LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN | ARNOLD SOMMERFELD CENTER FOR THEORETICAL PHYSICS

Sommerfeld Theory Colloquium

Wednesday, December 4, 2019
16:15h

Room A 348, Theresienstr. 37, III

Prof. Werner Krauth

Laboratoire de Physique, Ecole normale supérieure
Paris, France

Fast irreversible Markov chains in statistical physics

The Monte Carlo method is an outstanding computational tool in science. Since its origins, it has relied on the detailed-balance condition (that is, the absence of flows in equilibrium) to map general computational problems onto equilibrium-statistical-physics systems.

Irreversible Markov chains violate the detailed-balance condition. They realize the equilibrium Boltzmann distribution as a steady state with non-vanishing flows. For one-dimensional particle models we have proven rigorously that local algorithms reach equilibrium on much faster time scales than the reversible algorithms that satisfy detailed balance. The event-chain Monte Carlo algorithm (ECMC) generalizes these irreversible Markov chains to higher dimensions. It relies on a factorized Metropolis filter which is based on a consensus rule rather than on an energy criterion.

As applications I will briefly discuss our solution of the two-dimensional melting problem for hard disks and related systems. I will then present the use of ECMC for the general classical all-atom N-body problem. Here, the Boltzmann distribution exp(-beta E) is sampled (without any discretization or truncation error) but the potential energy E remains unknown. This is of great interest in the Coulomb problem, where E or its derivatives, the forces, are hard to compute. Our recent JeLLyFysh open-source Python application implements ECMC for models from hard spheres to three-dimensional water systems. I will finish by discussing parallel implementations of event-driven algorithms.

gez. Prof. Ulrich Schollwöck