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**Spatial Grand Canonical Monte Carlo Algorithms for Fluid Simulation** RUICHAO REN, C.J. O'KEEFFE, GERASSIMOS ORKOULAS, UCLA — Strict detailed balance is essentially unnecessary for Markov chain Monte Carlo simulations to converge to equilibrium. Recently, we proposed a general Monte Carlo algorithm based on sequential updating that only satisfies the weaker balance condition. We have shown analytically that the new algorithm identifies the correct equilibrium distribution of states. Analysis of the diagonal elements of the transition matrices shows that the new algorithm is more mobile than the conventional Metropolis algorithm. Monte Carlo simulations of the Ising model and the lattice gas show that the new algorithm reduces autocorrelation time and thus improves the statistical quality of sampling. By exploiting the equivalence of the Ising model and the lattice gas, we demonstrate that the new method can also be applied to continuum systems, such as Lennard-Jones, in the grand canonical ensemble. Potential applications of the new algorithm are simulations of 1st and 2nd order phase transitions. Any massively parallel Monte Carlo simulation based on spatial decomposition involves simultaneous moves of atoms/molecules on multiple CPUs. Parallel Monte Carlo simulations based on spatial decomposition suffer from loss of precision due to the periodic switching of active domains. On the other hand, our algorithms are intrinsically sequential, and can be parallelized easily without compromising precision.

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