization of the equal-area rule which allowed us to explain the obtained simulation behaviour of the real microcanonical ensemble. For comparisons we introduced the transition barrier of an ensemble as

$$B = \ln\left[P^{\mathrm{eqh}}\left(E_p^{\pm}\right)/P^{\mathrm{eqh}}\left(E_p^{0}\right)\right], \tag{10.6}$$

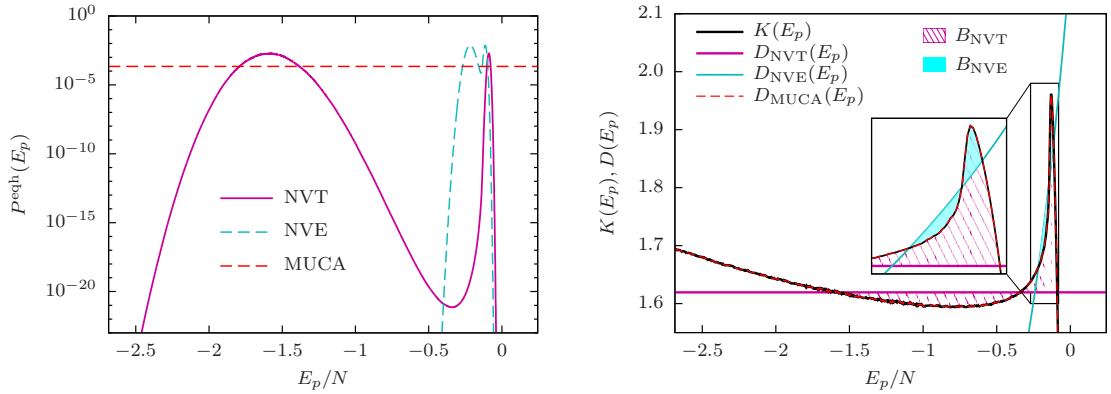


Figure 10.26: (a) The potential-energy histogram at equal height for three different ensembles for the $N = 2048$ Lennard-Jones system [6]. (b) The system dependent quantity $K(E_p)$ and the ensemble dependent $D(E_p)$ for the considered ensembles as defined in [6].

where $P^{\mathrm{eqh}}\left(E_p^{\pm}/E_p^0\right)$ denotes the equal-height histogram emerging due to phase coexistence, $E_p^{\pm}$ the positions of the two maxima and E_p^0 the position of the minimum in between. This quantity hence allows one to evaluate how "hard" the first-order transition between two phases is within an ensemble. This framework leads to the conclusion that the barrier in the canonical ensemble is always larger than in the microcanonical ensemble, $B_{\mathrm{NVT}} > B_{\mathrm{NVE}}$. In the microcanonical ensemble the transition barrier can even vanish as it was observed in [4, 7] for polymer aggregation and by reproducing the data from Ref. [5]. For the example of the Lennard-Jones system with $N = 2048$ particles we discovered that the sampling with the microcanonical ensemble is of the order of $\exp\left(B_{\mathrm{NVT}} - B_{\mathrm{NVE}}\right) \approx 10^{16}$ more efficient than simulations in the canonical ensemble due to the difference of the barriers.

[1] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
[2] W. Janke: Int. J. Mod. Phys. C **03**, 1137 (1992); Physica A **254**, 164 (1998)
[3] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001)
[4] P. Schierz et al.: J. Chem. Phys. **143**, 134114 (2015)
[5] V. Martin-Mayor: Phys. Rev. Lett. **98**, 137207 (2007)
[6] P. Schierz et al.: Phys. Rev. E **94**, 021301(R) (2016)
[7] W. Janke et al.: *Transition barrier at a first-order phase transition in the canonical and microcanonical ensemble*, Leipzig preprint (2017), to appear in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2017), in print

10.22 Convergence of Stochastic Approximation Monte Carlo and modified Wang-Landau algorithms: Tests for the Ising model

S. Schneider, M. Müller, W. Janke

The Wang-Landau algorithm [1] has proven to be a very efficient tool for determining the density of states (DOS) of statistical systems near phase transitions where traditional

local importance sampling algorithms like the Metropolis algorithm are likely to run into critical slowing down or become trapped in local free-energy minima [2]. It has, however, been pointed out that the error of the estimator for the DOS obtained by the Wang-Landau algorithm cannot be made arbitrarily small just by using longer simulations [3], the (systematic) error saturates at some (small) value. To overcome this, it has been suggested to change the behaviour of the refinement parameter in the $1/t$ modification ($1/t$-WL) of the Wang-Landau algorithm in order to circumvent the error saturation [4, 5].

Another approach is the Stochastic Approximation Monte Carlo (SAMC) algorithm first introduced in Ref. [6] and refined in Ref. [7], which works similar to the modified Wang-Landau algorithm regarding the choice of refinement scheme. While the algorithm proposed by Belardinelli and Pereyra has been tested for the Ising model, for the calculation of multidimensional integrals and was applied to lattice polymer models, the SAMC algorithm has only been tested for an artificial, non-physical model with a very small number of states [7] compared to models currently studied in statistical physics and for an off-lattice polymer model [8]. The standard test case, the Ising model, however, was still missing and we closed this gap [9].

The $1/t$-method inherits the problem of needing to know the range of admissible energies for the considered model from the Wang-Landau algorithm. In SAMC, this needs not to be known beforehand, since histogram checking is not necessary in principle. The SAMC algorithm, on the other hand, sometimes failed to converge in our examined run times. This is caused by the simulation failing to explore the low-energy states. Therefore no flat histogram can be produced, see Fig. 10.27. Since both variants of the Wang-Landau algorithm regularly check the histogram for adequate flatness, it is ensured that all energies are visited at least once. While the SAMC algorithm should converge to the desired distribution if all conditions are met, it is necessary to check if the histogram measured during the simulation was really flat at the end. This dampens the advantage of a predictable run time, since it is possible that a complete run of the algorithm turns out to be unusable due to an inappropriate choice of t_0. Monitoring the flatness of the histogram during the run is no help, because this would introduce a stochastic quantity into the algorithm, making the run time unpredictable and require the same *a-priori* knowledge of the admissible energy range as the Wang-Landau algorithm and its modifications. The rule of thumb for the choice of t_0 given by Liang et al. [7] is violated even by the 128×128 Ising model, showing that finding an appropriate t_0 can be a quite cumbersome task. The $1/t$-WL algorithm suffers from a similar restriction in this regard: While we could not find anything comparable in the Ising model, other studies suggest that the overall convergence behaviour can also be sensitive to the details of the $1/t$-refining scheme for more complicated models [5, 10]. Regarding the common features of the SAMC and $1/t$-WL algorithms, it seems reasonable to assume that the proof of convergence for SAMC also extends to the $1/t$-WL algorithm as well, since their long-time behaviour is the same. Therefore the choice of algorithm to apply to a certain problem is a practical one. With the modifications proposed in Refs. [10, 11], allowing it to adapt to *a-priori* unknown energy ranges, and in Refs. [5, 10], allowing it to find the right time for the onset of the $1/t$-refinement, the $1/t$-WL algorithm might be able to overcome its drawback for complicated systems with unknown ground states. SAMC still has the advantage of allowing to generate weights not only according to the density of states, but also according to other distributions [6, 7], which can improve

estimators [12] and might prove useful for complex systems like spin glasses or polymers, because sampling with distributions other than the inverse density of states can speed up round trip times significantly [13].

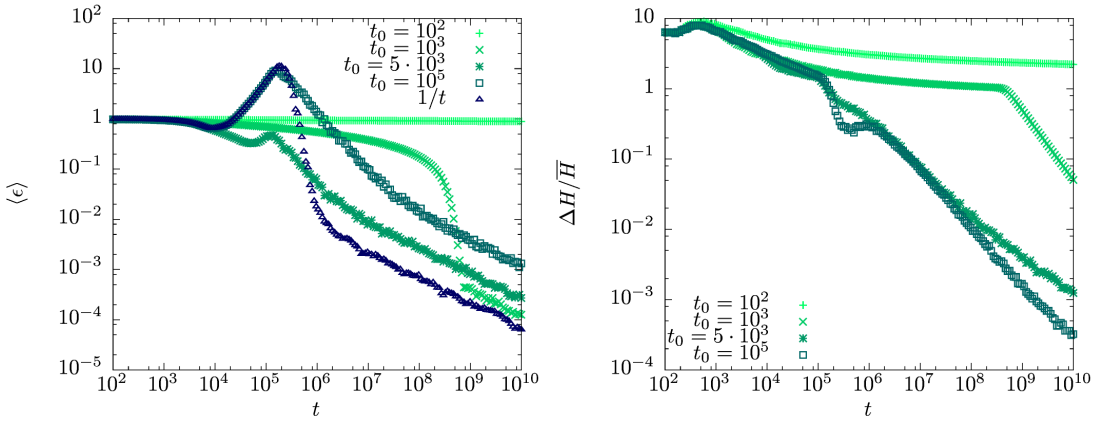


Figure 10.27: (a) The behaviour of the average deviation from the exact solution $\langle\epsilon(t)\rangle_E$ over MC time t for SAMC for different t_0 and $1/t$-WL simulations of the 16×16 Ising model. Obviously, tweaking the free parameter t_0 is essential for practical convergence. (b) The flatness of the histogram over MC time t for different choices of t_0. All data was obtained by averaging over 40 independent runs of the algorithm to reduce statistical noise.

[1] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001)
[2] W. Janke, W. Paul: Soft Matter **12**, 642 (2016)
[3] Q. Yan, J.J. de Pablo: Phys. Rev. Lett. **90**, 035701 (2003)
[4] R.E. Belardinelli, V.D. Pereyra: J. Chem. Phys. **127**, 184105 (2007); Phys. Rev. E **75**, 046701 (2007)
[5] C. Zhou, J. Su: Phys. Rev. E **78**, 046705 (2008)
[6] F. Liang: J. Stat. Phys. **122**, 511 (2006)
[7] F. Liang et al.: J. Amer. Statist. Assoc. **102**, 305 (2007)
[8] B. Werlich et al.: Comput. Phys. Commun. **186**, 65 (2015)
[9] S. Schneider et al.: Comput. Phys. Commun. **216**, 1 (2017)
[10] A. D. Swetnam, M. P. Allen: J. Comput. Chem. **32**, 816 (2011)
[11] T. Wüst, D.P. Landau: Phys. Rev. Lett. **102**, 178101 (2009)
[12] B. Hesselbo, R.B. Stinchcombe: Phys. Rev. Lett. **74**, 2151 (1995)
[13] S. Trebst et al.: Phys. Rev. E **70**, 046701 (2004)

10.23 Population annealing: Massively parallel simulations in statistical physics

M. Weigel[*], L.Yu. Barash[†‡], M. Borovský[§], L.N. Shchur[†‡¶], W. Janke

[*]Applied Mathematics Research Centre, Coventry University, England, UK
[†]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia

‡Science Center in Chernogolovka, 142432 Chernogolovka, Russia
§P.J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovak Republic
¶National Research University Higher School of Economics, 101000 Moscow, Russia

The canonical technique for Monte Carlo simulations in statistical physics is importance sampling via a suitably constructed Markov chain [1]. While such approaches are quite successful, they are not particularly well suited for parallelization as the chain dynamics is sequential, and if replicated chains are used to increase statistics each of them relaxes into equilibrium with an intrinsic time constant that cannot be reduced by parallel work. Population annealing is a sequential Monte Carlo method that simulates an ensemble of system replica under a cooling protocol. This method was first suggested in 2001 by Iba [2] and later on discussed in more detail by Hukushima and Iba [3] as a method to tackle potentially difficult sampling problems, but with no particular view to a parallel implementation. More recently, Machta [4] used a variant that avoids the recording of weight functions through population control in every step. This is the variant we adapted in our own implementation.

The population element makes this method naturally well suited for massively parallel simulations, and bias can be systematically reduced by increasing the population size. To demonstrate this, we developed an implementation of population annealing on graphics processing units (GPUs) [5] and benchmarked its behaviour for different systems undergoing continuous and first-order phase transitions [6, 7].

[1] D.P. Landau, K. Binder: *A Guide to Monte Carlo Simulations in Statistical Physics*, 4th ed. (Cambridge University Press, Cambridge, 2015)
[2] Y. Iba: Trans. Jpn. Soc. Artif. Intell. **16**, 279 (2001)
[3] K. Hukushima, Y. Iba: AIP Conf. Proc. **690**, 200 (2003)
[4] J. Machta: Phys. Rev. E **82**, 026704 (2010)
[5] L.Yu. Barash et al.: *GPU accelerated population annealing algorithm*, Moscow/Coventry/Košice/Leipzig preprint (2017), arXiv:1703.03676 [physics.comp-ph], to appear in Comput. Phys. Commun., in print
[6] L.Yu. Barash et al.: Eur. Phys. J. – Special Topics **226**, 595 (2017)
[7] M. Weigel et al.: *Population annealing: Massively parallel simulations in statistical physics*, to appear in: *Computer Simulation Studies in Condensed-Matter Physics XXX*, Coventry/Moscow/Košice/Leipzig preprint (2017), eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2017), in print

10.24 Framework for programming Monte Carlo simulations (βMC)

M. Marenz, J. Zierenberg, W. Janke

Monte Carlo (MC) computer simulations are a very powerful tool for investigating and understanding the thermodynamic behaviour of a wide variety of physical systems. These systems range from such simple ones like the Ising spin model to complex ones like the adsorption properties of proteins on surfaces [1]. In contrast to Molecular

Dynamics (MD) simulations, the other important class of algorithm to simulate microscopic systems, MC simulations are not suitable to investigate dynamical properties. On the other hand, the ability of modern MC methods to explore effectively the phase space of physical systems, especially those with a phase transition, makes them a very powerful and indispensable tool.

Another difference to MD simulations is the lack of a widely used program package for generic MC simulations. One reason for this lack is the versatility of modern MC algorithms – there are various different algorithm and many different possibilities to adjust a MC simulation to a specific problem. This was the starting point for the development of our framework for advanced MC algorithms. The aim of the framework is to enable the programmer to implement specific simulations in an easy and efficient way, without the need to implement all the tricky details for every new problem. The framework is implemented in the C++ programming language and is designed such that it separates basics parts of a MC algorithm in separate building blocks. These building blocks can be used by the programmer to implement a specific simulation.

There are 5 basic building blocks as illustrated in Fig. 10.28: The first one is the "system", which defines the Hamiltonian and the structure of the physical system. This means that the "system" building block encapsulates the energy calculation and the structure of the considered physical problem. For off-lattice system this block contains a smaller subpart, the "atom" block, which encodes the geometry of the system (e.g., boundary conditions). As systems we have implemented so far different kinds of coarse-grained homopolymers, the Lennard-Jones gas, the TIP4P water model, lattice polymers and the Potts model in different dimensions. On top of the "system" are the last two other building blocks, the "move" and the "MC technique". A "move" defines a single update proposal, propagating the system from the current state to the next one. Additionally a "constraint" can be added to every "move" in order to simulate efficiently systems with geometrical confinements. The "MC technique" implements the Monte Carlo algorithm itself. At the moment we have implemented various algorithms such as Metropolis MC, parallel tempering, multicanonical MC, multimagnetic MC and the Wang-Landau MC algorithm. One of the most advanced MC algorithms we have implemented is a parallel version of the multicanonical algorithm [2], see Fig. 10.29.

The boundaries between these blocks are well defined, so that one can easily exchange one of them. For example one can use two different algorithm to simulate a specific system without implementing a completely new program. The framework is already in practical use for different studies, for example the investigation of the influence of bending stiffness on a coarse-grained homopolymer, the influence of a spherical confinement to pseudo-phase transitions of homopolymers, and the study of polymer aggregation of several polymers for a large set of parameters (temperature, bending stiffness). Thus, the framework is very useful and has led already to several publications [2–10].

[1] M. Bachmann et al.: Angew. Chem. Int. Ed. **49**, 9530 (2010) [Angew. Chem. **122**, 9721 (2010), in German]
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] M. Marenz et al.: Condens. Matter Phys. **15**, 43008 (2012)
[4] J. Zierenberg et al.: J. Phys.: Conf. Ser. **510**, 012017 (2014)

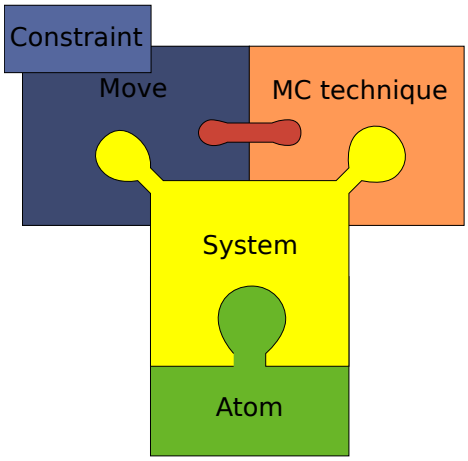


Figure 10.28: The 5 basic building blocks.

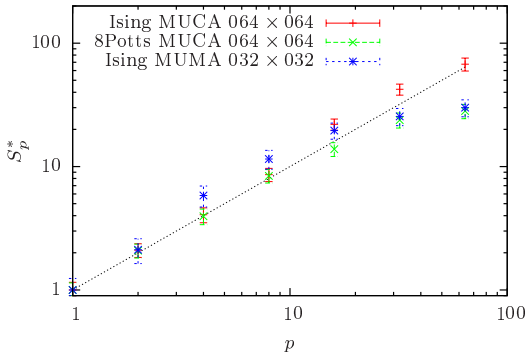


Figure 10.29: Scaling properties of the parallel multicanonical algorithm as a function of the number of processors p.

[5] J. Zierenberg et al.: J. Chem. Phys. **141**, 114908 (2014)
[6] J. Zierenberg, W. Janke: Europhys. Lett. **109**, 28002 (2015)
[7] M. Mueller et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXVIII*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, Physics Procedia **68**, 95 (2015)
[8] M. Marenz, W. Janke: Phys. Rev. Lett. **116**, 128301 (2016)
[9] J. Zierenberg et al: Polymers **8**, 333 (2016)
[10] J. Zierenberg et al.: Nat. Commun. **8**, 14546 (2017)

10.25 Funding

Graduate School *"BuildMoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-objects*
W. Janke (Principal Investigator)

Doctoral College *Statistical Physics of Complex Systems* ($\mathbb{L}^4$)
W. Janke (with B. Berche, Nancy)
Deutsch-Französisches Doktorandenkollegium (DFDK) with "Co-tutelle de Thèse", jointly with Université de Lorraine, Nancy, France, and Coventry University, UK, and National Academy of Sciences of Ukraine, Lviv, Ukraine, as associated partners
Deutsch-Französische Hochschule (DFH-UFA), Grant No. CDFA-02-07

International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
W. Janke (Scientific Member)
Max Planck Society and Klaus Tschira Foundation

Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
W. Janke (Principal Investigator, project B04)
Deutsche Forschungsgemeinschaft (DFG)

Molecular Conformation Mechanics of Proteins and Polymers

W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/24-3

Mass Transport Models on Networks
W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/27-1

Free-Energy Landscapes of Semiflexible Theta-Polymer Aggregation with and without External Force
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/31-1

Stable Knotted Phases in Semiflexible Polymers
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/33-1

Institute Partnership with the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, *Polymers in Porous Environments and on Disordered Substrates*
W. Janke (with V. Blavatska, Lviv)
Alexander von Humboldt Foundation (AvH)

Marie Curie IRSES Network *DIONICOS: Dynamics of and in Complex Systems*
W. Janke (Principal Investigator, Head of Leipzig node)
European Union (EU), Contract No. PIRSES-GA-2013-612707.

Free-Energy Landscapes of Semiflexible Polymer Aggregation
W. Janke, J. Zierenberg
NIC Jülich (computer time grant for "JURECA"), Grant No. HLZ24

10.26 Organizational Duties

Wolfhard Janke

- Director, Institute for Theoretical Physics (ITP), Universität Leipzig
- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Member of Department Council ("Fakultätsrat"), Faculty for Physics and Earth Sciences, Universität Leipzig
- Member of the Steering Committee ("Direktorium") of the Graduate Centre *Mathematics/Computer Science and Natural Sciences*, Research Academy Leipzig
- Principal Investigator of the Graduate School "BuildMoNa"
- Scientific Member of the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
- Principal Investigator of the DFG Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
- Principal Investigator of "Profillinie" *Complex Matter*, Universität Leipzig
- Principal Investigator of "Profillinie" *Mathematical and Computational Sciences*, Universität Leipzig

- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems* with Nancy (France), and associated partners in Coventry (England, UK) and Lviv (Ukraine), of the Deutsch-Französische Hochschule (DFH-UFA)
- Spokesperson of the German-Ukrainian Institute Partnership Leipzig-Lviv of the Alexander von Humboldt Foundation (AvH)
- External Member of the Jagiellonian University Graduate School *International Ph.D. Studies in Physics of Complex Systems*, Krakow, Poland
- *International Visiting Professor* of Coventry University, England, UK
- *Adjunct Professor* of The University of Georgia, Athens, Georgia, USA
- Permanent Member of the International Advisory Board for the Annual *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Organizer (with J. Gross, P. Schierz) of the Contribution *3D-Visualisierung von Polymeren – oder: Wie verkleben Spaghetti* to the "Lange Nacht der Wissenschaften", Universität Leipzig, 24. June 2016
- Organizer of the Workshop *CompPhys16* – 17th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 24.–26. November 2016
- Organizer of the Workshop *CompPhys17* – 18th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 30. November – 01. December 2017
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- External Reviewer for Deutsche Forschungsgemeinschaft (DFG), Humboldt-Stiftung (AvH), Studienstiftung des deutschen Volkes, Fond zur Förderung der wissenschaftlichen Forschung (FWF), Österreich, The Royal Society, UK, The Engineering and Physical Sciences Research Council (EPSRC), UK, Israel Science Foundation, Israel, National Science Foundation (NSF), USA, Natural Sciences and Engineering Research Council of Canada (NSERC), Canada, The Jeffress Memorial Trust, Bank of America, Virginia, USA, Universität Mainz, Germany, The University of Warwick, England, UK, Coventry University, England, UK, CECAM, Lyon, France
- Referee for Physical Review Letters, Physical Review B, Physical Review E, Journal of Chemical Physics, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Proceedings of the Royal Physical Society, Journal of Physics A, Computer Physics Communications, JSTAT, Condens. Matter Phys., PLOS ONE, New Journal of Physics, International Journal of Modern Physics C

10.27 External Cooperations

Academic

- Institute of Physics, Jagiellonian University, Kraków, Poland
  Prof. Dr. Piotr Białas, Dr. Leszek Bogacz, Prof. Dr. Zdzisław Burda
- CEA/Saclay, Service de Physique Théorique, France
  Dr. Alain Billoire

- Institut für Physik, Universität Mainz, Germany
  Prof. Dr. Kurt Binder, Andreas Nußbaumer, Prof. Dr. Friderike Schmid
- Institut für Theoretische Physik, Universität Heidelberg, Germany
  Dr. Elmar Bittner
- Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Université de Lorraine, Nancy, France
  Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Dr. Olivier Collet, Prof. Dr. Malte Henkel, Prof. Dr. Dragi Karevski
- Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- SUPA, School of Physics and Astronomy, University of Edinburgh, Scotland, UK
  Dr. Richard A. Blythe, Prof. Dr. Martin R. Evans, Dr. Bartłomiej Wacław
- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
  Prof. Dr. Pablo Butera
- Applied Mathematics Research Centre, Coventry University, England, UK
  PD Dr. Christian von Ferber, Dr. Nikolaos G. Fytas, Prof. Dr. Ralph Kenna, Dr. Thierry Platini, Dr. Martin Weigel
- Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich, Germany
  Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- IAC-1, Universität Stuttgart, Germany
  Prof. Dr. Rudolf Hilfer, Prof. Dr. Christian Holm
- Max Planck Institute for Polymer Research, Mainz, Germany
  Dr. Hsiao-Ping Hsu, Prof. Dr. Kurt Kremer
- Complex Systems Division, Department of Theoretical Physics, Lunds Universitet, Lund, Sweden
  Prof. Dr. Anders Irbäck
- Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
  Prof. Dr. Desmond A. Johnston
- Inst. für Theoretische Physik, FU Berlin, Germany
  Prof. Dr. Hagen Kleinert
- Department of Physics, University of Athens, Greece
  Prof. Dr. Anastasios Malakis
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum
- Jacobs Universität Bremen, Germany
  Prof. Dr. Hildegard Meyer-Ortmanns, Darka Labavić
- Applied Mathematics, Universitat Pompeu Fabra, Barcelona, Spain
  Prof. Dr. Ramon Villanova
- CERN (PH-SFT), Geneva, Switzerland
  Dr. Sandro Wenzel

- Department of Engineering of Physics, Ankara University, Ankara, Turkey
  Prof. Dr. Handan Arkın (Olgar), Mustafa Bilsel, Buket Taşdizen
- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Dept. of Physics Engineering, Hacettepe University, Ankara, Turkey
  Prof. Dr. Fatih Yaşar
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Alikhanyan National Science Laboratory, Yerevan, Armenia
  Prof. Dr. Nerses Ananikyan, Dr. Nikolay Izmailyan
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Dr. Lev Yu. Barash, Prof. Dr. Lev N. Shchur
- Center for Simulational Physics, The University of Georgia, Athens, USA
  Prof. Dr. Michael Bachmann, Prof. Dr. David P. Landau
- Dept. of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. Bernd A. Berg
- Dept. of Chemistry and Biochemistry, University of Oklahoma, Norman, USA
  Prof. Dr. Ulrich H.E. Hansmann
- Los Alamos National Laboratory, Los Alamos, USA
  Dr. Christoph Junghans
- Dept. of Physics and Astronomy, Texas A&M, College Station, USA
  Prof. Dr. Helmut G. Katzgraber
- Dept. of Physics, Virginia Tech, Blacksburg, USA
  Prof. Dr. Michel Pleimling, Prof. Dr. Royce K.P. Zia
- Physics Department, Carnegie Mellon University, Pittsburgh, USA
  Prof. Dr. Robert H. Swendsen
- Stetson University, DeLand, USA
  Dr. Thomas Vogel
- Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, India
  Prof. Dr. Subir K. Das
- Computational Chemistry Unit Cell (CCUC), Department of Chemistry, Chulalongkorn University, Bangkok, Thailand
  Prof. Dr. Supot Hannongbua, Dr. Oraphan Saengsawang
- Ramkhamhaeng University, Department of Chemistry, Faculty of Science, Bangkok, Thailand
  Dr. Tatiya Chokbunpiam
- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan
  Prof. Dr. Chin-Kun Hu

- The University of Tokyo, Tokyo, Japan
  Prof. Dr. Nobuyasu Ito
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Nagoya University, Nagoya, Japan
  Dr. Tetsuro Nagai, Prof. Dr. Yuko Okamoto
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

10.28 Publications

Journals

S. Basu, S. Majumder, S. Sutradhar, S.K. Das, R. Paul: *Phase Segregation in a Binary Fluid Confined Inside a Nanopore*, Europhys. Lett. **116**, 56003-1–7 (2016)

T. Chokbunpiam, S. Fritzsche, C. Chmelik, J. Caro, W. Janke, S. Hannongbua: *Gate Opening Effect for Carbon Dioxide in ZIF-8 by Molecular Dynamics – Confirmed, but at High CO_2 Pressure*, Chem. Phys. Lett. **648**, 178–181 (2016)

T. Chokbunpiam, S. Fritzsche, C. Chmelik, J. Caro, W. Janke, S. Hannongbua: *Gate Opening, Diffusion, and Adsorption of CO_2 and N_2 Mixtures in ZIF-8*, J. Phys. Chem. C **120**, 23458–23468 (2016)

J. Gross, M. Ivanov, W. Janke: *Comparing Atomistic and Coarse-Grained Simulations of P3HT*, in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012009-1–5 (2016)

W. Janke, M. Marenz: *Stable Knots in the Phase Diagram of Semiflexible Polymers: A Topological Order Parameter?*, in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012006-1–5 (2016)

W. Janke, W. Paul: *Thermodynamics and Structure of Macromolecules from Flat-Histogram Monte Carlo Simulations* (invited review), Soft Matter **12**, 642–657 (2016)

S. Kumar, R. Kumar, W. Janke: *Periodically Driven DNA: Theory and Simulation*, Phys. Rev. E **93**, 010402(R)-1–5 (2016)

S. Majumder, W. Janke: *Evidence of Aging and Dynamic Scaling in Collapse of a Polymer*, Phys. Rev. E **93**, 032506-1–6 (2016)

S. Majumder, W. Janke: *Aging and Related Scaling During the Collapse of a Polymer*, in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012020-1–5 (2016)

M. Marenz, W. Janke: *Knots as a Topological Order Parameter for Semiflexible Polymers*, Phys. Rev. Lett. **116**, 128301-1–6 (2016)

H. Nagel, W. Janke: *Emergence of Dynamic Phases in the Presence of Different Kinds of Open Boundaries in Stochastic Transport with Short-Range Interactions*, J. Stat. Mech.: Theor. Exp., 013207-1–19 (2016)

H. Nagel, W. Janke: *Dynamics of Condensate Formation in Stochastic Transport with Pair-Factorized Steady States: Nucleation and Coarsening Time Scales*, Phys. Rev. E **93**, 052112-1–12 (2016)

A. Nußbaumer, J. Zierenberg, E. Bittner, W. Janke: *Numerical Test of Finite-Size Scaling Predictions for the Droplet Condensation-Evaporation Transition* (invited talk), in Conference Proceedings *CCP2015*, IIT Guwahati, India, J. Phys.: Conf. Ser. **759**, 012009-1–8 (2016)

P. Schierz, J. Zierenberg, W. Janke: *First-Order Phase Transitions in the Real Microcanonical Ensemble* (Editors' Suggestion), Phys. Rev. E **94**, 021301(R)-1–5 (2016)

J. Zierenberg, W. Janke: *Finite-Size Scaling of Lennard-Jones Droplet Formation at Fixed Density*, in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012017-1–5 (2016)

J. Zierenberg, M. Marenz, W. Janke: *Dilute Semiflexible Polymers with Attraction: Collapse, Folding and Aggregation* (invited review), Polymers **8**, 333-1–19 (2016)

in press

K. Austin, J. Zierenberg, W. Janke: *Interplay of Adsorption and Semiflexibility: Structural Behavior of Grafted Polymers under Poor Solvent Conditions*, Macromolecules **50**, 4054–4063 (2017)

L. Yu. Barash, M. Weigel, L.N. Shchur, W. Janke: *Exploring First-Order Phase Transitions with Population Annealing*, Eur. Phys. J. – Special Topics **226**, 595–604 (2017)

T. Chokbunpiam, S. Fritzsche, J. Caro, C. Chmelik, W. Janke, S. Hannongbua: *Importance of ZIF-90 Lattice Flexibility on Diffusion, Permeation, and Lattice Structure for an adsorbed H_2/CH_4 Gas Mixture: A Re-Examination by Gibbs Ensemble Monte Carlo and Molecular Dynamics Simulations*, J. Phys. Chem. C **121**, 10455–10462 (2017)

N. Fricke, W. Janke: *Exact Enumeration of Self-Avoiding Walks on Critical Percolation Clusters in 2–7 Dimensions*, J. Phys. A **50**, 264002-1–17 (2017)

N. Fricke, J. Zierenberg, M. Marenz, F. P. Spitzner, V. Blavatska, W. Janke: *Scaling Laws for Random Walks in Long-Range Correlated Disordered Media*, Condens. Matter Phys. **20**, 13004-1–11 (2017)

J. Gross, M. Ivanov, W. Janke: *Single-Chain Behavior of Poly(3-hexyl-thiophene)*, Eur. Phys. J. – Special Topics **226**, 667–681 (2017)

D.A. Johnston, M. Mueller, W. Janke: *Plaquette Ising Models, Degeneracy and Scaling*, Eur. Phys. J. – Special Topics **226**, 749–764 (2017)

S. Majumder, J. Zierenberg, W. Janke: *Kinetics of Polymer Collapse: Effect of Temperature on Cluster Growth and Aging*, Soft Matter **13**, 1276–1290 (2017)

M. Mueller, D.A. Johnston, W. Janke: *Exact Solutions to Plaquette Ising Models with Free and Periodic Boundaries*, Nucl. Phys. B **914**, 388–404 (2017)

S. Schneider, M. Mueller, W. Janke: *Convergence of Stochastic Approximation Monte Carlo and Modified Wang-Landau Algorithms: Tests for the Ising Model*, Comp. Phys. Comm. **216**, 1–7 (2017)

J. Zierenberg, N.G. Fytas, M. Weigel, W. Janke, A. Malakis: *Scaling and Universality in the Phase Diagram of the 2D Blume-Capel Model*, Eur. Phys. J. – Special Topics **226**, 789–804 (2017)

J. Zierenberg, P. Schierz, W. Janke: *Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation*, Nat. Commun. **8**, 14546-1–7 (2017)

J. Zierenberg, K. Tholen, W. Janke: *Effect of Grafting on the Binding Transition of Two Flexible Polymers*, Eur. Phys. J. – Special Topics **226**, 683–692 (2017)

L.Yu. Barash, M. Weigel, M. Borovský, W. Janke, L.N. Shchur: *GPU Accelerated Population Annealing Algorithm*, arXiv:1703.03676, to appear in Comput. Phys. Commun. (2017), in print

W. Janke, M. Marenz, J. Zierenberg: *Generalized Ensemble Computer Simulations for Structure Formation of Semiflexible Polymers*, to appear in Proceedings of the International Conference *Supercomputer Simulations in Science and Engineering (SSSE2016)*, Moscow, Russia, Lobachevskii J. Math., in print

W. Janke, P. Schierz, J. Zierenberg: *Transition Barrier at a First-Order Phase Transition in the Canonical and Microcanonical Ensemble*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2017), in print

S. Schnabel, W. Janke: *Dynamic Greedy Algorithms for the Edwards-Anderson Model*, to appear in Comput. Phys. Commun. (2017), in print

M. Weigel, L.Yu. Barash, M. Borovský, W. Janke, and L.N. Shchur: *Population Annealing: Massively Parallel Simulations in Statistical Physics*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, H.B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2017), in print

Talks

J. Bock: *Computer Simulations of Semiflexible Polymers in Disordered Media*, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, 11. November 2016

J. Gross, M. Ivanov, W. Janke: *Comparing Atomistic and Coarse-Grained Simulations of P3HT*, 29th Annual CSP Workshop *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 22.-26. February 2016

J. Gross, M. Ivanov, W. Janke: *Comparing Atomistic and Coarse-Grained Simulations of P3HT*, Spring Meeting of the German Physical Society, Regensburg, Germany, 07.–11. March 2016

J. Gross, J, Zierenberg, M. Weigel, W. Janke: *Massively Parallel Multicanonical Simulations on GPUs*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

W. Janke, J. Zierenberg, P. Schierz: *Finite-Size Scaling of Free-Energy Barrier in Droplet Formation and Nucleation-Like Processes*, Conference of the Middle European Cooperation in Statistical Physics – MECO41, Vienna, Austria, 15. February 2016

W. Janke, M. Marenz: *Knots as a Topological Order Parameter for Semiflexible Polymers*, 29th CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 22.–26. February 2016

W. Janke, M. Mueller, D.A. Johnston: *Planar Order in the 3D Plaquette Gonihedric Ising Model*, DPG Frühjahrstagung 2016, Regensburg, Germany, 07.–11. March 2016

W. Janke: *Introduction to Monte Carlo Simulations*, SFB/TRR 102 Advanced Training Module *Introduction to Monte Carlo and Molecular Dynamics Simulation*, Leipzig/Halle, 27./28. April 2016

W. Janke: *Generalized Ensemble Computer Simulations of Macromolecules*, invited *Ising Lectures 2016*, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, 17.–19. May 2016

W. Janke, M. Marenz: *Knots as Stable Order Parameter for Semiflexible Polymers*, invited talk, Workshop *From Computational Biophysics to Systems Biology* (CBSB16), Hacettepe University Ankara, Turkey, 23.–25. May 2016

W. Janke: *Generalized Ensemble Computer Simulations for Structure Formation of Semiflexible Polymers*, invited plenary talk, International Conference *Supercomputer Simulations in Science and Engineering (SSSE)*, Higher School of Economics, Moscow, Russia, 6.–10. September 2016

S. Majumder, W. Janke: *Evidence of Aging and Dynamical Scaling During Collapse of a Polymer* 29th Annual CSP Workshop *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 25. February 2016

S. Majumder, W. Janke: *Aging and Dynamical Scaling During Collapse of a Polymer*, Soft-Matter Day, Universität Leipzig, Germany, 10. June 2016

S. Majumder, H. Christiansen, W. Janke: *Scaling Laws in Polymer Collapse: Lattice vs Off-Lattice*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 24. November 2016

M. Mueller, D.A. Johnston, W. Janke: *Exact Solutions to Plaquette Ising Models with Free and Periodic Boundaries*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 24. November 2016

P. Schierz, J. Zierenberg, W. Janke: *The Microcanonical Barrier and the Ensemble Tailoring Framework*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

S. Schnabel, W. Janke: *Local Energy Minima of the 3d Edwards-Anderson Model*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

J. Zierenberg, W. Janke: *Exploring Different Regimes in Finite-Size Scaling of the Droplet Condensation-Evaporation Transition*, 29th Annual CSP Workshop *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 24. February 2016

J. Zierenberg, P. Schierz, W. Janke: *Finite-Size Scaling of Free-Energy Barrier in Droplet Formation and Nucleation-Like Processes*, DPG Frühjahrstagung, Regensburg, Germany, 09. March 2016

J. Zierenberg, P. Schierz, W. Janke: *Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 24. November 2016

Posters

H. Christiansen, S. Majumder, W. Janke: *Coarsening and Aging of Lattice Polymers*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

N. Fricke, W. Janke: *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

J. Gross, J. Zierenberg, M. Weigel, W. Janke: *Parallel Multicanonical Simulations on GPUs*, Conference on *Phase Transitions and Critical Phenomena*, Coventry University, United Kingdom, 6.–8. April 2016

W. Janke, N. Fricke: *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*, 26th IUPAP International Conference on *Statistical Physics – StatPhys26*, Lyon, France, 22.–28. July 2016

R. Kumar: *Approximate Ground States of the Random-Field Potts Model from a Graph-Cut Method and Parallel Tempering*, 17th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys16*, Universität Leipzig, Germany, 25. November 2016

S. Majumder, W. Janke: *Evidence of Aging and Dynamical Scaling During Collapse of a Polymer*, Conference of the Middle European Cooperation in Statistical Physics – MECO41, Vienna, Austria, 15.-17. February 2016

M. Mueller, D.A. Johnston, W. Janke: *Planar ("Fuki-Nuke") Ordering and Finite-Size Effects for a Model with Four-Spin Interactions*, 26th IUPAP International Conference on *Statistical Physics – StatPhys26*, Lyon, France, 22.–28. July 2016

P. Schierz, J. Gross, W. Janke: *3D-Visualisierung von Polymeren – oder: Wie verkleben Spaghetti*, Lange Nacht der Wissenschaften, Universität Leipzig, Germany, 24. June 2016

J. Zierenberg, W. Janke: *From Amorphous Aggregates to Polymer Bundles: The Role of Stiffness on Structural Phases in Polymer Aggregation*, NIC Symposium, Forschungszentrum Jülich, Germany, 11.-12. February 2016

10.29 Graduations

Doctorate

- Niklas Fricke
  Polymers in Fractal Disorder
  28. April 2016

Master

- Benjamin Schott
  Aggregation of Lattice Polymers
  28. January 2016
- Jan Meischner
  Knotted Polymers
  17. March 2016
- Marius Bause
  Fisher-Zeros of Semiflexible Interacting Self-Avoiding Walk
  30. June 2016
- Henrik Christiansen
  Kinetics of the Collapse Transition in Lattice Polymers
  20. September 2016

Bachelor

- Katharina Tholen
  Metropolis-Simulationen von Polymeren bei externer Kraft
  04. May 2016

- Robert Wiesen
  Step-Size Dependence of Update Moves in Monte Carlo Simulations
  27. June 2016
- Lisa Fiedler
  (1+1)D Ising Ladder under Constraints
  05. July 2016
- Shane Carlson
  Persistence, Domain Growth, and Fractality in Quenched 2D Ising and Potts Spin Lattices
  15. October 2016
- Jan Philipp Hess
  Monte Carlo Simulation of the Surface Tension in the 2D Ising Model
  20. November 2016

10.30 Guests

- Dr. Peter Virnau
  Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany
  Physik-Kolloquium (19. January 2016)
  Knots in Polymers, Proteins and DNA – A Tangled Challenge
  19.–20. January 2016
- Prof. Dr. Nerses Ananikyan
  Alikhanyan National Science Laboratory, Yerevan, Armenia
  NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (12. May 2016)
  Magnetization Plateau and Partition Function Zeros on a Diamond Chain: Spin-1/2 & 1 Ising-Heisenberg models
  17. April – 16. June 2016
- Prof. Dr. Ulrich H.E. Hansmann
  University of Oklahoma, Norman, USA
  Physik-Kolloquium (10. June 2016)
  Modeling Protein Aggregation
  09.–11. May 2016
- Prof. Dr. Subir K. Das
  Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
  NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (06. July 2016)
  Continuously Varying Growth Exponent in Kinetics of Vapor-Solid Phase Transitions
  01.–07. July 2016
- Dr. Martin Weigel
  Applied Mathematics Research Centre, Coventry University, England, UK
  Physik-Kolloquium (25. October 2016)
  Fragmentation of Fractal Random Structures
  Joint NTZ-SFB/TRR 102 Colloquium (24. November 2016)
  Population Annealing: Massively Parallel Simulations in Statistical Physics
  01. August – 31. December 2016

- Dr. Lev Yu. Barash
  Landau Institute, Chernogolovka, Russia
  NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (27. October 2016)
  Monte Carlo Calculations with the Population Annealing Algorithm and its Massively Parallel Realization
  10.–30. October 2016
- Dr. Nikolay Izmailyan
  Yerevan Physics Institute, Armenia
  NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (17. November 2016)
  Ising Model on Plane: Numerical Solution
  15. October – 15. December 2016
- Liliia Ziganurova
  Landau Institute, Chernogolovka, and Higher School of Economics, Moscow, Russia
  17. October – 13. November 2016
- Prof. Dr. George Savvidy
  Demokritos Nat. Res. Center, Athens, Greece
  NTZ/DFH-UFA Colloquium (03. November 2016)
  The Gonihedric Ising Model
  01. November – 31. January 2017
- Dr. Nikolaos G. Fytas
  Coventry University, England, UK
  Phase Transitions in Disordered Systems: The Example of the Random-Field Ising Model in Four Dimensions
  22.–26. November 2016
- Prof. Dr. Hans Werner Diehl
  Univ. Duisburg-Essen, Germany
  Fluctuation-Induced Forces in Confined He and Bose Gases
  23.–25. November 2016
- Hamid Khoshbakht
  Applied Mathematics Research Centre, Coventry University, England, UK
  On the Uniform Sampling of Ground States in the 2D $\pm J$ Ising Spin-Glass Model
  23.–25. November 2016
- Dr. Francesco Parisen Toldin
  Universität Würzburg, Germany
  Critical Behavior in the Presence of an Order-Parameter Pinning Field
  23.–25. November 2016
- Dr. Hsiao-Ping Hsu
  MPI für Polymerforschung, Mainz, Germany
  Detailed Analysis of Rouse Mode and Dynamic Scattering Function of Highly Entangled Polymer Melts in Equilibrium
  23.–26. November 2016
- Prof. Dr. Nobuyasu Ito
  Univ. of Tokyo, Japan

Joint NTZ-DFH/UFA Colloquium (25. November 2016)
Social Simulation with Exascale Computer
23.–26. November 2016

- Dr. Sebastian Kapfer
FAU Erlangen, Germany
Melting in 2D and a Fresh Perspective on Monte Carlo
23.–26. November 2016

- Dr. Arnab Barua
IIT Bombay, India
23.–27. November 2016

- Pascal Fieth
Universität Oldenburg, Germany
Improving Causal Gaussian Bayesian Network Inference using Parallel Tempering
23.–27. November 2016

- Prof. Dr. Ferenc Igloi
Wigner Research Centre, Budapest, Hungary
Random Quantum Systems with Long-Range Interactions
23.–27. November 2016

- Dr. Benjamin Jäger
ETH Zürich, Switzerland
Towards the QCD Phase Diagram using Complex Langevin
23.–27. November 2016

- Hendrik Schawe
Universität Oldenburg, Germany
Convex Hulls of Self-Avoiding Random Walks: A Large-Deviation Study
23.–27. November 2016

- Dr. Arnulf Möbius
IFW Dresden, Germany
24.–25. November 2016

- Prof. Dr. Walter Selke
RWTH Aachen, Germany
24.–25. November 2016

- Dr. Elmar Bittner
Universität Heidelberg, Germany
24.–26. November 2016