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A splitting scheme for highly dissipative smoothed particle dynamics

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ABSTRACT

Smoothed particle dynamics refers to Smoothed Particle Hydrodynamics (SPH) when simulating macroscopic flows and to Smoothed Dissipative Particle Dynamics (SDPD) when simulating mesoscopic flows. When the considered flow is highly dissipative, this otherwise very attractive method faces a serious time-step limitation. This difficulty, known in literature as Schmidt number problem for Dissipative Particle Dynamics (DPD), prevents the application of SDPD for important cases of liquid micro-flows. In this paper we propose a splitting scheme which allows to increase significantly the admissible time-step size for SPH and SDPD. Macroscopic and mesoscopic validation cases, and numerical simulations of polymer in shear flows suggest that this scheme is stable and accurate, and therefore efficient simulations at Schmidt numbers of order $O(10^6)$ are possible.

1. Introduction

Smoothed particle dynamics is a fully Lagrangian, grid free method, where a smoothing kernel is introduced to approximate functions and their spatial derivatives from data carried by neighboring particles. It is referred to as Smoothed Particle Hydrodynamics (SPH) when simulating macroscopic flows [1], and as Smoothed Dissipative Particle Dynamics (SDPD) when simulating mesoscopic flows [2,3]. SDPD also can be viewed as a modification of Dissipative Particle Dynamics (DPD), a popular mesoscopic particle-based method [4]. Compared to DPD, in SDPD transport coefficients can be prescribed as input parameters rather than being an indirect result of other model parameters. Thermal fluctuations can be introduced adaptively according to the size of the fluid particles.

When the smoothed particle dynamics method is used to simulate low-Reynolds-number and mesoscopic liquid flows, the time-step size limit for stable time integration is usually determined by the viscous effects as such flows are highly dissipative. Specifically, this issue is referred to as Schmidt number problem in DPD [5,6] and obviously also applies to SDPD. The Schmidt number is defined as the ratio of momentum diffusivity (viscosity) and mass diffusivity

$$\mathrm{Sc} = \frac{\mu}{D\rho}, \tag{1}$$

where μ is dynamic viscosity, ρ is density and D is the diffusion coefficient. Typical Sc number achieved by SDPD and DPD simulations are of order $O(1)$, which is similar to that of a gas rather than a liquid with Sc $\sim O(10^3)$.

Peters [7] suggested that the diffusion coefficient D appearing in the definition of Sc refers to the molecular diffusivity and therefore is an ill-defined quantity for coarse-grained systems. Accordingly, one would not need to achieve realistically large Sc to capture correct hydrodynamic interactions [8–10]. However, it has been pointed out by Groot and Warren [11] that in order to achieve a realistic liquid behavior it is essential to recover the correct magnitude of Sc in DPD simulation. Furthermore, it was observed by Symeonidis et al. [5,12] that an agreement between simulations and experiments with

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respect to the non-equilibrium properties of a DNA molecule in a shear flow requires Sc numbers with a magnitude of that for a liquid.

For increasing Sc in DPD simulation one could generate a higher viscosity by increasing the stiffness of the conservative force or the number density of DPD particles, or the dissipative force. Since the represented length scale decreases with the increase of the former two quantities, these approaches contradict the intended coarse-graining property of the DPD method. Therefore, a common approach for increasing Sc is to increase the magnitude of the dissipative force. However, if the DPD particle velocity is updated explicitly, as in the traditional velocity-Verlet method [11], the time integration requires a very small, computationally inefficient time-step size to achieve correct equilibrium properties. To cope with this difficulty, Pagonabarraga et al. [13] have proposed an iterative method where the particle velocity is updated implicitly. However, it is found that such a method is not very practical due to large computational cost. Lowe [14] developed an alternative DPD method where the dissipative and random forces of the traditional DPD method are replaced by a pairwise momentum-conservative Andersen thermostat, which relates the resulting viscosity to a prescribed random relaxation parameter. Due to the Andersen thermostat the method recovers the correct kinetic temperature independently of the time-step size and can be used for simulating a DPD fluid with high Sc. One issue of this method is that the deterministic dissipative term in DPD is replaced by a stochastic term which may lead to strong spatial–temporal fluctuations of the dissipation rate when the time-step size is large.

More recently, a splitting scheme for DPD was proposed by Shardlow [15]. While updating the contribution of the conservative force explicitly, similarly to that of Lowe's method, this method updates the contributions of the dissipative and random forces in pairwise fashion. By this procedure the original DPD formulation of dissipative and random forces is preserved. Nikunen et al. [16] showed that the accuracy and performance of Shardlow's scheme is superior to that of several other schemes commonly used in DPD. However, compared to that of Lowe's method, the kinetic temperature is still significantly overestimated when a large time-step size is used. It is interesting to note that in an earlier work of Monaghan [17] a splitting scheme similar to that of Shardlow [15] was described for handling the drag force on dust particles when modeling dust-gas flow with an SPH method. To recover very large drag coefficients the pairwise interactions are computed by sweeping over all the dust-gas particle pairs several times. Although this method originally has been developed for a drag-force model an extension to general viscous flows appears to be straightforward.

In this work we present a splitting scheme for the smoothed particle dynamic method which can be viewed as a combination and extension of Shardlow's and Monaghan's schemes. The scheme achieves significantly larger time-step sizes than is possible by the standard predictor–corrector and velocity-Verlet schemes, and can be applied for general macroscopic and mesoscopic viscous flows. To demonstrate the robustness and efficiency of the method, a number of validation tests and examples for macroscopic and microscopic flows are given.

2. SPH and SDPD

For SPH the temporal evolution of discrete-particle location and properties is given by

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \tag{2a}$$

$$\rho_i = m_i \sum_j W_{ij} = m_i \sigma_i, \tag{2b}$$

$$\frac{d\mathbf{v}_i}{dt} = -\frac{1}{m_i} \sum_j \left(\frac{p_i}{\sigma_i^2} + \frac{p_j}{\sigma_j^2} \right) \frac{\partial W_{ij}}{\partial r_{ij}} \mathbf{e}_{ij} + \frac{\mu}{m_i} \sum_j \left(\frac{1}{\sigma_i^2} + \frac{1}{\sigma_j^2} \right) \frac{\mathbf{v}_{ij}}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}}, \tag{2c}$$

representing a Lagrangian discretization of the Navier–Stokes equations for isothermal, weakly compressible flow [3]. Here, $\mathbf{e}_{ij}$ and r_{ij} are the normalized vector and distance from particle i to particle j, respectively. $\mathbf{r}_i$,$\mathbf{v}_i$,m_i,ρ_i and p_i are position, velocity, mass, density and pressure of a particle i, respectively. σ_i is the inverse of particle volume, and $W_{ij} = W(r_{ij},h)$ is a kernel function with smoothing length h. An isothermal equation of state is given as

$$p = p_0 \left(\frac{\rho}{\rho_0} \right)^{\gamma} + b, \tag{3}$$

where p_0,ρ_0, b and γ are parameters which may be chosen based on a scale analysis so that the density variation is less than a given value, usually 1% [18].

Within the SDPD formulation [2] Eq. (2) presents the deterministic part of the particle dynamics. Using the GENERIC formalism [19,20] thermal fluctuations can be taken into account by postulating the following expressions for mass and momentum fluctuations

$$d\tilde{m}_i = 0, \tag{4a}$$

$$d\widetilde{\mathbf{P}}_i = \sum_j B_{ij} d\overline{\overline{W}}_{ij} \mathbf{e}_{ij}, \tag{4b}$$

where $\overline{\overline{dW}}_{ij}$ is the traceless symmetric part of a tensor of independent increments of a Wiener process, and B_{ij} is defined as