Coarse-Grained Monte Carlo Simulations of Continuous Systems

XIAO LIU, WARREN SEIDER, TALID SINNO, University of Pennsylvania — Various types of Monte Carlo simulations are used extensively to simulate an enormous range of material properties. Restricting particle positions to fixed lattice sites can substantially increase the computational efficiency of a simulation, and this benefit increases as the lattice becomes coarser. However, the confinement of particle positions to a rigid lattice necessarily reduces the available configurational degrees of freedom in a system and this constraint can become very important at elevated temperatures. In this presentation, we discuss a new framework for performing Metropolis Monte Carlo and kinetic Monte Carlo (KMC) simulations of continuous systems on coarse, rigid lattices, while preserving the phase-space contributions of the missing degrees-of-freedom. The approach relies on the pre-computation of coarse-grained interaction potentials using equilibrium sampling of small systems. The coarse-grained simulation methodologies are shown to reproduce both equilibrium (e.g. phase diagram), and non-equilibrium (e.g. aggregation dynamics) features in the corresponding fully resolved systems. In the latter case, the coarse potential is used to compute rates for moves in a coarse-grained KMC system.

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