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A numerical study of strongly overdamped Dissipative Particle Dynamics (DPD) systems

N. Mai-Duy [a,b], N. Phan-Thien [a,*], B.C. Khoo [a]

[a] Department of Mechanical Engineering, Faculty of Engineering, National University of Singapore, Singapore
[b] Computational Engineering and Science Research Centre, Faculty of Engineering and Surveying, University of Southern Queensland, Toowoomba, QLD 4350, Australia

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ABSTRACT

In this paper, we investigate the behaviour of a Dissipative Particle Dynamics (DPD) system in the overdamped limit where the particles approach zero mass limit. In this limit, the DPD system becomes singular. We propose two numerical schemes to deal with this system - one results in a fully-populated but well-conditioned matrix system, while the other employs a deflation technique to handle the system in an iterative manner, where the eigenvalue of -1 corresponding to a rigid-body motion is mapped to zero. The latter iterative scheme is to be preferred, with the possibility of parallel implementations. Some numerical results are presented to verify the two proposed schemes.

1. Introduction

Dissipative Particle Dynamics (DPD) is a particle-based method for simulating hydrodynamic phenomena, originally derived as a coarse-grained method for molecular dynamics (MD) simulation [1–5]. One salient feature of DPD is that the method is based on simple pairwise interactions, which allows mean quantities (density, linear momentum, etc.) to satisfy conservation laws (thus qualifies the method as a particle-based solver for continuum problems). The interparticle forces, namely conservative, dissipative and random, are functions of relative pairwise positions and velocities in pairs. The method is particularly powerful for dealing with complex fluid systems, such as colloidal suspensions and polymer solutions, on physically interesting length and time scales. For example, in simulating colloidal suspensions, a colloidal particle can be simply modelled by a set of standard but constrained DPD particles located on a rigid surface [6], or by a single DPD particle with a different set of DPD parameters [7].

It should be pointed out that a DPD fluid is compressible in nature and its dynamic response is rather slow - the Schmidt number (Sc) is about unity because of the soft interaction between particles in the DPD system. On the other hand, many practical applications involve incompressible flows that exhibit strongly viscous behaviour at low fluid inertia, (*i.e.*, low Reynolds number (Re) flows) [8]. Incompressibility is a good approximation in many practical flows at low Mach numbers ($M < 0.3$) [9]. For real fluids of physical properties like those of water, the Schmidt number is $O(10^3)$. One effective way to induce an incompressible slow viscous flow in a DPD fluid and simultaneously enhance its dynamic response is to reduce the mass of the particles (m). In the limit of $m \to 0$, a strongly overdamped system results, with $Re \to 0, M \to 0$ and $Sc \to \infty$.

* Corresponding author. Tel.: +65 6601 2054; fax: +65 6779 1459.
E-mail address: nhan@nus.edu.sg (N. Phan-Thien).

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In the context of Brownian dynamics simulations, the motion of a Brownian particle is governed by a Langevin equation which also involves viscous friction and fluctuating forces [10]. The highly overdamped case (i.e., viscous limit), in which the friction is strong enough so that the inertia term may be neglected, has been well studied. In the context of DPD, to our knowledge, there has been no previous report concerning the overdamped limit. In this study, we examine the DPD equations, in which inertia terms are ignored. Despite the similar appearances of the DPD and Langevin equations, the mathematical properties of strongly overdamped systems of the former are fundamentally different from those of the latter. For example, due to the presence of the pairwise velocities in the governing equations, the DPD system is singular. The aim of this work is to provide numerical schemes that are able to yield a solution to the DPD system in the limit of $m \to 0$, where the dynamic response of the DPD fluid becomes fast.

The remainder of the paper is organised as follows. In Section 2, a brief overview of the DPD equations is given. In Section 3, the highly overdamped case of DPD is studied, in which two numerical schemes are proposed to deal with the singularity of the system. In Section 4, some numerical simulations are carried out to verify the two proposed schemes. Section 5 concludes the paper.

2. DPD equations

The DPD equations can be written as

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \tag{1}$$

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1, j\neq i}^{N} a_{ij} w_C \mathbf{e}_{ij} - \sum_{j=1, j\neq i}^{N} \gamma w_D \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}\right)\mathbf{e}_{ij} + \sum_{j=1, j\neq i}^{N} \sigma w_R \theta_{ij} \mathbf{e}_{ij}, \tag{2}$$

where $i = (1, 2, \cdots, N), N$ is the number of particles, m_i, $\mathbf{r}_i$ and $\mathbf{v}_i$ the mass, position and velocity vector of the ith particle, t the time, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j, \mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, r_{ij} = |\mathbf{r}_{ij}|$), a_{ij}, γ and σ are constants, and θ_{ij} a Gaussian white noise ($\theta_{ij} = \theta_{ji}$) with stochastic properties

$$\langle \theta_{ij} \rangle = 0, \tag{3}$$

$$\langle \theta_{ij}(t)\theta_{kl}(t') \rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta(t - t'), \text{ with } i \neq k \text{ and } j \neq l. \tag{4}$$

The first term on the right side of (2) is the conservative force, the second the dissipative force and the last the random force. The equilibrium and detailed balance of the system requires

$$w_D(r_{ij}) = \left(w_R(r_{ij})\right)^2, \tag{5}$$

$$k_B T = \frac{\sigma^2}{2\gamma}, \tag{6}$$

where $k_B T$ is the Boltzmann temperature (mean kinetic energy of the particles).

In this paper, we consider the commonly used form

$$w_C(r_{ij}) = 1 - \frac{r_{ij}}{r_c}, \tag{7}$$

$$w_D(r_{ij}) = \left(1 - \frac{r_{ij}}{r_c}\right)^{1/2}, \tag{8}$$

where r_c is the cutoff radius that limits the range of interaction for the forces. It is noted that r_c can be different for different types of forces.

3. Overdamped limit of DPD

In the limit of $m\gamma^2 \to 0$, Eq. (2) reduces to

$$\mathbf{0} = \sum_{j=1, j\neq i}^{N} a_{ij} w_C \mathbf{e}_{ij} - \sum_{j=1, j\neq i}^{N} \gamma w_D \left(\mathbf{e}_{ij}\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}\right) + \sum_{j=1, j\neq i}^{N} \sigma w_R \theta_{ij} \mathbf{e}_{ij}. \tag{9}$$

When necessary, we use the superscript k on relevant variables to denote the time level $t = t^k$. Note that this limit is not equivalent to a steady-state flow assumption - it only guarantees that the inertial terms (Reynolds number) in the momentum equations are zero, but any other time-dependent behaviour inherited, for example from the boundary conditions, has not been eliminated.