Mesoscale modelling of fluctuating fluids: colloids, active particles and polymers in flow

THOMAS IHLE, DANIEL KROLL, Department of Physics, North Dakota State University, Fargo, ND 58105., ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455., MARTIN HECHT, Institute for Computational Physics 1, Stuttgart University, Germany

A recently introduced stochastic model for fluid flow, called Stochastic Rotation Dynamics (SRD), is a promising tool for the coarse-grained modelling of a fluctuating solvent, particularly for colloidal and polymer suspensions. The solvent is represented by "fluid"-particles which follow a simple dynamics and undergo efficient multiparticle collisions. SRD can be thought of a "hydrodynamic heat bath" which provides the correct hydrodynamic interactions between embedded particles. It is shown how exact analytical expressions for the transport coefficients of this model can be derived by means of discrete Green-Kubo relations. We will discuss several extensions of the original model such as obtaining a non-ideal equation of state. Colloids and polymers can be coupled to this fluid and are treated by Molecular Dynamics. Results for the sedimentation of colloids and the pattern formation of active particles and polymers in flow will be presented.

Thomas Ihle
Department of Physics, North Dakota State University, Fargo, ND.

Date submitted: 01 Dec 2004  Electronic form version 1.4