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Discontinuous Molecular Dynamics for Rigid Bodies: Applications. S. OPPTS, Univ. of Prince Edward Island, L. HERNANDEZ DE LA PENA, R. VAN ZON, J. SCHOFIELD, Univ. of Toronto — Event-driven molecular dynamics simulations are carried out on two rigid body systems which differ in the symmetry of their molecular mass distributions. First, simulations of methane in which the molecules interact via discontinuous potentials are compared with simulations in which the molecules interact through standard continuous Lennard-Jones potentials. It is shown that under similar conditions of temperature and pressure, the rigid discontinuous molecular dynamics method reproduces the essential dynamical and structural features found in continuous-potential simulations at both gas and liquid densities. Moreover, the discontinuous molecular dynamics approach is demonstrated to be between 3 to 100 times more efficient than the standard molecular dynamics method, depending on the specific conditions of the simulation. The rigid discontinuous molecular dynamics method is also applied to a discontinuous-potential model of a liquid composed of rigid benzene molecules, and equilibrium and dynamical properties are shown to be in qualitative agreement with more detailed continuous-potential models of benzene. The few qualitative differences in the angular dynamics of the two models are related to the relatively crude treatment of variations in the repulsive interactions as one benzene molecule rotates by another. *This work was supported by grants from the National Sciences and Engineering Research Council of Canada (NSERC).

Sheldon Opps
University of Prince Edward Island

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