Abstract Submitted
for the DFD15 Meeting of
The American Physical Society

Polarizable protein model for Dissipative Particle Dynamics
EMANUEL PETER, KIRILL LYKOV, IGOR PIVKIN, Institute of Computational Science, Faculty of Informatics, University of Lugano — In this talk, we present a novel polarizable protein model for the Dissipative Particle Dynamics (DPD) simulation technique, a coarse-grained particle-based method widely used in modeling of fluid systems at the mesoscale. We employ long-range electrostatics and Drude oscillators in combination with a newly developed polarizable water model. The protein in our model is resembled by a polarizable backbone and a simplified representation of the sidechains. We define the model parameters using the experimental structures of 2 proteins: TrpZip2 and TrpCage. We validate the model on folding of five other proteins and demonstrate that it successfully predicts folding of these proteins into their native conformations. As a perspective of this model, we will give a short outlook on simulations of protein aggregation in the bulk and near a model membrane, a relevant process in several Amyloid diseases, e.g. Alzheimers and Diabetes II.

Igor Pivkin
Institute of Computational Science, Faculty of Informatics, University of Lugano

Date submitted: 29 Jul 2015 Electronic form version 1.4