Pressure control in dissipative particle dynamics and its application in simulating micro- and nano-bubbles

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Abstract

The interest of studying property as a function of temperatures and pressures is much more extensive than the interest of using volume and energy as the independent variables. In dissipative particle dynamics [1] (DPD) and many-body DPD (MDPD) [2], a natural thermostat has been already incorporated. Therefore, the barostat for pressure control could be a very important part for the (M)DPD application. In current work, the Berendsen barostat [3] from molecular dynamics simulation is applied in both DPD and MDPD simulations. The original Berendsen barostat works well in (M)DPD simulation of single-component system under constant pressure condition and in non-equilibrium dynamic processes. The novel partial Berendsen barostat is proposed for multi-component system simulation with (M)DPD. The displacement rescaling process of Berendsen barostat is only applied on the particles outside the center region, acting as a pressure 'boundary condition'. The center part forms the free zone, in which the interface shape, non-equilibrium dynamic behavior between different phases can be captured properly. Immiscible bubble in the second fluid under constant pressure condition is studied, and the oscillation of bubble radius and fluctuation of system pressure can be obtained by current barostat. Preliminary models for bubble growing and collapsing under square pressure wave and bubble oscillation under harmonic pressure wave are also reported in current simulation. It shows that the partial Berendsen barostat is suitable for the modeling of non-equilibrium process of single or few droplets/bubbles in multi-component systems.

Keywords: pressure control; Berendsen barostat; non-equilibrium dynamic process; (many-body) dissipative particle

References

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