

## **Novel formulas for thermodynamics and correlation functions in computer simulation of hard spheres**

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Paper presents application of the mapped-averaging framework for generating ensemble averages for thermodynamic properties and correlation functions in molecular dynamics simulations of a system modelled with impulsive dynamics. Specifically completely new formulas of ensemble averages for the pressure, the singlet and pair correlation functions of a one-component hard-sphere system are presented. The pressure formula in particular is constructed such that it gives an ensemble average that exactly corrects the second-order virial equation of state. The performance of these formulas in relation to conventional approaches is examined. We found that mapped averaging has some advantage at low density, while both approaches perform equally well (in terms of uncertainties for a given amount of sampling) at higher densities.