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.

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