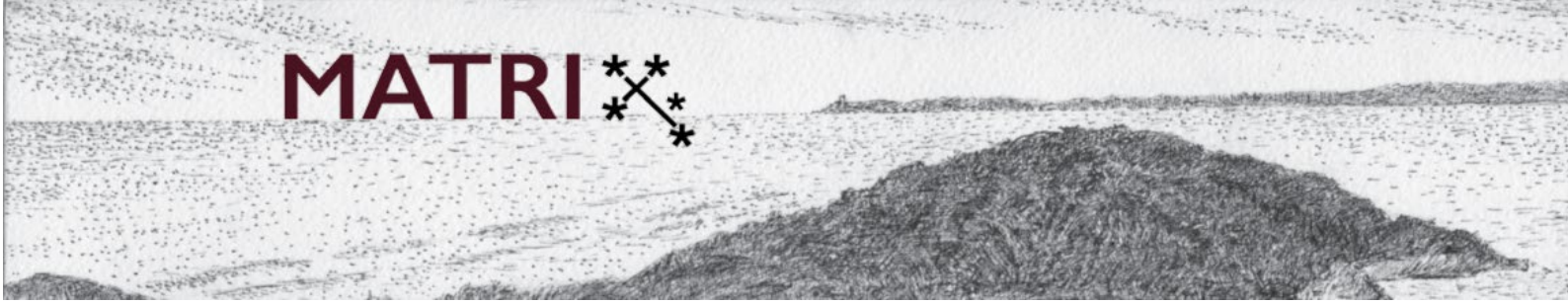
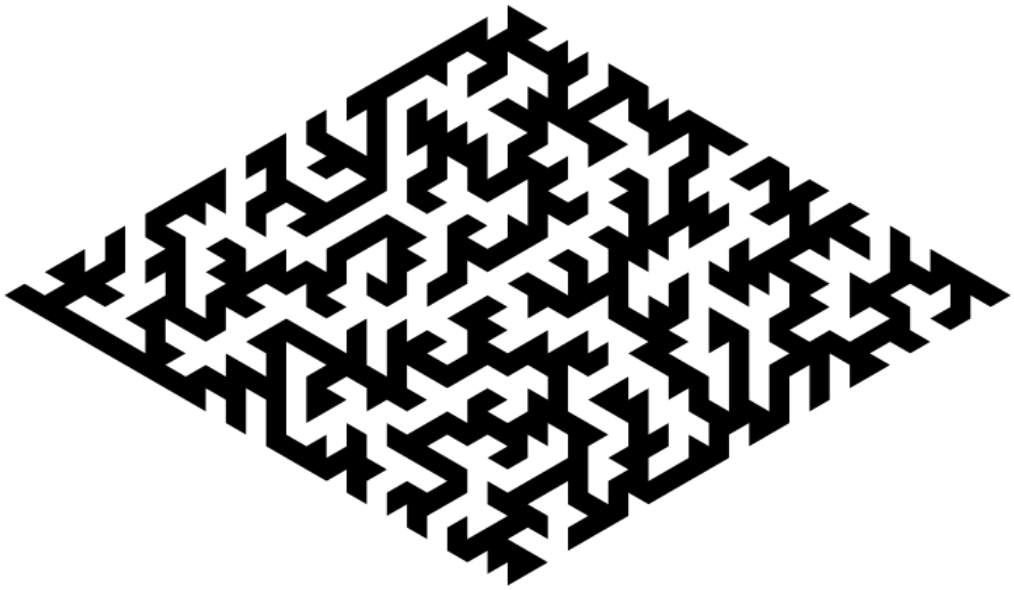


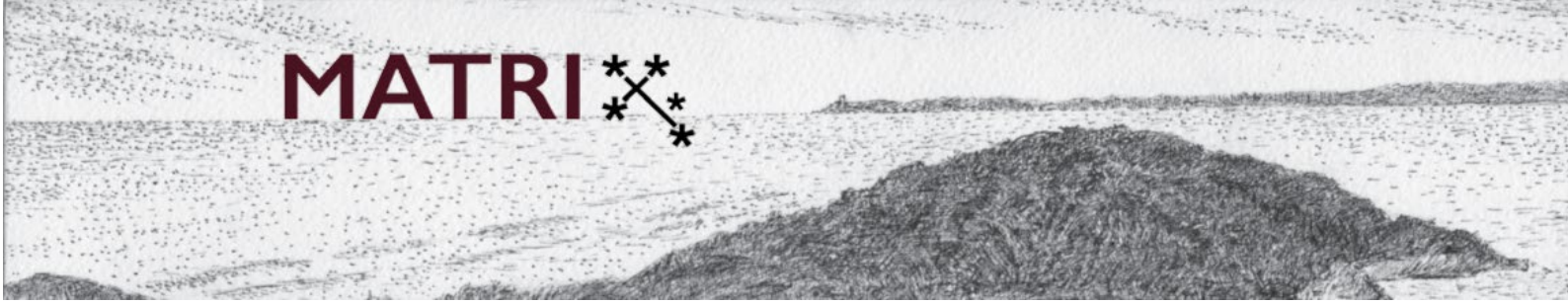

## MATRIX Research Program:

# Monte Carlo Algorithms in Statistical Mechanics



## Talks - Titles & Abstracts

**26 June – 7 July 2023**
**MATRIX, Creswick**




# Talk Titles and Abstracts

**Speaker:** David Landau

**Titles:** Insights from Monte Carlo Simulations: Yesterday, Today, and Tomorrow

**Speaker:** Catherine Greenhill

**Titles:** Triangle switches, reconstruction and mixing

**Abstract:** In a uniformly random graph with a given degree sequence, if the maximum degree is constant then the number of triangles in the graph is asymptotically Poisson with constant mean. In particular, this implies that a uniformly random graph is not well-suited as a model for a network which contains many triangles, such as a social network.

**Speaker:** Nick Beaton

**Titles:** Lattice models of theta-shaped polymers and other branching structures

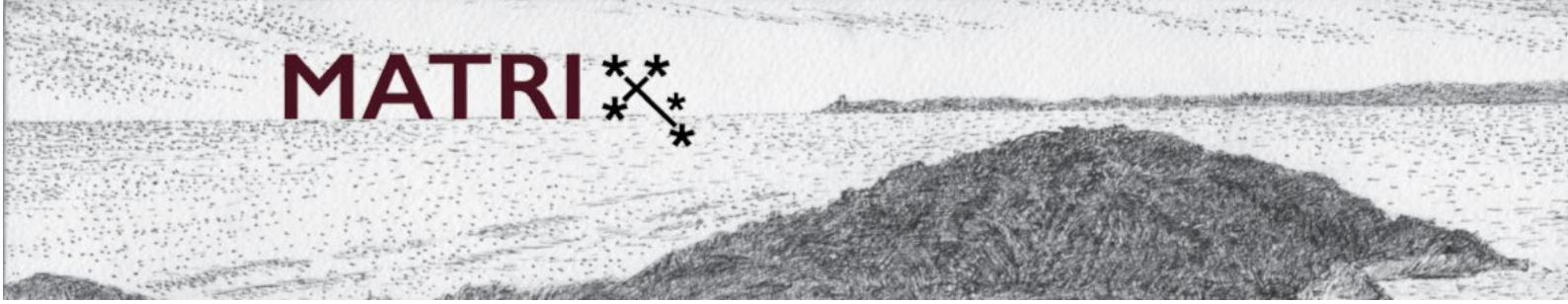
**Abstract:** We implement a new version of the BFACF algorithm combined with the Wang-Landau method to sample lattice polymers with a theta shape. The initial goal is to understand how the three "arms" scale in length, and if this resembles the scaling of a large knotted polygon in dilute solution. Other shapes like "tadpoles" are also studied.

This is joint work (still in progress) with Aleks Owczarek and James Gleeson.

**Speaker:** Mikhail Isaev

**Titles:** High-order Laplace approximations for the number of Eulerian orientations

**Abstract:** An Eulerian orientation is an orientation of edges of a graph such that every vertex is balanced: the in-degree equals the out-degree. Counting Eulerian orientations corresponds to the crucial partition function in so-called "ice-type models" in statistical physics and is known to be hard for general graphs. There is a reduction to enumeration perfect matchings for a class of graphs for which the Markov Chain Monte Carlo method applies. In this work, for graphs with good expansion properties, we derive an asymptotic formula for approximating this count up to a multiplicative error $O(n^{-c})$, where $c$ is an arbitrary fixed constant. Using the Laplace method, we estimate the number of Eulerian orientations via cumulants of a polynomial of Gaussian random variables. The proof relies on the new tail bound for the cumulant expansion series, which is of independent interest.




**Speaker:** Werner Krauth

**Titles:** Non-reversible Markov chains: From the TASEP to applications in chemical physics

**Abstract:** I discuss recent developments in the theory and practice of Markov chains.

**Speaker:** Antonio Blanca

**Titles:** Sampling from the ferromagnetic Potts model on random graphs

**Abstract:** We present new mixing time bounds for the Glauber dynamics of the random-cluster model for a general family of random graphs that includes random regular graphs and the classical Erdos-Renyi model. Our results reveal a novel and significant computational advantage of random-cluster-based algorithms for sampling from the Potts distribution at high temperatures. Namely, in the presence of high-degree vertices, random-cluster Markov chain mix quickly in near-linear time, but standard Potts Markov chains may require exponential (in the max degree) time to mix. We also provide generic conditions that imply fast mixing of the Glauber dynamics at low temperatures.

**Speaker:** Manon Michel

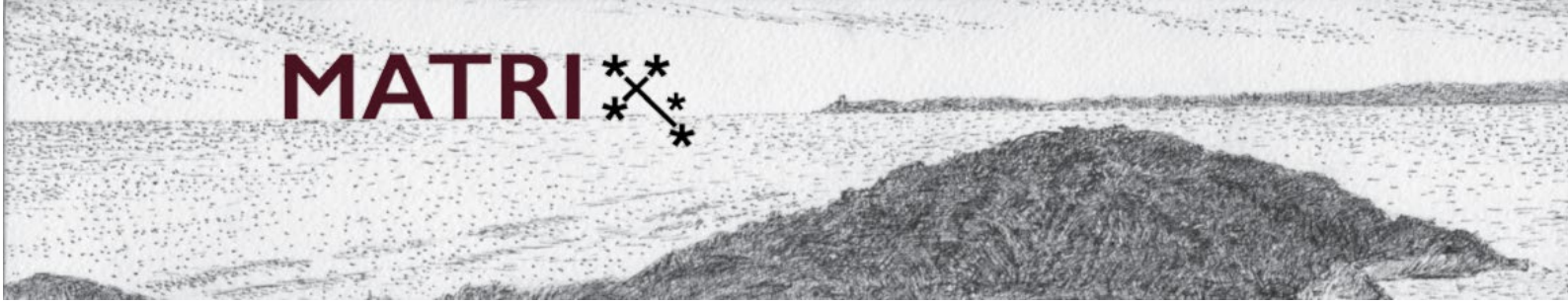
**Titles:** Non-reversible and continuous-time MCMC by piecewise deterministic markov processes

**Abstract:** Since the beginning of MCMC sampling and the Metropolis algorithm introduction, constant efforts have been made on developing fast Markov chains which do not present any diffusive behavior while sampling the correct distribution. However, almost all of the developed schemes are reversible, obey detailed balance and rely on rejections to achieve the correct invariant distribution. During this talk, I will present how the exploitation of system symmetries allows to break detailed balance, while satisfying the necessary condition of the global one. This leads to the design of continuous-time and non-reversible Markov processes, which, being rejection-free, display interesting dynamical properties. First known as Event-Chain Monte Carlo algorithms, these processes can actually be characterized as Piecewise Deterministic Markov Processes (PDMP). I will then discuss how this powerful characterization allows to probe deeper what is necessary from what is actually sufficient to achieve a correct exploitation and how it can be exploited for algorithmic design.

**Speaker:** Stefan Schnabel

**Titles:** Long Lennard-Jones polymers at the Theta-point

**Abstract:** Polymers in dilute solution undergo a phase transition from extended random coils to collapsed globules when the solvent changes from good to bad. At the critical (Theta) point the polymer behaves on large enough scales like an ideal chain or a pure random walk. Renormalization group calculations predict logarithmic corrections to scaling which so far have not been confirmed




by computer simulation or experiment. The main challenge is that very long chains have to be considered, a feat that has only been possible for systems on lattice geometries.

Recently [1] we devised a Monte Carlo method for the simulation of long off-lattice polymers with untruncated interaction. It allows for the simulation of polymers with ten thousands of fully interacting repeat units. Here, we determine the Theta-temperature and investigate the scaling properties at the critical point of a bead-stick polymer model whose monomers (beads) interact pairwise via a Lennard-Jones potential.

[1] S. Schnabel and W. Janke, Comput. Phys. Commun. 256, 107414 (2020).

**Speaker:** Xusheng Zhang

**Titles:** The Chayes-Machta dynamics for the mean-field random-cluster model at the critical point

**Abstract:** Markov Chain Monte Carlo (MCMC) sampling algorithms have been intensively studied for the use of sampling from probabilistic models. Despite their simplicity and wide use in practice, the efficiency of this approach was often not rigorously examined. It is not uncommon that the rates of convergence (i.e., mixing time) of a well-known Markov chain is not clear from the theoretical perspective. We focus on a specific Markov chain called the Chayes-Machta dynamics for the random-cluster model. The random-cluster model is a probabilistic model that has applications in random graphs, spin systems, and other combinatorial distributions. The Chayes-Machta dynamics is a non-local Markov chain associated with the random-cluster model. We provide a nearly optimal bound for the mixing time of the mean-field Chayes-Machta dynamics in the only regime of parameters where no non-trivial bound was previously known.

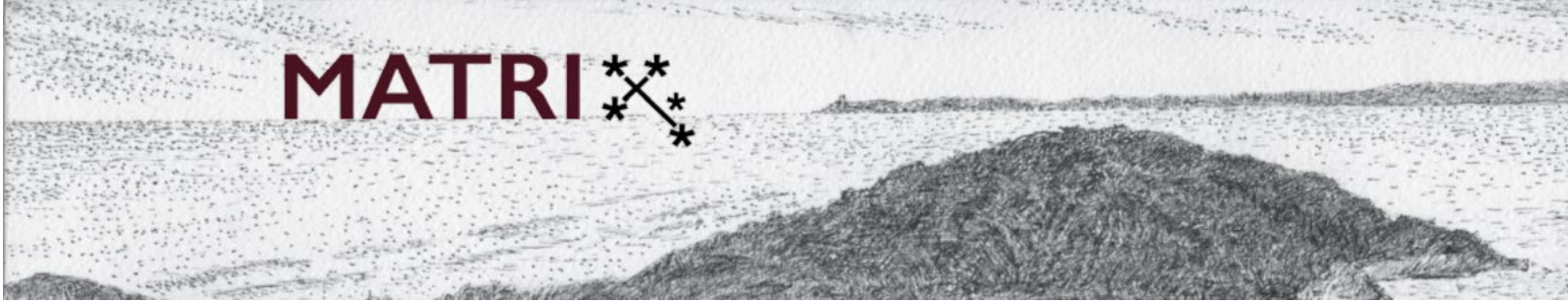
**Speaker:** Wolfhard Janke

**Titles:** Thermodynamically Stable Knots in Semiflexible Polymers

**Abstract:** Semiflexible polymers are widely used as a paradigm for understanding struc-

tural phases in biomolecules including folding of proteins. As function of temperature and bending stiffness they exhibit a rich phase structure. Here, we compare bead-stick and bead-spring homopolymer models that cover the whole range from flexible to stiff and, by employing extensive replica-exchange Monte Carlo simulation, focus on phases with stable knots. We find that the presence of stable knots in the phase diagram is dependent on the ratio rb/rmin where rb is the equilibrium bond length and rmin the distance for the strongest nonbonded contacts. For both models, our results provide evidence that if the ratio rb/rmin is outside a small window around unity, then depending on the bending stiffness, one always encounters stable knotted phases along with the usual frozen and bent-like structures at low temperatures. These findings prompt us to conclude that knots are generic stable phases in semiflexible polymers.

[1] S. Majumder, M. Marenz, S. Paul, and W. Janke, Macromolecules 54, 5321–5334 (2021).




**Speaker:** Martin Weigel

**Titles:** News from population annealing: From weighted averages to quantum Monte Carlo

**Abstract:** Population annealing is a generalized-ensemble Monte Carlo simulation algorithm that proves useful for the simulation of systems with complex free-energy landscapes and that offers superior parallelizability properties.

As a meta-algorithm, population annealing can be combined with a wide range of simulation methods, including Monte Carlo and molecular dynamics. In the past, we have analyzed the approach regarding the scaling of statistical and systematic errors, proposed improvements and implemented the method on highly-efficient graphics processing units. In the present talk I will discuss recent developments regarding the optimal choice of the resampling protocol and the combination of several population annealing simulations using weighted averages.

Finally, I will discuss a combination of population annealing with quantum Monte Carlo simulations.

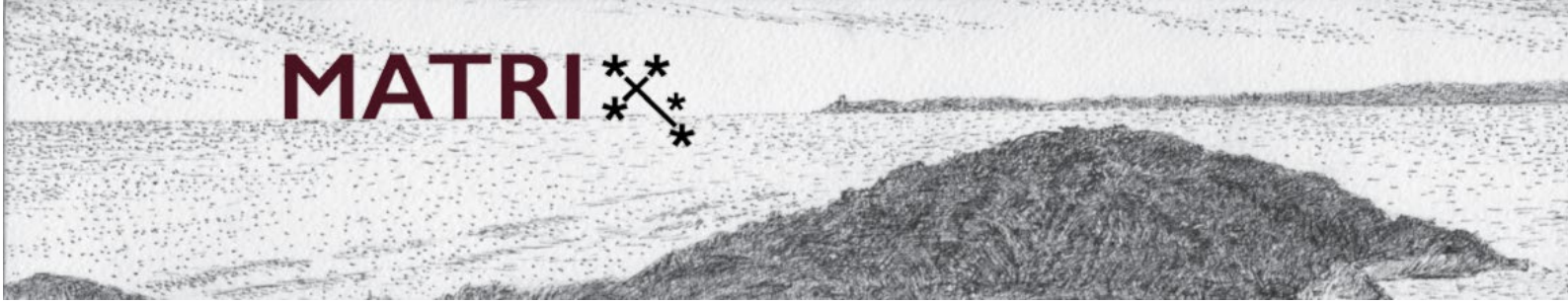
**Speaker:** Philipp Höllmer

**Titles:** Molecular simulation from modern statistics: Continuous-time, continuous-space, exact

**Abstract:** Classical molecular simulations are widespread in molecular sciences to study, e.g., protein folding. Here, chemical systems are modeled empirically by a set of atomic positions with parameterized interaction potentials. In this talk, we develop a modern-statistics paradigm for thermodynamic averages in classical molecular simulations based on efficient non-reversible and rejection-free Markov-chain Monte Carlo methods. It is an alternative to the thermostatted molecular-dynamics (MD) approach. In MD, a symplectic integrator combined with a sensible choice of the finite time step leads to long-time stability of the trajectories with a bounded error on conserved quantities. Still, there can be undesirable artifacts for many reasons that were understood and overcome in a rich literature over the last decades. Examples include too large time steps, ergodicity problems because of MD's deterministic nature, thermostats that only approximately generate the canonical ensemble, and too inaccurate evaluation of long-range forces. In this talk, we present the alternative modern-statistics paradigm, which is approximation-free from the very start and treats all short- and long-range interactions numerically exact. We explore how the non-reversible event-chain Monte Carlo (ECMC) algorithm samples the equilibrium Boltzmann distribution exactly, although it uses non-equilibrium dynamics and never computes the total system potential. We discuss how ECMC's sole restriction of the global-balance condition yields a great freedom to implement quickly decorrelating dynamics. Finally, we show that the modern-statistics approach has a competitive computational scaling with system size and explores the configuration space efficiently for the example of a long-range-interacting water model.

**Speaker:** Chris Soteros

**Titles:** Monte Carlo methods for studying entanglements in lattice models of polymers under tubular confinement




**Speaker:** Thomas Prellberg

**Titles:** On the universality class of the special adsorption point of two-dimensional lattice polymers

**Abstract:** In 2019 we found evidence that the surface adsorption transition of interacting self-avoiding trails (ISATs) placed on the square lattice displays a non-universal behaviour at the special adsorption point where the collapsing polymers adsorb, with surface exponents depending on the orientation of the surface with respect to the lattice axes. Here, we revisit these systems and study other ones.

Through extensive Monte Carlo simulations, utilising much longer configurations than previously, we can now demonstrate that the different exponents observed earlier are due to the presence of a previously unseen surface-attached-globule (SAG) phase which changes the multicritical nature of the special adsorption point. We confirm this observation by considering other modified surfaces. These results strongly indicate that at least two universality classes exist for the special adsorption point of adsorbing ISATs on the square lattice.

https://arxiv.org/abs/2305.09803

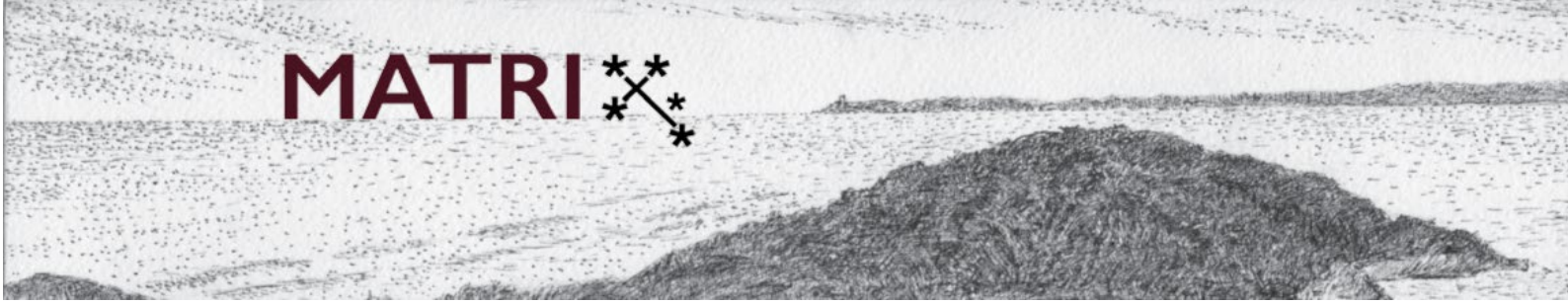
**Speaker:** Matthew Schmirler

**Titles:** Optimizing An Interacting Lattice Polygon Model Using Stochastic Approximation

**Abstract:** The main focus of this talk will be on discussing an application of the Simultaneous Perturbation Stochastic Approximation (SPSA) Algorithm (Spall, 1992), an iterative method which can efficiently optimize parameters for multi-parameter models using Monte Carlo simulation data. At each step in the SPSA algorithm, all parameters are updated simultaneously using a gradient estimated from only two simulations (regardless of the parameter dimension).

The utility of the SPSA algorithm will be exhibited for two equilibrium statistical mechanics models of DNA, where conformations of randomly cyclized DNA in a salt solution are modelled using self-avoiding polygons in the simple cubic lattice. The first model considers a long-range Yukawa potential with a short-range contact potential, an approach first proposed by Tesi et al (1994). The second model uses the same Yukawa potential but replaces the contact potential with another short-range interaction based on bending rigidity. This bending potential is used in discrete worm-like chain models, a popular off-lattice choice for modelling DNA.

The goal of this research is to obtain an improved lattice polygon model for DNA by tuning model parameters to best fit the Shaw and Wang (1993) experimental results for DNA knotting probability as a function of salt concentration. To estimate knot probabilities, samples from the stationary distribution of our models are generated using a two-point pivot Markov Chain Monte Carlo (MCMC) approach. In order to obtain reliable estimates of knotting probabilities, MCMC simulations are sometimes required to run for multiple days. This extreme time cost makes this model a perfect candidate for SPSA; we will show how parameter convergence was obtained for our model in as little as 15 iterations and how the lattice model for DNA has been improved.




**Speaker:** Ying Wai Li

**Titles:** Irreversible Monte Carlo algorithms and its applications to machine learning

**Speaker:** Sarat Moka

**Titles:** Importance Sampling for Estimation of Rare-event Probabilities in Random Graphs.

**Abstract:** Erdös-Rényi graphs and geometric random graphs are two fundamental models for network analysis and spatial networks, respectively. We present a novel method using importance sampling for estimating rare-event probabilities in these graphs. By connecting pairs of nodes randomly, Erdos-Renyi graphs capture network properties, while by placing nodes in a geometric space, geometric random graphs model spatial arrangements. Our approach enables efficient estimation of low-probability events (i.e., rare-events) associated with these networks. Through simulation experiments, we demonstrate the effectiveness of our method.

**Speaker:** Buks van Rensburg

**Titles:** Monte Carlo method for dense confined self-avoiding walks using GAS and PERM

**Speaker:** Eric Zhou

**Titles:** Loop-cluster algorithm and geometric properties of the Ising model in high dimensions

**Abstract:** The Ising model is the most fundamental model in statistical mechanics. Apart from the original spin representation, it is well known there are two geometric representations; one is the 2-state Fortuin-Kasteleyn random-cluster model and the other one is the loop model. The algorithm connects the spin and random-cluster representations is the famous Swendsen-Wang algorithm, which can be well understood using the Edwards-Sokal coupling. In this talk, I will introduce a recently proposed loop-cluster joint model which connects the random-cluster and the loop representations, and the application of the corresponding algorithm to understand the anomalous geometric properties of the Ising model in high dimensions.

**Speaker:** Tim Garoni

**Titles:** The running time of coupling from the past for the Ising Glauber process

**Abstract:** Coupling from the past is a method for obtaining perfect samples from Markov chain Monte Carlo algorithms. The price paid is that the running time becomes random. We will discuss some results concerning the limit behaviour of this running time for the Ising Glauber process on large tori. The strategy employed is to combine compound Poisson approximation with the information percolation machinery of Lubetzky and Sly.