Monte Carlo Algorithms in Statistical Physics – Program

Location

Executive Lounge on Level 1 of the Alan Gilbert Building, The University of Melbourne, 161 Barry St, Carlton, on the corner of Barry St and Grattan St. Google maps url: http://bit.ly/bfJcOU.

Monday

8:30am *Registration*

9:00am Jon Machta – *Parallel Tempering and Population Annealing for Rough Free Energy Landscapes*

9:45am David Yllanes – *The low-temperature phase of Ising spin glasses: parallel-tempering simulations with sample-dependent thermalisation on the Janus computer*

10:10am Yukito Iba – *Rare Event Sampling using Multicanonical Monte Carlo*

10:35am *Morning tea / Late registration*

11:10am Peter Young – *Monte Carlo Simulations of Heisenberg Spin Glasses*

11:55am Piotr Kowalczyk – *Microscopic model of carbonaceous nanoporous molecular sieves - anomalous transport in molecularly confined spaces*

12:20pm Michael Bachmann – *Hierarchical Subphase Transitions in Molecular First-Order Nucleation Processes*

12:45pm *Lunch*

2:00pm Victor Martín-Mayor – *Monte Carlo simulations of (quasi) constrained ensembles*

2:45pm Beatriz Seoane – *Effective potential study of hard-spheres crystallization*

3:10pm Gerd Schröder-Turk – *Hard Sphere Liquids in Complex Pores*

3:35pm *Afternoon tea*

4:00pm Alan Sokal – *Overcoming critical slowing-down: Where do we stand 23 years after Swendsen and Wang?*

5:00pm *Finish*

Tuesday

9:00am Wolfhard Janke – *Error Estimation and Reduction with Cross Correlations*

9:45am Ebrahim Foulaadvand – *Ground state energy of simple atoms by variational quantum Monte Carlo method: steepest descent approach*

10:10am Manolo Per – *Efficient calculation of unbiased estimates in diffusion quantum Monte Carlo*

10:35 *Morning tea*

11:10am Henk Blöte – *Potts models with long-ranged interactions*

11:55am Munetake Sasaki – *Stochastic Cutoff Method for Long-Range Interacting Systems*

12:20pm Peter Anders – *Diagrammatic Monte Carlo method for bosonic impurity problems*

12:45pm *Lunch*

2:00pm Jesus Salas – *Dynamic critical behavior of the Wang-Swendsen-Kotecky algorithm for two-dimensional Potts antiferromagnets*

2:45pm Elmar Bittner – *Replica-Exchange Cluster Algorithm*

3:10pm Hidemaro Suwa – *Markov Chain Monte Carlo without Detailed Balance and Bounce-free Worm Algorithm*

3:35pm *Afternoon tea*

4:00pm David Landau – *Exploring Complex Free Energy Landscapes with Wang-Landau Sampling*

5:00pm *Finish*

7:00pm *Dinner at Bokchoy Tang*

Wednesday

9:00am Ian Snook – *The observation of formation and annihilation of solitons and standing strainwave superstructures in a two-dimensional colloidal crystal*

9:45am George Opletal – *Hybrid Reverse Monte Carlo Modelling of Disordered Materials*

10:10am Peter Zoontjens – *Kinetic Monte Carlo Modelling of Pt on Au (111) in Bimetallic Catalysis*

10:35am *Morning tea*

11:15am Thomas Prellberg – *PERM and all that - a comparison of growth algorithms*

12:00pm Ofer Biham – *Reaction networks with fluctuations: from inter-stellar chemistry to intracellular biology*

12:45pm *Lunch*

2:00pm Martin Weigel – *Simulating spin models on GPU*

2:45am Phani Nukala – *Low-rank updates in statistical physics applications*

3:10pm Wenan Guo – *A worm simulation of the loop model on the square lattice*

3:35pm *Afternoon tea*

4:00pm Werner Krauth – *The event-chain algorithm and the melting transition for two-dimensional hard spheres*

4:45pm *Finish*

Abstracts

Title: Diagrammatic Monte Carlo method for bosonic impurity problems

Authors: **Peter Anders**[1], Emanuel Gull[2], Lode Pollet[3], Matthias Troyer[1] and Philipp Werner[1]

Affiliation:

1. Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland

2. Department of Physics, Columbia University, New York, NY 10027, USA

3. Department of Physics, Harvard University, Cambridge, MA 02138, USA

Abstract:

We present a continuous-time Monte Carlo method for bosonic impurity models which allows the study of bosonic lattice models within the recently developed bosonic dynamical mean field (B-DMFT) framework. The method is based on a Monte Carlo sampling of a perturbation expansion in the hybridization functions as well as the condensate wave function. It allows us to solve the B-DMFT equations and to calculate the Green's function for various temperatures and coupling parameters. As an application we present the B-DMFT phase diagram for the bosonic Hubbard model on the 3d cubic lattice.

Title: Hierarchical Subphase Transitions in Molecular First-Order Nucleation Processes

Author: **Michael Bachmann**

Affiliation: Soft Matter Systems Research Group, Institut fuer Festkoerperforschung (IFF-2), Germany

Abstract:

Thermodynamic transitions in nucleation processes of finite systems often exhibit an interesting first-order-like signature, represented by a convex region of the microcanonical entropy. This is conveyed to the caloric temperature which in the transition region possesses a little intuitive behavior: With increasing energy, the system gets colder. Independently of the physical interpretation of this "backbending effect", its characteristic change in monotony not only enables a systematic and quantitative analysis of the transition. It even allows to reduce the nucleation process to a hierarchical sequence of subphase transitions. We discuss this in detail for the exemplified aggregation transition of a system consisting of a few polymers.

Title: Reaction networks with fluctuations: from inter-stellar chemistry to intra-cellular biology

Author: **Ofer Biham**

Affiliation: Racah Institute of Physics, Hebrew University, Jerusalem, Israel.

Abstract:

Complex reaction networks are common in physical, chemical and biological systems. In many cases, the reactive species are confined to a small volume, in which the copy number of each species is low. Relevant examples include biochemical networks in cells and reactions on dust grains in the interstellar medium. In these systems the reaction rates are often dominated by fluctuations and cannot be evaluated by rate equations. Stochastic methods such as the direct integration of the master equation or Monte Carlo simulations (e.g. using the Gillespie algorithm) are needed. However, the number of microscopic states (and the number of equations) increase exponentially with the complexity of the network. This makes the stochastic simulations infeasible for complex networks.

In this talk I will describe the effects of fluctuations on the reaction rates in interstellar chemistry networks and on bistability and oscillations in genetic regulatory networks in cells. I will also present two methods that provide a dramatic reduction in the number of equations, and enable efficient stochastic simulations of complex reaction networks. In the multiplane method [1], the reduction is achieved by breaking the network into a set of maximal fully connected sub-networks (cliques). Lower-dimensional master equations are constructed for the marginal probability distributions associated with the cliques, with suitable couplings between them. In the moment equations method [2], the reduction is achieved by writing a closed set of equations for the first and second moments, using a suitable closure condition. Applications of the two methods will be shown and their advantages and limitations in comparison with the Gillespie algorithm will be discussed.

[1] A. Lipshtat and O. Biham, Efficient simulations of gas-grain chemistry in interstellar clouds, Phys. Rev. Lett. 93, 170601 (2004).
[2] B. Barzel and O. Biham, Efficient stochastic simulations of complex reaction networks on surfaces, J. Chem. Phys 127, 144703 (2007).
[3] F. Le Petit, B. Barzel, O. Biham, E. Roueff and J. Le Bourlot, Incorporation of stochastic chemistry on dust grains in the Meudon PDR code using moment equations: I. Application to the formation of H2 and HD, Astron. Astrophys. 505, 1153 (2009).
[4] B. Barzel and O. Biham, Stochastic analysis of dimerization systems, Phys. Rev. E 80, 031117 (2009).

Title: Replica-Exchange Cluster Algorithm

Author: **Elmar Bittner** and Wolfhard Janke
Affiliation: Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ) – Universität Leipzig, Germany

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

Title: Potts models with long-ranged interactions

Author: **Henk W.J. Blöte**
Affiliation: Lorentz Institute, Leiden University, Netherlands

Abstract:
Simulations of models with long-range interactions by means of cluster methods can, in many cases, be arranged such that the number of operations needed to update one particle becomes independent on the range of the interactions. This makes it possible to perform very efficient simulations of long-range Potts models. Application to three- and four-state Potts models shows that the transition turns first-order when the range of the interactions is increased.

Title: Optimisation of quantum Monte Carlo wave function: steepest descent method

Author: **M. Ebrahim Foulaadvand**
Affiliation: Department of Physics, Zanjan University, P.O. Box 45196-313, Zanjan, Iran

Abstract:
We have employed the steepest descent method to optimise the variational ground state quantum Monte Carlo wave function for He, Li, Be, B and C atoms. We have used both the direct energy minimisation and the variance minimisation approaches. Our calculations show that in spite of receiving insufficient attention, the steepest descent method can successfully minimise the wave function. All the derivatives of the trial wave function respect to spatial coordinates and variational parameters have been computed analytically. Our ground state energies are in a very good agreement with those obtained with diffusion quantum Monte Carlo method (DMC) and the exact results.

Title: A worm simulation of the loop model on the square lattice

Author: **Wenan Guo**
Affiliation: Physics Department, Beijing Normal University, Beijing 100875, P. R. China

Abstract:
We develop a worm algorithm for the O(n) intersecting loop model on the square lattice. We show that our

algorithm has little critical slowing-down when $1 \leq n \leq 2$. We tested this algorithm by investigating the critical properties of the model, for which we determine the critical points and several critical exponents. The present of crossing bonds is found to be irrelevant at the critical branch of the loop model.

Title: Rare Event Sampling using Multicanonical Monte Carlo

Author: **Yukito Iba**

Affiliation: The Institute of Statistical Mathematics, Japan

Abstract:

Since Metropolis et al. (1953), dynamic Monte Carlo methods have been used for calculation of canonical averages in statistical physics (and path integrals in field theories). However, they are universal tools for sampling from multivariate non- Gaussian/discrete distributions with unknown normalization constants, hence should be useful in problems in other fields.

We have been interested in applications of dynamic Monte Carlo methods to rare event sampling and calculation of large deviation probabilities. Examples include:

- Sampling rare events in random matrices and networks [1, 2]
- Sampling rare trajectories in chaotic dynamical systems [3, 4]
- Numerical studies on Griffiths singularity [5]

To treat these examples using dynamic Monte Carlo, the physical energy in usual simulations should be replaced by a quantity that characterizes rare events; for example, when we are interested in large deviation in the largest eigenvalue $\lambda^{\max}$ of random matrices, we use $\lambda^{\max}$ as a fictitious energy in a Monte Carlo simulation.

Slow mixing of the Markov chain caused by local optima is common in these applications. Extended ensemble methods such as replica exchange algorithm or multicanonical algorithms are useful for avoiding this difficulty. Among them, the Wang-Landau algorithm, which directly gives tails of the density of states in an efficient way, is particularly convenient for our purpose.

In this talk, we will discuss selected examples of our studies on rare event sampling using dynamic Monte Carlo, as well as earlier studies on this subject.

[1] Saito, N., Iba, Y., and Hukushima, K. (2010): Multicanonical sampling of rare events in random matrices, arXiv:1002.4499v1.

[2] Saito, N. and Iba, Y. (2010): Probability of graphs with large spectral gap by multicanonical Monte Carlo, arXiv:1003.1023.

[3] Yanagita,T, and Iba, Y. (2009): Exploration of order in chaos using the replica exchange Monte Carlo method, Journal of Statistical Mechanics, P02043.

[4] Kitajima, A. and Iba, Y. (2010): Multicanonical sampling of rare trajectories in chaotic dynamical systems, arXiv:1003.2013.

[5] Hukushima, K. and Iba, Y. (2008): A Monte Carlo algorithm for sampling rare events: Application to a search for the Griffiths singularity, Journal of Physics: Conference Series, 95, 012005.

Title: Error Estimation and Reduction with Cross Correlations

Authors: Martin Weigel[1] and **Wolfhard Janke**[2]

Affiliation:

1. University of Mainz, Germany

2. University of Leipzig, Germany

Abstract:

Besides the well-known effect of autocorrelations in time series of Monte Carlo simulation data resulting from the underlying Markov process, using the same data pool for computing various estimates entails additional cross correlations. This effect, if not properly taken into account, leads to systematically wrong error estimates

for combined quantities. Using a straightforward recipe of data analysis employing the jackknife or similar resampling techniques, such problems can be avoided. In addition, a covariance analysis allows for the formulation of optimal estimators with often significantly reduced variance as compared to more conventional averages. The basic ideas will be illustrated for finite-size scaling analyses of the two- and three-dimensional Ising model.

M. Weigel and W. Janke, Cross Correlations in Scaling Analyses of Phase Transitions, Phys. Rev. Lett. 102, 100601-1–4 (2009) [arXiv:0811.3097] (see also Phys. Rev. Lett. Highlights Synopsis of April 13, 2009);

M. Weigel and W. Janke, Error Estimation and Reduction with Cross Correlations, Phys. Rev. E81, 066701-1–15 (2010) [arXiv:1002.4517].

Title: Microscopic model of carbonaceous nanoporous molecular sieves - anomalous transport in molecularly confined spaces

Authors: **Piotr Kowalczyk**

Affiliation: Applied Physics, School of Applied Science, RMIT University, P.O. Box 2476V, 3001 Victoria, Australia

Abstract:

To model the equilibrium and transport properties of carbonaceous molecular sieves (CMS) the new microscopic turbostratic carbon pore model (TCPM) is developed. Analysis of experimental Gibbs excess of methane adsorption on Shirasagi CMS 3K-161 at 298 K indicates that investigated CMS is structurally heterogeneousss material (i.e., it is composed of slit-shaped and turbostratic carbon nanopores of different sizes). Predicted absolute methane isotherm, total pore volume of 0.22 cm^3 g^{-1}, enthalpy of methane adsorption of 17.5-18.6 kJ mol^{-1} on Shirasagi CMS 3K-161 at 298 K are in good agreement with existing experimental and theoretical data. Applying TCPM, we model the equilibrium and kinetic separation of hydrogen and methane mixtures adsorbed in CMS turbostratic carbon nanopores at infinite dilution and 194.7, 293.2, 313.2, 423.2, and 573.2 K. We found that near ambient temperatures one can reach equilibrium selectivity of methane over hydrogen (CH_4/H_2) of 10^2 in the turbostratic carbon nanopores having effective cage sizes of ≈ 5 Å. Lowering an operating temperature down to the dry ice one, increases the equilibrium CH_4/H_2 selectivity in these nanopores up to 10^3. The kinetic selectivity of hydrogen over several investigated fluids, including: methane, argon, xenon, nitrogen, and carbon dioxide at studied operating conditions does not depend on the size of the carbon nanopore cage. This simply means that kinetic separation factor is controlled by the size of the carbon nanopore constriction. Taking this into account, we predicted the effective size of the carbon nanopore constriction of real CMS from the experimentally measured kinetic H_2/CH_4 selectivities at infinite dilution. The high kinetic H_2/CH_4 selectivity of 10^2-10^3 corresponds to the effective size of the carbon nanopore constriction of ≤ 2.958 Å(i.e., lower or equal to the collision diameter of hydrogen molecule). However, decreasing/increasing of the effective size of the carbon nanopore constriction by ≈ 0.1–0.2 Åexponentially increases/decreases kinetic H_2/CH_4 separation factor.

Title: The event-chain algorithm and the melting transition for two-dimensional hard spheres

Author: **Werner Krauth**

Affiliation: Laboratoire de Physique Statistique, Ecole Normale Superieure, Paris, France.

Abstract:

I discuss cluster Monte Carlo algorithms for hard-sphere systems, especially the event-chain algorithm, which moves long chains of particles without any rejection. This powerful method was used for large-scale simulations of two-dimensional hard disks. I will discuss convergence criteria for this system, and show fully converged samples of hard disks which leave no doubt that this system undergoes a Kosterlitz-Thouless transition with a hexatic phase sandwiched in between the liquid and the solid.

Title: Exploring Complex Free Energy Landscapes with Wang-Landau Sampling

Author: **David Landau**

Affiliation: Department of Physics and Astronomy, University of Georgia, USA.

Title: Parallel Tempering and Population Annealing for Rough Free Energy Landscapes

Author: **Jon Machta**

Affiliation: University of Massachusetts Amherst and Santa Fe Institute, USA

Abstract:

I will describe parallel tempering (replica exchange Monte Carlo) and discuss its efficiency for various free energy landscapes. For some simple model free energy landscapes, the performance of parallel tempering can be analyzed and the results highlight strengths and weaknesses of the method. I will also discuss population annealing, a related algorithm for glassy systems introduced by Iba and Hukushima, and contrast it to parallel tempering. Applications to spin glasses will be discussed.

Title: Monte Carlo simulations of (quasi) constrained ensembles

Author: **Víctor Martín-Mayor**

Affiliation: Universidad Complutense de Madrid, Spain

Abstract:

The standard Monte Carlo simulation of systems displaying metastability is very inefficient, (think of first-order phase transitions, spin glasses, structural glasses, lattice polymers, etc.). One may use constrained statistical ensembles in order to guide the simulation inside those rare but crucial regions where it does not want to get into. We combine a generalization of Lustig's microcanonical Monte Carlo with a fluctuation-dissipation formalism. Thermodynamic integration allows for an accurate reconstruction of the effective potential. Cluster algorithms can sometimes be made to work within this framework. In the context of the Statistical Mechanics of disordered systems, this approach amounts to a redefinition of the quenched average in terms of an effective potential, rather than Gibb's free energy. This choice automatically cures the rare-events syndrome that has hampered progress for quite a long time.

Title: Low-rank updates in statistical physics applications

Author: **Phani Nukala**

Affiliation: Oak Ridge National Laboratory, USA

Abstract:

This paper presents efficient low-rank updating algorithms for a variety of materials science and statistical physics applications. In particular, we present efficient algorithms for (1) simulating fracture of disordered materials, (2) modeling colossal magnetoresistance effect in manganites using spin-fermion models, (3) describing strongly correlated systems using the Hubbard model, and (4) describing many-body problems using Quantum Monte Carlo (QMC). These algorithms are based on low-rank updating of underlying linear algebra problem and result in significant computational savings often in the range of three to ten times faster than competing algorithms.

References:

1) P.K.V.V. Nukala et al, Fast Update Algorithm for the Quantum Monte Carlo Simulation of the Hubbard Model, Phys. Rev. B (in print)

2) P.K.V.V. Nukala and P. Kent, A Fast Algorithm for Slater Determinant Updates in Quantum Monte Carlo Simulations, Journal of Chemical Physics 130(20), 204105 (2009).

3) G. Alvarez, P. K. V. V. Nukala, and E. D'Azevedo, Fast diagonalization of evolving matrices: Application to Spin-Fermion Models, J. Stat. Mech.: Theory and Experiment P08007 (2007).

Title: Hybrid Reverse Monte Carlo Modelling of Disordered Materials

Author: **G. Opletal**, S. Russo and I. Snook

Affiliation: Applied Physics, School of Applied Science, RMIT University, Melbourne, Australia

Abstract:

In the construction of models of amorphous materials, the Reverse Monte Carlo modelling methodology,

which traditionally only fits experimental diffraction data, suffers from a lack of uniqueness. For a particular data set, many unphysical atomic configurations are possible. The Hybrid Reverse Monte Carlo (HRMC) method addresses this by incorporating an energetic constraint which ensures realistic local bonding while at the same time fitting to the experimental diffraction data. We discuss applications to amorphous carbon and silicon and the incorporation of a variety of other constraints including porosity and internal surface area.

Title: Efficient calculation of unbiased estimates in diffusion quantum Monte Carlo

Author: **Manolo Per**

Affiliation: Applied Physics, School of Applied Science, RMIT University, Melbourne, Australia

Abstract:

The diffusion quantum Monte Carlo (DQMC) method is a powerful and relatively straightforward technique for calculating quantum mechanical properties of a wide variety of systems at zero temperature. However, expectation values of operators which do not commute with the Hamiltonian exhibit large variances and a systematic bias. Individual solutions to these problems exist but are mutually incompatible. In this talk I will describe a new approach which enables efficient calculation of unbiased estimates in DQMC.

Title: PERM and all that - a comparison of growth algorithms

Author: **Thomas Prellberg**

Affiliation: Queen Mary, University of London

Abstract:

Over the last few years, there have been a variety of growth-like algorithms, such as PERM, IGW, GARM, and GAS. Some of these have been coupled with flat-histogram techniques, resulting in multicanonical PERM, flatPERM, flatIGW.

In this talk we will describe these various algorithms, point out their differences, and discuss their respective strengths.

Title: Dynamic critical behavior of the Wang-Swendsen-Kotecky algorithm for two-dimensional Potts antiferromagnets

Author: **Jesus Salas**

Affiliation: Universidad Carlos III de Madrid, Spain

Abstract:

The phase diagram of the antiferromagnetic q-state Potts model is not universal: it depends, in addition to the number of states q and the dimensionality of the lattice, on the lattice structure. Therefore, one has to study this model on a case-by-case basis. For q large enough, the system is always disordered, even at zero temperature (T=0), and in some cases, there are also critical points at T=0. Monte Carlo simulations provide a fruitful way to investigate this phase diagram, and the (non-local) Wang-Swendsen-Kotecky (WSK) dynamics is one of the algorithms of choice for such simulations. (For non-frustrated systems, WSK contains single-site moves as a particular case.)

In this talk, we briefly review the main properties of the WSK algorithm. For bipartite lattices, it can be proven that WSK satisfies all the required properties to converge to the right probability distribution. For q=3, we provide several examples (on the square, hexagonal, and diced lattices) that demonstrate that the dynamic critical behavior of WSK also depends strongly on the lattice structure of the model. For non-bipartite lattices, we show that the WSK algorithm for the q=4 model on the triangular lattice and the closely related q=3 model on the kagome lattice are non-ergodic at T=0. (This also implies that single-site dynamics is non-ergodic at T=0.) Therefore, new Monte Carlo algorithms are needed for such systems.

Title: Stochastic Cutoff Method for Long-Range Interacting Systems

Authors: **Munetaka Sasaki** and Kazuya Watanabe

Affiliation: Tohoku University, Japan

Abstract:
In this work, we present an efficient Monte-Carlo (MC) method called stochastic cutoff method for long-range interacting systems. This method enables us to reduce the computational time per MC step from O(N^2) to O(N) (or O(N log N)) without any approximation, where N is the number of elements. The efficiency of the method is demonstrated by applying it to magnetic dipolar systems. We also show how this method is combined with other MC methods such as the replica exchange method and the Wang-Landau method.

Title: Hard Sphere Liquids in Complex Pores
Author: **G.E. Schröder-Turk**, S. Kuczera, R. Roth and K. Mecke
Affiliation: Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany
Abstract:
The thermodynamic properties of fluids confined in topologically and geometrically complex pores depend on the shape of the confining geometry. Here we use grand-canonical Monte Carlo simulation to compute equilibrium densities η of a hard sphere fluid confined to pores given by triply-periodic minimal and constant-mean-curvature surfaces, sufficiently far from the fluid's critical point. We show that the MC simulation results and DFT results are in agreement with a morphometric theory which assumes that thermodynamic potentials are additive w.r.t. the pore shape and can hence be expressed as a linear combination of volume, interface area, integrated mean curvature and Euler index of the pore.

Title: Effective potential study of hard-spheres crystallization
Author: **Beatriz Seoane**
Affiliation: Universidad Complutense de Madrid, Spain
Abstract:
We use tethered Monte Carlo to study the fluid-solid phase transition in hard spheres at constant pressure. Tethered Monte Carlo features directly the effective potential by simulation of constrained statistical ensembles. In order to avoid metastabilities, we have found it crucial to constraint the values of two crystalline order parameters, namely Q_6 and C. Parameter Q_6 is the standard rotationally-invariant bond-ordering parameter and C is a variation of Q_6 which is only invariant with respect to the cubic group, thus allowing us to determine the alignment of the crystal planes. A sort of Maxwell construction yields the critical pressure and the densities of the coexisting phases. In the system sizes explored so far, up to N=864 particles, exponential critical slowing-down is not present. Note that state-of-the-art methods, such as phase-switch Monte Carlo, nowadays seem limited to N=500 due to strong exponential critical slowing-down.

Title: The observation of formation and annihilation of solitons and standing strainwave superstructures in a two-dimensional colloidal crystal
Authors: **Ian K. Snook**,[1] Yu-Hang Chui,[2] Surajit Sengupta,[3,4] and Kurt Binder[2]
Affiliation:
1. Applied Physics, School of Applied Science, RMIT University, P.O. Box 2476V, 3001 Victoria, Australia
2. Institute of Physics, Johannes-Gutenberg University, D-55099 Mainz, Staudinger Weg 7, Germany
3. Indian Association for the Cultivation of Science, Centre for Advanced Materials, Jadavpur, Kolkata 700032, India
4. S. N. Bose National Centre for Basic Science, Block JD, Sector III, Salt Lake, Kolkata 70098, India
Abstract:
Confining a colloidal crystal within a long narrow channel produced by two parallel walls can be used to impose a mesoscale superstructure of a predominantly mechanical elastic character. When the crystal is compressed in the direction perpendicular to the walls, we obtain a structural transition when the number of rows of particles parallel to the walls decreases by one. All the particles of this vanishing row are distributed throughout the crystal. If the confining walls are structured (say with a corrugation along the length of the walls), then these extra particles are distributed neither uniformly nor randomly; rather, defect structures are

created along the boundaries resembling "soliton staircases", inducing a nonuniform strain pattern within the crystal. Here, we study the conditions of stability, formation, and annihilation of these solitons using a coarse grained description of the dynamics based on the Monte Carlo method. The processes are shown by comparing superimposed configurations as well as molecular animations obtained from our simulations. Also, the corresponding normal and shear stresses during the transformation are calculated. A study of these dynamical processes should be useful for controlling strain wave superstructures in the self-assembly of various nano- and mesoscaled particles.

Title: Overcoming critical slowing-down: Where do we stand 23 years after Swendsen and Wang?

Author: **Alan Sokal**

Affiliation: Department of Physics, NYU, USA

Abstract:

I begin by reviewing the Swendsen-Wang algorithm for ferromagnetic q-state Potts models — and its extension to noninteger q due to Chayes and Machta — and our current state of knowledge about these algorithms' dynamic critical behavior. I then discuss recent results concerning the dynamic critical behavior of Sweeny's local algorithm for the random-cluster model, notably the surprising phenomenon of critical speeding-up. Finally, I discuss similar but more complicated phenomena in the worm algorithm for the ferromagnetic Ising model.

Title: Markov Chain Monte Carlo without Detailed Balance and Bounce-free Worm Algorithm

Author: **Hidemaro Suwa**

Affiliation: Department of Applied Physics, the University of Tokyo, Japan

Abstract:

In the Markov chain Monte Carlo method, the detailed balance is usually imposed as a sufficient condition for the balance condition. If the Markov sequence goes beyond the detailed balance, however, rejection rates can get minimized. Although it has been considered to be difficult to generally construct a transition matrix beyond the detailed balance, we have invented a new Monte Carlo algorithm that surely makes it possible with minimized rejection rates. As a benchmark, we have confirmed that our algorithm significantly boosts up the relaxation speed in 4-state Potts model to nearly 7 times more than the heat bath algorithm and 30 times more than the Metropolis algorithm. In the same manner, we have also developed a bounce-free worm algorithm in the quantum Monte Carlo method. In one dimensional Heisenberg model with magnetic field, it is confirmed that the relaxation by the bounce-free worms gets about 50 times faster than by the conventional method called the generalized directed-loop.

Title: Simulating spin models on GPU

Authors: **Martin Weigel**

Affiliation: Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Germany

Abstract:

Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses.

In this presentation I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards- Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis [1] and cluster updates [2], as well as computional tricks such as multi-spin coding are taken into account.

References

[1] M. Weigel, Performance potential for simulating spin models on GPU, Mainz preprint (2010).

[2] M. Weigel, Cluster update simulations of spin models on GPU, Mainz preprint (2010).
[3] M. Weigel, Simulating spin models on GPU, Preprint arXiv:1006.3865.

Title: The low-temperature phase of Ising spin glasses: parallel-tempering simulations with sample-dependent thermalisation on the Janus computer

Author: **David Yllanes**

Affiliation: Universidad Complutense de Madrid, Spain

Abstract:

We have performed a large-scale equilibrium simulation of the three-dimensional Ising spin glass at low temperatures, achieving thermalisation for lattices up to L=32 at temperatures as low as T=0.64Tc. This has been possible thanks to the Janus supercomputer, a custom-built massively parallel machine designed specifically for Monte Carlo simulations, which outperforms conventional computers by several orders of magnitude (during the whole simulation campaign we performed a total of 10^{20} spin updates, which we believe is a record). Since the energy landscape of the Ising spin glass at such low temperatures is extremely complicated, parallel tempering is employed to accelerate equilibration. In this kind of simulations one typically takes the same number of Monte Carlo steps for each sample and studies the quality of the thermalisation through the time evolution of disorder averages. However, relaxation times vary wildly (several orders of magnitude) from one sample to another, so this usual simulation strategy is suboptimal. In this talk I will show how to use the random walk in temperature space during the parallel-tempering process to assess thermalisation on a sample-by-sample basis. This is more efficient than simulating all samples for a very long time and safer, too, because it exposes thermalisation biases that can be concealed by the disorder average.

We demonstrate the relevance of equilibrium finite-size simulations to understand experimental non-equilibrium spin glasses in the thermodynamical limit by establishing a time-length dictionary. We conclude that non-equilibrium experiments performed on a time scale of one hour can be matched with equilibrium results on L=110 lattices.

Title: Monte Carlo Simulations of Heisenberg Spin Glasses

Author: **Peter Young**

Affiliation: University of California Santa Cruz, USA

Abstract:

Whereas most numerical studies on spin glasses have focussed on the Ising case, since this is the simplest, there are new features associated with vector spin glasses which need to be elucidated. Here I will discuss results of simulations on 3-component (Heisenberg) spin glasses. Equilibration is hard at low temperatures because of the "many-valley" energy landscape, and so, as with the Ising case, the method of "parallel tempering" is used to speed things up. From a computational perspective, there are two surprises. The first is that, although the code to update a spin is much more complicated and hence more time consuming than that for the Ising case, one can actually equilibrate much larger sizes for the Heisenberg spin glass, indicating that the barriers between valleys are smaller for Heisenberg spin glasses. Presumably vector spins can, to some extent, go round barriers rather than over them. The second surprise is that adding "overrelaxation" moves, introduced initially just because they are simpler and hence execute more quickly than "heatbath" moves, equilibrates the system much more efficiently than if one had just heatbath moves. I will also discuss some of the physics results that have emerged from these simulations.

Title: Kinetic Monte Carlo Modelling of Pt on Au (111) in Bimetallic Catalysis

Authors: **P. Zoontjens**, G. Grochola, S. Russo and I. Snook

Affiliation: Applied Physics, School of Applied Science, RMIT University, P.O. Box 2476V, 3001 Victoria, Australia

Abstract:

Catalytically active nanoparticles play significant roles in electrocatalysis [1]. Pt is of considerable interest as it catalyses the oxidation of methanol, which is a very promising fuel cell reaction [2]. Also, Pt is a catalyst

for many other technologically important reactions [3].

It has recently been shown that PtAu nanoparticles can act as efficient nanocatalysts for formic acid oxidation [4]. Furthermore, bimetallic PtAu nanoparticles have been shown to function as electrocatalysts for the oxygen reduction reaction [5]. Nanoparticles such as these have potential applications in fuel cells with the advantage of minimising the amount of Pt required.

In view of these results we are led to consider other Pt on Au nanostructures as possible nano catalysts. We investigate by simulation, the creation of extended Pt nanostructures on an Au surface via a physical deposition process. Extended structures maximise the surface area of the deposited Pt which is positively correlated with catalytic activity.

The low energy and low flux deposition of Pt adatoms onto an Au (111) surface, which incorporated a mono layer Au island, was studied. The Au island acts as a template for the organisation of extended structures composed of the deposited Pt atoms, which are trapped by the island edge. These structures form as a result of long time scale diffusion processes, which are impractical to simulate with Molecular Dynamics (MD). Consequently we use the Kinetic Monte Carlo (KMC) method to study the development of Pt nanostructures on Au. The ability to alter the morphology of the Pt nanostructures by varying the readily controlled parameters of temperature and deposition rate was studied.

REFERENCES

[1] M L Satter and P N Ross. Ultramicroscopy, 20 21, (1986).

[2] K R Williams. An Introduction to Fuel Cells, Elsevier, (1966).

[3] J M Chapuzet, A Laisa and J Lessard. Electrocatalysis, WileyVCH, (1998).

[4] N Kristian, Y Yan and X Wang. Chem. Comm., 353355, (2008).

[5] P Hernandez Fernandez, S Rojas, P Ocon, J L Gomez de la Fuente and J San Fabian. J. Phys. Chem. C, 111(7), 29132923, (2007).