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ABSTRACTS

of contributions to the

19th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys18

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Preface

Welcome to the 19th International NTZ-Workshop *CompPhys18* on *New Developments in Computational Physics*. As in previous years, also this year's Workshop will cover a broad spectrum of different fields ranging from general aspects of computational and statistical physics over computer simulation studies in condensed and soft matter physics, including applications to biological systems, and random networks to the intriguing properties of quantum systems and high-energy physics. Following the traditional setup of the Workshop, it is also this year designed to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig at the beginning of Christmas time.

The main part of the Workshop takes place from 29 – 30 November 2018 in the Theory Lecture Hall ("Hörsaal für Theoretische Physik") and the "Aula" of the Experimental Physics building in Linnéstr. 5. We are very grateful to all colleagues who helped moving their regular lecture courses to another location or date. We also wish to thank the secretary of the Computational Physics Group at the Institute for Theoretical Physics, Ms. Gabriele Menge, for her invaluable help with all administrative matters.

As in previous years, the Saturday, 01 December 2018, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that a few years ago the Institute for Theoretical Physics has moved from the old location "Vor dem Hospitaltore 1" to the *new* office building in "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", Leipzig Graduate School of Natural Sciences "BuildMoNa", and Research Academy Leipzig (RALeipzig).

Leipzig,
November 2018

Wolfhard Janke

Abstracts

Universality in reaction-diffusion fronts (P)

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We have studied the dynamical critical behavior of the reversible process A + A $\leftrightarrow$ A whose macroscopic dynamics is described by the Fisher equation. We have revisited this discrete model in two dimensions, performing extensive numerical simulations of the time evolution of the interface separating the stable and unstable phases. In particular we have measured the critical exponents which characterize the spatio-temporal fluctuations of such front for different lattice sizes. These exponents are in very good agreement with the Kardar-Parisi-Zhang (KPZ) universality class for one-dimensional interfaces.

Quantum Hamilton equations for n-body quantum systems (P)

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Within a stochastic picture quantum systems can be described in terms of kinematic and dynamic equations where the particles follow a conservative diffusion process. We here deal with an extension of the recently established quantum Hamilton equations of motion to n-particle systems. With this, one has a mathematical structure for describing n-body quantum systems which is very closely related to n-body classical systems. The relation of symmetries and conservation laws in classical mechanics, like the decoupling of the center-of-mass motion in multi-particle systems or the solution of the Kepler problem, as a special case of the two-body problem, using space-time symmetries, are translated to the quantum Hamilton equations.

Short peptides – thermodynamics and the effect of dyes: A Monte Carlo study (P)

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Although the number of structures in the PDB is continuously growing, the topic of protein folding still requires great attention and is being treated with a variety of methods. In spectroscopic experiments like FRET or FCS, one or more chromophores are grafted to a protein and their fluorescence after excitation then provides insight into the structure and dynamics of the chain. However, typically being at least the size of a large amino acid, it is conceivable that these chromophores influence the very conformations they are used to observe. Since the experiments cannot be performed without chromophores, we use a simulation approach in order to characterise their effect on the folding transition and resulting configurations of peptides. To fully capture the thermodynamics, we use a Flat Histogram Monte Carlo algorithm which provides thermodynamic information about the system in an efficient way at the expense of dynamics. We apply this algorithm to an intermediate resolution protein model which distinctly parametrises all 20 proteinogenic amino acids. Poly-Alanines, -Glutamines and -Serines of variable length act as our systems of investigation, chromophores are represented by Tryptophans. We find a limited influence of the chromophores on thermodynamic quantities and global configurational observables like the radius of gyration, but more detailed, local analysis reveals that chromophores at the chain ends cause a preference of loop structures regardless of the original peptide's folded ensemble. As individual residue positions cannot be accessed experimentally, results like these may be of interest in spectroscopy in order to obtain a setup wich minimizes disturbance of the objects and structures being investigated.

Accelerating molecular dynamics simulations with population annealing

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We adapt Population Annealing to Molecular Dynamics simulations and demonstrate its ability to accurately simulate systems with rugged-free energy landscapes. For this we simulate the folding of met-enkephalin, a short peptide commonly used to test the performance of algorithms. A comparison with Parallel Tempering, the de facto standard for the simulation of complex systems with a rugged free-energy landscape using Molecular Dynamics, is presented. Further, we show that it is possible to use adaptive temperature steps in Population Annealing, i.e., the temperature set has not to be known beforehand, like in Parallel Tempering, but can be determined on-the-fly.

An overview of recent numerical results on the random-field Ising model

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A lot of progress has been made recently in our understanding of the random-field Ising model (RFIM) thanks to large-scale numerical simulations. In particular, it has been shown that, contrary to previous statements, the critical exponents for different probability distributions of the random fields and for diluted antiferromagnets in a field are the same. Therefore, critical universality, which is a perturbative renormalization-group prediction, holds beyond the validity regime of perturbation theory. Most notably, dimensional reduction appears to be restored at five dimensions, i.e., the estimated values of the critical exponents of the 5D random-field Ising model are statistically compatible to those of the pure 3D Ising ferromagnet. In this talk, I will review some aspects of these results obtained via high-precision ground-state simulations of the RFIM at several spatial dimensions below the upper critical dimension.

Does KPZ describe pushed interfaces with quenched disorder?

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We will present simulation data for generalized percolation (including the $T = 0$ random-field Ising model without spontaneous nucleation) in 3–6 dimensions. In all these dimensions they show a second topological transition in addition to the pinning (= percolation) transition, and they suggest that KPZ does not describe the asymptotic behavior of the moving interface in either one of the two phases. In $d = 2$ the second transition is absent, and KPZ does describe the asymptotics.

Conformational transitions in prions and amyloids

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Presence of amyloid fibrils is a hallmark of Alzheimer's and many other metabolic or neurodegenerative diseases. However, in the case of Alzheimer's disease, the primary neurotoxic agents appear to be small soluble

oligomers formed either on-pathway or off-pathway to fibril assembly. Hence, it is important to understand how the equilibrium between the polymorphous fibrils and oligomers is shifted by mutations, changing environmental conditions, or in the presence of prion-like amyloid strains. These processes are difficult to probe in experiments. An alternative are computer simulations; however, the assembly of mis-folded proteins into oligomers and fibrils happens on time scales that often cannot be covered in all-atom simulations. We have proposed to overcome this problem by a Replica-Exchange with Tunneling method. We will discuss this approach and present recent work.

Phase transition in detecting causal relationships from obervational and interventional data

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Analysing data of, e.g., gene-expression experiments, and modelling it via network-based approaches is one of the main data analysis tasks in modern science. A first step is to use the observation of correlation to infer the structure of the underlying network, for example in the context of the inverse Ising model. Although this is already a algorithmically hard problem, it becomes even more challenging, when one is even interested in causal relationships between the network entities. When just using correlations obtained from observational data, such causal relationships can only be resolved partially. One way out is to include interventions to the system, e.g., by knocking out genes when studying gene expression. This allows one, in principle, to get a grip on the causal structure of a system. Here, we model the data using Gaussian Bayesian networks defined on directed acyclic graphs (DAGs). By applying an approach which allows for multiple interventions in each single experiment and which takes large-scale interaction effects into account by calculating joint maximum likelihoods (MLs) for rather large (sub) networks, causal relationships can be detected, in principle, with high accuracy. The algorithm which achieves this needs on top of the ML calculation to sample different causal orderings, which induce different DAGs. We present a new Monte Carlo approach to sample orderings, which is based on approximating the full ML by probabilities of orderings of triplets. We show that this approximation is rather good and efficient. This allows us to study the quality of the causality detection as a function of the fraction of interventional experiments. We observe a (information) phase transition between phases where the causal structure cannot be detected and where it can be detected. The transition point occurs roughly where only one intervention per network node is necessary.

Axiomatic construction of quantum Langevin equations

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A phenomenological construction of quantum Langevin equations, based on the physical criteria of (i) the canonical equal-time commutators, (ii) the Kubo formula, (iii) the virial theorem and (iv) the quantum fluctuation-dissipation theorem is presented. The case of a single harmonic oscillator coupled to a large external bath is analysed in detail. This allows to distinguish a markovian semi-classical approach, due to Bedeaux and Mazur, from a non-markovian full quantum approach, due to to Ford, Kac and Mazur. The quantum-fluctuation-dissipation theorem is seen to be incompatible with a markovian dynamics. Possible applications to the quantum spherical model are discussed.

Indication of chain retraction in highly entangled polymer melts after a large step deformation

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(with Kurt Kremer)

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Anisotropic stress relaxation of strongly deformed polymer melts in a non-linear viscoelastic regime and the resulting anisotropic structures of chains after isochoric elongation are studied [1]. Both the classical Doi-Edward tube theory and refined GLaMM tube theory incorporating contour length fluctuation, and convective constraint release predict that the process of retraction in entangled linear chains sets in immediately after the deformation, while there exist contradiction between experiment and theory. From our simulations, we show that results of radius of gyration in the direction perpendicular to the stretching direction indicate chain retraction in the initial relaxation process. Applying the harmonic spherical expansion approach to the 2D scattering function along the parallel and perpendicular to the stretching direction, the profiles of the first anisotropic term of scattering function also qualitatively agree with the theoretical prediction by GLaMM around Rouse time. The influence of entanglement effects and the strength of strain are also investigated.

[1] H.-P. Hsu and K. Kremer, Phys. Rev. Lett. **121** (2018) 167801.

A multiplicative Monte Carlo rate for nonequilibrium dynamics

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In this talk we present a multiplicative Monte Carlo rate for nonequilibrium single spin flip dynamics that can be treated analytically in several cases [1]. We argue that, at least for the considered systems, the well known Metropolis and Heat-bath rates introduce dynamical multi-spin correlations that modify the acceptance rates of the algorithms, while the proposed multiplicative rate does not introduce such correlations and has the same acceptance rate as an exact solution of the dynamics. We discuss implications for other applications.

[1] A. Hucht, *Nonequilibrium phase transition in an exactly solvable driven Ising model with friction*, Phys. Rev. E **80** (2009) 061138.

Quantum relaxation and metastability of lattice bosons with cavity-induced long-range interactions

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The coupling of cold atoms to the radiation field within a high-finesse optical resonator, an optical cavity, induces long-range interactions which can compete with an underlying optical lattice. The interplay between short- and long-range interactions gives rise to new phases of matter including supersolidity (SS) and density waves (DW), and interesting quantum dynamics. Here it is shown that for hard-core bosons in one dimension the ground state phase diagram and the quantum relaxation after sudden quenches can be calculated exactly in the thermodynamic limit. Remanent DW order is observed for quenches from a DW ground state into the superfluid (SF) phase below a dynamical transition line. After sufficiently strong SF to DW quenches beyond a static metastability line DW order emerges on top of remanent SF order, giving rise to a dynamically generated SS state. Our method to handle infinite- and short-range interactions in the infinite system size limit opens a way to solve exactly other Hamiltonians with infinite- and short-range interactions as well.

Simulation of quantum computer

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Recent results of simulations of quantum computers using massively-parallel classical computers are given. Using the K computer of RIKEN, the JUQUEEN of Forschungszentrum Jülich and Sunway Taihu Light of the National Supercomputer Center in Wuxi in China, simulations of up to 45 qbits quantum gate circuits are realized with double-precision, 46 with single-precision and 48 with much reduced precision in reasonable execution time. These simulators can be applied directly to simulate quantum-spin systems.

Specific heat and partition function zeros for the dimer model on the checkerboard B lattice: Finite-size effects

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There are three possible classifications of the dimer weights on the bonds of the checkerboard lattice and they are denoted as checkerboard A, B and C lattices. The dimer model on the checkerboard B and C lattices has much richer critical behavior comparing with the dimer model on the checkerboard A lattice. In this paper we study in full details the dimer model on the checkerboard B lattice. The dimer model on the checkerboard B lattice has two types of the critical behaviors associated with different universality classes, namely $c = -2$ and $c = 1$. In one limit this model is the anisotropic dimer model on rectangular lattice with algebraic decay of correlators and in another limit it is the anisotropic generalized Kasteleyn model with radically different critical behavior. We analyze the partition function of the dimer model on an $2M \times 2N$ checkerboard B lattice wrapped on a torus obtained in Ref. [1]. We find that for this lattice the correlation length exponent is unequal to the shift exponent. We also find very unusual behavior of the partition function zeros and the specific heat of the dimer model. Remarkably, we find out that the number of the specific heat peaks and the number of the circle of the partition function zeros increases with the system size.

[1] N. Sh. Izmailian, C.-K. Hu, and R. Kenna, Phys. Rev. E **91** (2015) 062139.

Fractons

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One of the (many) things Wolfhard has simulated in recent years has been the (classical) 3D plaquette Ising model. The peculiar finite-size scaling properties of this at its first-order phase transition can be traced back to a subsystem symmetry, midway between a global and a gauge symmetry. In the same way that gauging a quantum 2D Ising model gives the Toric Code, gauging the quantum 3D plaquette Ising model gives the X-cube model whose topological excitations, fractons, have unusual properties.

Critical exponent ν of the Ising model in three dimensions with long-range correlated disorder (P)

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We analyze the critical behavior of the site-diluted Ising model in three dimensions using Monte-Carlo simulation techniques. The case of uncorrelated defects is compared to the long-range correlated case where the space correlation function between the defects obeys a power-law decay. We discuss different methods of critical exponent ν extraction and compare our results to theoretical predictions.

Irreversible, totally asymmetric Markov chains in statistical physics

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The Markov-chain Monte Carlo method is an outstanding computational tool in science. Since its origins in 1953, it has relied on the detailed-balance condition to solve general computational problems under the conditions of thermodynamic equilibrium with vanishing probability flows. In this talk, I discuss irreversible Markov chains that violate detailed balance, yet satisfy global balance. Equilibrium is reached as a steady state with non-vanishing probability flows. I will concentrate on the case of one-dimensional particle systems, for which simulations [1] and mathematical results [2] became available recently, but also mention the 2-d melting problem for hard disks (that was solved using the above framework [3]. I will further discuss the N-body Coulomb problem [4], that relies on the factorized Metropolis algorithm [5] to sample the Boltzmann distribution without engaging in the costly computation of the system energy.

[1] S. C. Kapfer and W. Krauth, *Irreversible local Markov chains with rapid convergence towards equilibrium*, Phys. Rev. Lett. **119** (2017) 240603.
[2] Z. Lei and W. Krauth, *Mixing and perfect sampling in one-dimensional particle systems*, arXiv:1806.06786 (2018), to appear in Europhys. Lett. (in print).
[3] E. P. Bernard and W. Krauth, *Two-step melting in two dimensions: First-order liquid-hexatic transition*, Phys. Rev. Lett. **107** (2011) 155704.
[4] M. F. Faulkner, L. Qin, A. C. Maggs, and W. Krauth, *All-atom computations with irreversible Markov chains*, J. Chem. Phys. **149** (2018) 064113.
[5] M. Michel, S. C. Kapfer, and W. Krauth, *Generalized event-chain Monte Carlo: Constructing rejection-free global-balance algorithms from infinitesimal steps*, J. Chem. Phys. **140** (2014) 54116.

Thermodynamics of supramolecular polymers with hydrogen bonding ends

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Rheological properties of supramolecular polymers (SMPs) depend on their equilibrium structure including the size, the number, and the topology of aggregates. A polymer with a hydrogen-bonding (H-bonding) motif at both ends is one widely used precursor to build SMPs. Due to the complex interplay between chain stiffness, H-bonding interaction, polarity along a chain, and polymer conformational entropy, it is difficult to theoretically predict the structure of SMPs. In this work we investigate thermodynamics of SMPs with H-bonding ends in wide range of densities. Replica exchange stochastic approximation Monte Carlo method simulation with a coarse-grained models for polyethylene and polybutylene glycols are used. Our simulation shows that SMPs with mono-functional stickers have two transition lines with increasing temperature, the first is a ring-linear transition and the second is a linear-free chain transition, which both are proven to be continuous. SMPs with multi-functional H-bonding

stickers which is described by weakly interacting sticker beads but wide allowance of bonding angle have one more transition line at very low temperature. This transition corresponds to the micelle-formation for dilute SMPs and the sol-gel transition for semi-dilute SMPs.

Steady state of a protein-ligand system in a temperature gradient

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The biological function of proteins is closely associated with their ability to bind ligands and change conformations in response to changing conditions. Since binding state and conformation of a protein affect its response to a temperature gradient, they may be probed with thermophoresis. In recent years, thermophoretic techniques to investigate biomolecular interactions, quantify ligand binding, and probe conformational changes have become established. However, it can be difficult to distinguish the effects of ligand binding, conformational change, and hydrogen bonding. To develop a better understanding of the mechanisms underlying the thermophoretic behavior of proteins, we investigate proteins and ligands in solution with the aid of density-of-states simulations with a Wang-Landau type algorithm. This method gives us access to the entropy of the system and allows us to calculate changes in entropy which may be related to the configurational part of the Soret coefficient. In this work, we focus on simple models for proteins and ligands to investigate thermodiffusion in explicit and implicit solvent models.

Dissipative dynamics of a single polymer in solution: A Lowe-Andersen approach

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We study the equilibrium dynamics of a single polymer chain under good solvent condition. Special emphasis is laid on varying the drag force experienced by the chain while it moves. To this end we model the solvent in a mesoscopic manner by employing the Lowe-Andersen approach of dissipative particle dynamics which is known to reproduce hydrodynamic effects. Our approach captures the correct static behavior in equilibrium. Regarding the dynamics, we investigate the scaling of the self-diffusion coefficient D with respect to the length of the polymer N, yielding results that are compatible with the Zimm scaling $D \sim N^{-3/5}$.

Nanopatterns of macromolecules (P)

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The poster presents the work of our group in the SFB/TRR 102 "Polymers under multiple constraints: restricted and controlled molecular order and mobility". The main objective of the project is to gain a better understanding of adsorption properties and recognition of surface patterns of macromolecules such as polymers and proteins when interacting with material surfaces and nanoparticles (external constraints), and of the interplay of these phenomena with polymer collapse, crystallization, aggregation and folding (internal constraints).

Dimension dependence of clustering dynamics in models of ballistic aggregation and freely cooling granular gas

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Via event-driven molecular dynamics simulations we study kinetics of clustering in assemblies of inelastic particles in various space dimensions. We consider two models, viz., the ballistic aggregation model (BAM) and the freely cooling granular gas model (GGM), for each of which we quantify the time dependence of kinetic energy and average mass of clusters (that form due to inelastic collisions). These quantities, for both the models, exhibit power-law behavior, at least in the long time limit. For the BAM, corresponding exponents exhibit strong dimension dependence and follow a hyperscaling relation. In addition, in the high packing fraction limit the behavior of these quantities become consistent with a scaling theory that predicts an inverse relation between energy and mass. On the other hand, in the case of the GGM we do not find any evidence for such a picture. In this case, even though the energy decay, irrespective of packing fraction, matches quantitatively with that for the high packing fraction picture of the BAM, it is inversely proportional to the growth of mass only in one dimension, and the growth appears to be rather insensitive to the choice of the dimension, unlike the BAM.

Quench dynamics of the disordered quantum Ising chain

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By means of free fermionic techniques combined with multiple precision arithmetic we study the time evolution of the average magnetization, $m(t)$, of the random transverse-field Ising chain after global quenches. We observe different relaxation behaviors for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow described by $\ln m(t) \sim a \ln \ln t$, and in a finite sample of length L the average magnetization saturates at a size-dependent plateau $\ln m(L) \sim -b \ln L$, where the two exponents satisfy the relation $b/a = 1/2$. Starting from a fully disordered initial state, the magnetization increase until it saturates to an asymptotic value $\ln m(L) \sim b' \ln L$, with $b' = 1.5$. For both quenching protocols, finite-size scaling is satisfied in terms of the scaled variable $L^{b/a} \ln t$. Furthermore, the distribution of long-time limiting values of the magnetization shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behavior of the magnetization is explained through semi-classical theory.

Simulation of a large polymer with untruncated interaction near the collapse

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(with Wolfhard Janke)

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Off-lattice polymer models usually incorporate monomer-monomer interactions that act – at least in principle – at any distance. In consequence, calculating the energy and in particular the change in energy during a Monte Carlo move is typically an operation of computational complexity $\mathcal{O}(N^2)$, where N is the number of monomers. Since this complexity is inherited by the individual Monte Carlo move, only small polymers can be simulated without truncating the interaction potentials. We show how this can be avoided at temperatures near or above the collapse transition by using a Metropolis algorithm that tolerates inaccurate estimates of ΔE and present results for a polymer with Lennard-Jones interactions and $N \leq 65536$.

Aggregation of short polyethylene chains

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The aggregation of polymer chains has been under investigation since a long time, but the simulations were focused mostly on simplified coarse-grained models. We present results of a Wang-Landau type Monte Carlo simulation of polyethylene short-chain aggregates. Our simulation study is based on a chemically realistic united atom model [1]. Simulation results for low-temperature states of aggregates of different numbers of chains and chain lengths demonstrate a set of diverse ground-state configurations. Even aggregates of a few chains can exist in disordered and ordered states. Low-energy (or ground state) configurations differ from configurations of single chains having the same number of monomers. However, with increasing chain length, collapsed single chain and aggregate morphologies become more similar.

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

Inferring dynamical properties of subsampled networks

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Inferring system-wide dynamic properties when only observing a small subsystem remains a challenge in neuroscience: Even today, the most advanced millisecond-precision electrode measurements can only record a few hundred neurons out of millions. One dynamical property whose assessment is particularly biased by subsampling is the stability of a complex system. In case of neural networks, the collective stability depends on the average activity propagated by every single neuron. This can be well described by the *branching parameter* m, the average number of postsynaptic spikes triggered per presynaptic spike. This parameter serves not only as a proxy for activity propagation, but for the collective characteristic time scale, responses to stimuli, the fraction of recurrent activation and Fano factors. We have recently shown that conventional estimation of the branching parameter via linear regression can be severely biased under subsampling. This implies, for instance, that even small stimuli can lead to a much larger response than anticipated. To compensate the subsampling bias, we introduced a new multi-step regression (MR) estimator [1].

[1] J. Wilting and V. Priesemann, Nat. Commun. **9** (2018) 2325.

Entropy reduction and entropy driven folding for confined polymers

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Geometric confinement of a polymer chain results in a loss of conformational entropy. For a flexible N-site chain (with monomer diameter a) restricted in 1 or 2 dimensions to a confinement length D (such that $aN^{1/3} < D < 2R_g$, where R_g is the unconfined radius of gyration) this entropy reduction is expected to exhibit power-law scaling of the form $N(a/D)^{5/3}$. For 3-dimensional confinement the expected scaling is $N^2(a/D)^3$. For a chain that can fold into a compact native state, these confinement effects reduce the number of possible unfolded states, thereby providing an entropic stabilization of the folded state and shifting the location of the folding transition. This allows for the possibility of confinement (entropy) driven folding [1]. Here we investigate these confinement effects for a flexible square-well-sphere chain with short range interactions that undergoes a first-order-like folding transition analogous to the all-or-none folding characteristic of many small proteins [2]. We use a Wang-Landau simulation approach to construct the partition function for a polymer confined within a hard-wall slit, cylindrical pore, or a finite cylindrical box. For the confined chain, isothermal reduction of the confinement dimension can induce folding, unfolding, or crystallite restructuring. Scaling laws, phase diagrams, and analyses of the free-energy barrier to folding will be presented.

[1] M. Taylor, Macromolecules **50** (2017) 6967.
[2] M. Taylor, W. Paul, and K. Binder, J. Chem. Phys. **145** (2016) 174903.

Approximate ground states of the random-field Potts model from graph cuts

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While the ground-state problem for the random-field Ising model is polynomial, and can be solved using a number of well-known algorithms for maximum flow or graph cut, the analog random-field Potts model corresponds to a multiterminal flow problem that is known to be NP-hard. Hence an efficient exact algorithm is very unlikely to exist. As we show here, it is nevertheless possible to use an embedding of binary degrees of freedom into the Potts spins in combination with graph-cut methods to solve the corresponding ground-state problem approximately in polynomial time. We benchmark this heuristic algorithm using a set of quasiexact ground states found for small systems from long parallel tempering runs. For a not-too-large number q of Potts states, the method based on graph cuts finds the same solutions in a fraction of the time. We employ the new technique to analyze the breakup length of the random-field Potts model in two dimensions.

Extending the dynamic range by an ensemble of neural networks

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The capability of perceiving systems to accurately process different intensities of input is typically captured by the single quantity termed *dynamic range*. The greater this quantity is, the better the broad intensities of the external world are represented by the system. It was shown that the dynamic range of a single neural network is maximized at criticality. However, even the critical network cannot explain the huge dynamic range that human sensory systems are capable of, which points at some missing ingredients that increase the dynamic range by an order of magnitude. Aim of our study is to uncover a possible mechanism for such an increase. We demonstrate that the dynamic range is strongly affected by the inevitable convergences from a non-zero fraction of activity. We show that for all parameter settings, the neural network is capable to discriminate inputs within the same regime of stimuli. In other words, the dynamic range increases moderately towards *critical* dynamics but the sensitivity to the input is barely affected. We derive convergence-correcting network adaptation and show that the power-law scaling of avalanche sizes in such networks persist for much larger sizes compared to a fixed network. We prove that in the convergence-corrected network the sensitivity to a specific input range changes with the distance to criticality such that a properly constructed ensemble of networks can extend the dynamic range to infinity. We comment on implications for machine learning problems as well as a possible biological implementation in auditory midbrain.