

Abstract Submitted
for the DFD14 Meeting of
The American Physical Society

When hard spheres overlap - generalization of the Rotne-Prager-Yamakawa hydrodynamic tensors¹ ELIGIUSZ WAJNRYB, Institute of Fundamental Technological Research Polish Academy of Sciences, Poland, PAWEL ZUK, University of Warsaw, Physics Department, Poland, KRZYSZTOF MIZERSKI, Institute of Geophysics, Polish Academy of Sciences, Poland, PIOTR SZYMCZAK, University of Warsaw, Physics Department, Poland — The Rotne-Prager-Yamakawa (RPY) approximation is commonly used to model the hydrodynamic interactions between small spherical particles suspended in a viscous fluid at a low Reynolds number. It takes into account long-range contribution to hydrodynamic interactions and yields positive definite diffusion matrix, which is essential for Brownian dynamics modeling. However, when the particles overlap, the RPY tensors lose their positive definiteness, which leads to numerical problems in the Brownian dynamics simulations as well as errors in calculations of the hydrodynamic properties of rigid macromolecules using bead modeling. We extend the RPY approach to the case of overlapping spherical particles of different radii in a consistent way that preserves positive definiteness of diffusion tensors for translational, rotational and dipolar degrees of freedom. Moreover we show how the Rotne-Prager-Yamakawa approximation can be generalized for other geometries and boundary conditions.

¹E.W. acknowledges the support of the Polish National Science Centre (Grant No. 2012/05/B/ST8/03010)

Eligiusz Wajnryb
Institute of Fundamental Technological Research
Polish Academy of Sciences, Poland

Date submitted: 30 Jul 2014

Electronic form version 1.4