Do Your Hard-Spheres Have Tails? A Molecular Dynamics Integration Algorithm for Systems with Mixed Hard-Core/Continuous Potentials

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Abstract

Integration algorithms for molecular-dynamics simulation generally fall into two mutually exclusive classes: those for purely collisional systems, such as hard spheres, and those for continuous potentials. However, there exist theoretically important model systems, such as the restricted primative model for electolytes, that have both collisional and continuous potential components and for which no satisfactory molecular dynamics algorithm has been developed. For this reason simulation studies of such systems have been limited to Monte Carlo studies, which give no information as to dynamical properties. We present a new molecular-dynamics algorithm for integrating the equations of motion for a system of particles interacting with mixed continuous/impulsive forces. This method, which we call Collision Verlet, is constructed using operator splitting techniques similar to those that have been used successfully to generate a variety molecular-dynamics integrators . In numerical experiments, the Collision Verlet method is shown to be superior to previous methods with respect to stability and energy conservation in long simulations.

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