419h A Domain Decomposition Based Parallel Monte Carlo Simulation Scheme for Simulations of Very Large Systems

Joydeep Mukherjee, Stephanie L. Teich-McGoldrick, and Sharon C. Glotzer

Monte Carlo simulation methods have been used effectively to understand the thermodynamics of matter. However, calculation of size-independent statistics (thermodynamic limit) requires performing Monte Carlo simulations of very large systems, which may pose prohibitively high CPU time and memory requirements. To study the self-assembly of nanoparticle systems, we apply an efficient domain over-decomposition based parallel Monte Carlo scheme that overcomes such hardware limitations and allows the study of very large systems. The algorithm is particularly suited for systems with short-range interactions as in the self-assembly of nanoparticle systems and colloidal systems with screened charge interactions. We shall present our implementation of this algorithm on our Apple G5 computing cluster. Issues of load balancing and scalability of this algorithm with increasing system sizes will be discussed.