Streszczenie w języku angielskim

This work concentrates on the computational methods of statistical mechanics (microcanonical ensemble and canonical ensemble). A new pairwise Nosé-Hoover type thermostat for molecular dynamics simulations (MD), which is similar in construction to the pair-velocity thermostat of Allen and Schmid (AS), is proposed and tested. The Laplace Transform Technique (LTT) is used to derive thermodynamic properties of the soft sphere system in terms of the potential energy and its density derivative. The n-inverse power potential is used.

Pairwise thermostats generate the canonical velocity distribution, are Galilean invariant and conserve linear and angular momentum. The unique feature of the pairwise thermostat is an unconditional conservation of the total angular momentum which is important for thermalizing isolated systems and those non-equilibrium bulk systems manifesting local rotating currents. These thermostats were benchmarked against the corresponding non-pairwise additive thermostats, like the Nosé-Hoover (NH) and Braga-Travis (BT), based on the kinetic and configurational definitions of temperature, respectively. Some differences between the shear-rate dependent shear viscosity from Sllod non-equilibrium MD, are observed at high shear rates using the different thermostats. The thermostats based on the configurational temperature produced very similar monotically decaying shear viscosity (shear thinning) with increasing shear rate, while the NH method showed discontinuous shear thinning into a string phase, and the AS method produced a continuous increase of viscosity (shear thickening), after a shear thinning region at lower shear rates. Both pairwise additive thermostats are neither purely kinetic nor configurational in definition and possible directions for further improvement in certain aspects are discussed.

The derived expressions obtained from LTT method provide an analytic framework with which to explore thermodynamic properties of soft sphere system across the whole softness and density fluid domain. The trends in the thermodynamic properties as a function of fluid density and potential softness are described using these formulas supplemented by the simulation-derived equation of state. At low densities a minimum in the isobaric heat capacity with density is found which is a new feature for a purely repulsive pair interaction. The hard-sphere and very-soft sphere limits are obtained, and the low density limit specified analytically for any n is discussed. The softness dependence of calculated quantities indicates freezing criteria based on features of the radial distribution function or derived functions of it, are not expected to be universal. The thermodynamic properties and structural quantities indicate that three regions specified by a convex, concave and an intermediate density dependence can be expected as a function of n.