Stable and accurate schemes for smoothed dissipative particle dynamics

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Abstract Smoothed dissipative particle dynamics (SDPD) is a mesoscopic particle method that allows to select the level of resolution at which a fluid is simulated. The numerical integration of its equations of motion still suffers from the lack of numerical schemes satisfying all the desired properties such as energy conservation and stability. Similarities between SDPD and dissipative particle dynamics with energy (DPDE) conservation, which is another coarse-grained model, enable adaptation of recent numerical schemes developed for DPDE to the SDPD setting. In this article, a Metropolis step in the integration of the fluctuation/dissipation part of SDPD is introduced to improve its stability.

Key words smoothed dissipative particle dynamics (SDPD), numerical integration, Metropolis algorithm

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1 Introduction

The development of the computational capacities in the last decades has allowed physicists to use numerical simulations to study physical properties at the atomic scale with the help of statistical physics. In particular, molecular dynamics (MD) consists in integrating the equation of motions for the atoms in order to sample probability measures in a high dimensional space[1–3]. However, traditional microscopic methods suffer from limitations in terms of accessible time and length scales, which drives the development of mesoscopic coarse-grained methods. These mesoscopic models aim at greatly reducing the number of degrees of freedom explicitly described, and thus the computational cost, while retaining some properties absent from more macroscopic models such as hydrodynamics. Smoothed dissipative particle dynamics (SDPD)[4] belongs to this class of the mesoscopic method. It couples a particle Lagrangian discretization of

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the Navier-Stokes, smoothed particle hydrodynamics (SPH)\cite{5–6}, and the thermal fluctuations from models like dissipative particle dynamics with energy (DPDE) conservation\cite{7–8}. It is thus able to deal with hydrodynamics at nanoscale and has been shown to give results consistent with MD for a wide range of resolutions, at equilibrium and for shock waves\cite{9}, or for dynamical properties such as the diffusion coefficient of a colloid in an SDPD bath\cite{10–11}. SDPD has in particular been used to study colloids\cite{10–12}, polymer suspensions\cite{13}, and fluid mixtures\cite{14}.

One of the main challenges for mesoscopic models incorporating fluctuations is to develop efficient, stable, and parallelizable numerical schemes for the integration of their stochastic dynamics. Most schemes are based on a splitting strategy\cite{15–16} where the Hamiltonian part is integrated through a velocity Verlet scheme\cite{17}. A traditional and popular algorithm first proposed for dissipative particle dynamics\cite{18} and later extended to DPDE\cite{19} relies on a pairwise treatment of the fluctuation/dissipation part\cite{20}. The adaptation of this scheme to dynamics preserving various invariants has led to a class of schemes called Shardlow-like splitting algorithms (SSA)\cite{21}. A major drawback in this strategy is the complexity of its parallelization\cite{22}. Other schemes have been recently proposed in Ref.\cite{23} to enhance its use in parallel simulations.

All these schemes are, however, hindered by instabilities when internal energies become negative. This especially happens at low temperatures or when small heat capacities are considered, typically for small mesoparticles. It has been proposed to use Monte Carlo principles to sample the invariant measure of DPDE, by resampling the velocities along the lines of centers according to a Maxwell-Boltzmann distribution and redistributing the energy variation into internal energies according to some prescriptions\cite{24}. However, this approach leads to dynamics which is not consistent with DPDE. It was proposed in Ref.\cite{25} to correct discretization schemes for DPDE by rejecting unlikely or forbidden moves through a Metropolis procedure, which prevents the appearance of negative internal energies and improves the stability of the integration schemes.

There exist relatively few references in the literature about the integration of full SDPD. Most works focus on numerical schemes in the isothermal setting\cite{26}, avoiding the need to preserve the total energy during the simulation. In a previous article\cite{9}, we introduced an adaptation of the Shardlow splitting to SDPD, allowing a good control of the energy conservation. The aim of this work is to provide more details about the possible integration of SDPD in an energy conserving framework and most importantly to increase the stability for small particle sizes by adapting the metropolization procedure described in Ref.\cite{25}.

This article is organized as follows. We first present in Section 2 the equations of SDPD as reformulated in Ref.\cite{9}. In Section 3, we recall the Shardlow splitting for SDPD and introduce a Metropolis step to enhance the stability of the algorithm. We evaluate the properties of the Shardlow and Metropolis schemes by means of numerical simulations in Section 4. Our conclusions are gathered in Section 5.

2 SDPD

At the hydrodynamic scale, dynamics of the fluid is governed by the Navier-Stokes equations as below, which reads in their Lagrangian form when the heat conduction is neglected (for the time $t \geq 0$ and the position $\mathbf{x}$ in a domain $\Omega \subset \mathbb{R}^3$),

\[
\begin{align*}
D_t \rho + \rho \text{div}_x \mathbf{v} &= 0, \\
\rho \text{Div} \mathbf{v} &= \text{div}_x (\boldsymbol{\sigma}), \\
\rho D_t (u + \frac{1}{2} \mathbf{v}^2) &= \text{div}_x (\boldsymbol{\sigma} \mathbf{v}).
\end{align*}
\]

In these equations, the material derivative used in the Lagrangian description is defined as

\[
D_t f(t, \mathbf{x}) = \partial_t f(t, \mathbf{x}) + \mathbf{v}(t, \mathbf{x}) \nabla_x f(t, \mathbf{x}).
\]