

Determination of structural, thermodynamic and dynamic properties of basic models of classical particle systems

dr Sławomir Pieprzyk

Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Different aspects of determination of physical properties of the basic particles systems composed of particles interacting using the Lennard-Jones, Inverse Power and Hard Sphere potentials will be presented. Some of the recent achievements in the simulation methods used in calculations of these classical particle systems will be mentioned.

In the first part of the presentation a new pairwise Nosé-Hoover type thermostat based on the configurational thermostat will be presented. The unique feature of this thermostat is an unconditional conservation of the total angular momentum, which is important feature for thermalizing isolated systems and performing simulations of bulk systems with locally rotating units.

In the second, main part of the presentation the structural, thermodynamic and dynamic properties of the three model systems will be discussed. It will be shown, how using a new set of molecular dynamics data the different thermodynamic characteristics of the Lennard-Jones fluid have been deduced and details of the equation of state have been obtained. In the case of the purely repulsive soft-sphere system, where the interaction potential is inversely proportional to the pair separation, the results obtained with the Laplace transform technique will be demonstrated. In the last part of the presentation the recently obtained results for the hard sphere system will be presented along with short description of the DYNAMO program.