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REFRAMING DISSIPATIVE PARTICLE DYNAMICS

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Dissipative Particle Dynamics is a method for the simulation of hydrodynamic processes in complex fluids [1]. The dissipative particles are usually understood as a coarse-grained representation of some underlying atoms of the fluid or other mesostructures present (colloids, polymers, etc.) I will show that when the system is composed by atoms bonded together, like the monomers in a polymer molecule, it is possible to coarse-grain the atoms in favor of blobs (i.e. dissipative particles). In this case, by following a bottom-up strategy, we derive rigorously the mesoscopic dynamics of the blobs from the microscopic Hamiltonian dynamics of the atoms [2]. The resulting equations for the blobs turn out to have the structure of the DPD equations, although with microscopically defined effective potential and friction coefficients. When the atoms are not bonded, like in a simple fluid, a bottom-up derivation of the mesoscopic dynamics of blobs is doomed to fail because a blob has no simple definition in terms of the underlying atoms (atoms may diffuse away from the center of the blob). In this case, a top-down strategy is required. We show how, by discretizing the Navier-Stokes equations in a meshless cloud of points by following the thermodynamically consistent framework known as GENERIC, it is possible to construct a fluid particle method that allows one to address the mesoscale where thermal fluctuations are important. The resulting method, called Smoothed Dissipative Particle Dynamics [3], resembles DPD but does not suffer from its known problems,[4]. The inclusion of additional structural variables like conformation tensors within the GENERIC framework allows one to describe viscoelastic fluids at scales where thermal fluctuations are relevant [5].

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