Polarizable water model for Dissipative Particle Dynamics IGOR
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matics, University of Lugano — Dissipative Particle Dynamics (DPD) is an efficient
particle-based method for modeling mesoscopic behavior of fluid systems. DPD
forces conserve the momentum resulting in a correct description of hydrodynamic
interactions. Polarizability has been introduced into some coarse-grained particle-
based simulation methods; however it has not been done with DPD before. We
developed a new polarizable coarse-grained water model for DPD, which employs
long-range electrostatics and Drude oscillators. In this talk, we will present the
model and its applications in simulations of membrane systems, where polarization
effects play an essential role.

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