



On the Conservative Forces of Dissipative Particle Dynamics

By José Castro Arce

Shaker Verlag Sep 2012, 2012. Buch. Condition: Neu. Neuware - Dissipative Particle Dynamics (DPD) is one of the most promising methods to simulate complex flows of multicomponent systems. In DPD, matter is represented using coarse-grained models which interact via soft-forces. The DPD conservative forces are responsible for the thermodynamic properties of the systems and therefore, it is crucial to model these forces properly in order to obtain feasible results. Regretfully, the DPD fluid behaves like a pseudo-gas (squared equation of state) when the standard conservative forces are employed. Moreover, DPD lacks of a physical meaningful parameterization approach for polar species. For these reasons, the use of non-standard conservative forces is investigated in this work. First, adaptable polynomial interactions are employed to explore the effect of the potential softness on the numerical stability and efficiency of the DPD simulations. Further on, the cutoff radius is extended to take the attractive part of the interactions into account. As expected, the simulation results show that attractive interactions are essential in the modeling of condensed matter. As the computational demands remain affordable for the hardest semi-soft interaction employed in this work, the author proposes using Lennard-Jones 12-6 potentials to model the interactions between the...



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