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A novel Kinetic Monte Carlo algorithm for Non-Equilibrium Simulations PRATEEK JHA, Northwestern University, VLADIMIR KUZOVKOV, University of Latvia, BARTOSZ GRZYBOWSKI, MONICA OLVERA DE LA CRUZ, Northwestern University — We have developed an off-lattice kinetic Monte Carlo simulation scheme for reaction-diffusion problems in soft matter systems. The definition of transition probabilities in the Monte Carlo scheme are taken identical to the transition rates in a renormalized master equation of the diffusion process and match that of the Glauber dynamics of Ising model. Our scheme provides several advantages over the Brownian dynamics technique for non-equilibrium simulations. Since particle displacements are accepted/rejected in a Monte Carlo fashion as opposed to moving particles following a stochastic equation of motion, nonphysical movements (e.g., violation of a hard core assumption) are not possible (these moves have zero acceptance). Further, the absence of a stochastic "noise" term resolves the computational difficulties associated with generating statistically independent trajectories with definitive mean properties. Finally, since the timestep is independent of the magnitude of the interaction forces, much longer time-steps can be employed than Brownian dynamics. We discuss the applications of this scheme for dynamic self-assembly of photo-switchable nanoparticles and dynamical problems in polymeric systems.

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