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Comprehensive boundary method for solid walls in dissipative particle dynamics

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Abstract

Dissipative particle dynamics (DPD) is a particle-based mesoscopic simulation technique, especially useful to study hydrodynamic behaviour in the field of complex fluid flow. Most studies with DPD have focused on bulk behaviour by considering a part of an infinite region using periodic boundaries. To model a finite system instead, boundary conditions of the solid walls confining the system must be addressed. These conditions depend on the time and length scales of phenomena studied, i.e., the level of coarse graining. Here we focus on a mesoscopic level at which small scale atomistic effects near the wall are no longer visible. At this, more macroscopic, level a solid wall should be impenetrable, show no-slip and should not affect the fluid properties. Solid walls used in previous studies were unable to meet all three these conditions or met them with limited success. Here, we describe a method to create solid walls that does satisfy all requirements, producing the correct boundary conditions. The introduction of periodic conditions for curved boundaries makes this new wall method fit for curved geometries as well. And, an improved reflection mechanism makes the walls impenetrable without causing side effects. The method described here could also be implemented in other particle-based models.

Keywords: Dissipative particle dynamics; Boundary conditions; Solid walls

1. Introduction

The rheology in some flow problems, such as complex fluid or multiphase flow, depends on microscopic information of the fluids present. Often, only a low-level of molecular behaviour is relevant and should be captured by the numerical technique employed. Conventional continuum-based techniques are based on

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solving the Navier–Stokes equations and have difficulties to address effects on a microscopic scale. On the other hand, molecular dynamics simulations give a full description on atomistic scale that is too detailed and computationally very expensive. Mesoscopic simulation methods that are applicable in between microscopic and macroscopic time- and length-scales, are therefore particularly useful in these situations. Dissipative particle dynamics (DPD) is a particle-based form of such a mesoscopic method. DPD was introduced by Hoogerbrugge and Koelman [1] to study suspensions [2]. Later, the hydrodynamic behaviour in various other problems has been studied with DPD, involving polymers [3], multiple phases [4–6], and heat transfer [7].

Most of these studies simulate part of an infinite region using a system confined by periodic boundaries. Simple shear flow with a linear velocity profile is obtained in such systems with the Lees–Edwards boundary condition [8]. However, systems addressing more complex flow patterns or impenetrable boundaries require real solid walls. The desired behaviour of a solid wall, and hence the boundary conditions, depends on the scale at which a system is observed. On an atomic level it is likely that a wall induces structure in the fluid, as well as locking and slip, influencing the behaviour in the order of nanometers from the wall [9–12]. Nevertheless, when DPD is employed as particle-based flow solver at a mesoscopic level of micrometers, the degree of coarse graining is too high to show such atomistic effects near the wall.

The central question of the present work is how to construct a solid wall for this higher, more macroscopic, level of mesoscopic modelling. On this level three boundary conditions hold for a solid wall: (1) impenetrability; no particles are allowed to enter the wall, (2) no-slip; the wall should impose the correct velocity, and (3) the wall should not affect the fluid properties in the system. Previous studies managed to implement impenetrability and no-slip boundary conditions, but proved to show small scale effects like ordering near the wall, which affects a substantial portion of the system. Obviously, this is not correct from our "macroscopic" point of view, since the properties of a system should not change when a wall is placed around it.

In this paper we present a new method for constructing solid walls solving the problem of the above mentioned wall effects and related anomalies. The method is based on a novel periodic approach that utilizes a set of identical systems, instead of a single one. Besides, a technique is introduced to achieve the correct interaction across a curved boundary, making it possible to model systems with curved walls. Furthermore, we improved the reflection mechanism that guarantees the wall's impenetrability. Together with the existing knowledge about boundary conditions this leads to a comprehensive boundary method for solid walls in DPD.

2. Dissipative particle dynamics

The DPD method describes a fluid system in a coarse-grained fashion by dividing it up in small interacting fluid packages. Each package is represented by a DPD particle that is assumed to show the collective dynamic behaviour of the group of molecules it contains. The evolution of the positions ($\mathbf{r}_i$) and impulses ($\mathbf{p}_i$) of all interacting particles over time is governed by Newton's second law of motion:

$$\frac{\partial \mathbf{r}_i}{\partial t} = \mathbf{v}_i(t), \quad \frac{\partial \mathbf{v}_i}{\partial t} = \mathbf{f}_i(t), \tag{1}$$

where the mass is left out since we will work with particle masses of 1 for simplicity. The equations of motion are solved using the modified velocity-Verlet algorithm presented by Groot and Warren [13]. The total force acting on a particle i is composed of three pairwise additive forces, a dissipative ($\mathbf{F}_{ij}^{\mathrm{D}}$), random ($\mathbf{F}_{ij}^{\mathrm{R}}$) and conservative force ($\mathbf{F}_{ij}^{\mathrm{C}}$)