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Stable schemes for dissipative particle dynamics with conserved energy

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ABSTRACT

This article presents a new numerical scheme for the discretization of dissipative particle dynamics with conserved energy. The key idea is to reduce elementary pairwise stochastic dynamics (either fluctuation/dissipation or thermal conduction) to effective single-variable dynamics, and to approximate the solution of these dynamics with one step of a Metropolis–Hastings algorithm. This ensures by construction that no negative internal energies are encountered during the simulation, and hence allows to increase the admissible timesteps to integrate the dynamics, even for systems with small heat capacities. Stability is only limited by the Hamiltonian part of the dynamics, which suggests resorting to multiple timestep strategies where the stochastic part is integrated less frequently than the Hamiltonian one.

1. Introduction

Dissipative Particle Dynamics (DPD) [10] is a particle-based coarse-grained model in which atoms, molecules or even groups of molecules are represented by a single mesoscale particle. The time evolution of the mesoscale particles is governed by a stochastic differential equation. Dissipative and random forces allow to take into account some effect of the missing degrees of freedom. DPD was put on a firm theoretical ground in [6]. However, it is intrinsically is an equilibrium model, with a prescribed temperature, and cannot be used as such to study nonequilibrium systems. It should be replaced by a dynamics where the fluctuation/dissipation relation is based on variables which evolve in time. DPD with conserved energy (DPDE) is such a model [1,5]. In the DPDE framework, mesoparticles have an additional degree of freedom, namely an internal energy, which accounts for the energy of the missing degrees of freedom. The dynamics on the internal energies is constructed in order for the total energy of the system to remain constant. DPDE was initially used for thermal transport [23, 17], and later on to simulate shock and detonation waves [27,18,19].

While numerous efficient schemes were developed for DPD (see for instance [15] for a review and careful comparison of various schemes), the efficient numerical integration of DPDE still requires some effort. One appealing framework to integrate DPDE, as considered in [27,13] for instance, is based on the so-called Shardlow splitting algorithm (SSA) for DPD [25]. It consists in decomposing the dynamics into a Hamiltonian part and pairwise elementary dynamics – either fluctuation/dissipation or thermal conduction. There is a consensus on the integration of the Hamiltonian part, for which a Verlet scheme [28] should be used. There is on the other hand no definite way of integrating the fluctuation/dissipation and thermal conduction parts, even when they are split into elementary pairwise dynamics. In particular, to the author's knowledge, for all the numerical schemes currently used, it is observed that negative internal energies may appear when the

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fluctuation terms are large compared to the heat capacity. This sometimes puts a severe constraint on admissible timesteps. This issue has been explicitly acknowledged by various researchers [23,2,17,22,9] (and hidden under the rug by others), but no satisfactory answer was found yet.

Better integration schemes can be obtained by a dedicated treatment of the elementary fluctuation/dissipation and thermal conduction dynamics, instead of resorting to general purpose integration schemes such as Euler–Maruyama. The key observation is that the seemingly $2(d+1)$-dimensional elementary fluctuation/dissipation dynamics can be reduced to an effective one-dimensional dynamics, which can be integrated with a high precision and/or stabilized by a Metropolis–Hastings acceptance/rejection procedure [20,8]. In particular, the Metropolis procedure automatically corrects for negative internal energies. A similar reduction can be performed to obtain an effective one-dimensional dynamics for the elementary pairwise thermal conduction, which is a priori of dimension 2.

This article is organized as follows. DPDE and the general splitting strategy for its numerical discretization are recalled in Section 2. Section 3 is the core of this work: It is shown there how to numerically integrate elementary pairwise stochastic dynamics in order to exactly sample the invariant measure of DPDE. The resulting numerical method is tested on various systems in Section 4. Section 5 gathers the conclusions and some perspectives of this work.

2. Dissipative particle dynamics with conserved energy

The governing equations of DPDE are recalled in Section 2.1, while Section 2.2 discusses microscopic equations of state which allow to model temperature-dependent heat capacities (some technical derivations being postponed to Appendices A and B). A general framework for the numerical integration of DPDE is finally presented in Section 2.3.

2.1. Description of the dynamics

In dissipative particle dynamics with energy conservation, the variables describing the state of the system are the positions $q = (q_1, \ldots, q_N)$ of the N particles, their associated momenta $p = (p_1, \ldots, p_N)$ and the corresponding internal energies $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_N)$. The positions q_i belong to a position space $\mathcal{D}$ (typically, a simulation box with periodic boundary conditions), the momenta p_i can assume any value in $\mathbb{R}^d$ (with d the physical dimension), while the internal energies ε_i are scalar variables which should remain non-negative. Denoting by $V(q)$ the potential energy of the system, the evolution of the variables (q, p, ε) is governed by the following equations [1,5]:

$$\begin{cases} dq_i = \dfrac{p_i}{m_i}\,dt, \\ dp_i = -\nabla_{q_i} V(q) + \displaystyle\sum_{j\neq i}\left[-\gamma(\varepsilon_i,\varepsilon_j)\chi^2(r_{ij})\Big(e_{ij}\cdot v_{ij}\Big)e_{ij}\,dt + \sigma\,\chi(r_{ij})e_{ij}\,dW_{ij}\right], \\ d\varepsilon_i = \displaystyle\sum_{i\neq j}\frac{\chi^2(r_{ij})}{2}\left[\gamma(\varepsilon_i,\varepsilon_j)\Big(e_{ij}\cdot v_{ij}\Big)^2 - \frac{\sigma^2}{2}\left(\frac{1}{m_i}+\frac{1}{m_j}\right)\right]dt - \frac{\sigma}{2}\chi(r_{ij})\Big(v_{ij}\cdot e_{ij}\Big)dW_{ij} \\ \qquad + \displaystyle\sum_{i\neq j}\kappa\,\chi^2(r_{ij})\left(\frac{1}{T_i(\varepsilon_i)}-\frac{1}{T_j(\varepsilon_j)}\right)dt + \sqrt{2\kappa}\,\chi(r_{ij})\,d\widetilde{W}_{ij}, \end{cases} \tag{1}$$

where m_i is the mass of the ith particle,

$$e_{ij} = \frac{q_i - q_j}{|q_i - q_j|}$$

is the unit vector in the direction $q_i - q_j$, $r_{ij} = |q_i - q_j|$ is the distance between particles i and j, χ is a cut-off function, $(W_{ij})_{1\leq i<j\leq N}$ and $(\widetilde{W}_{ij})_{1\leq i<j\leq N}$ are two families of independent standard one-dimensional Brownian motions with $W_{ji} = -W_{ij}$ and $\widetilde{W}_{ji} = -\widetilde{W}_{ij}$ for $1 \leq i < j \leq N$. The fluctuation magnitude $\sigma \geq 0$ and the thermal conductivity $\kappa \geq 0$ are fixed (although they could depend on the particle pair). Note that the version of DPDE where the friction forces and fluctuation terms are projected along the lines of center of the dynamics is considered here. The extension of the numerical schemes presented to more general dynamics with both parallel and perpendicular fluctuation/dissipation terms (as in [11] for DPD) is straightforward; see Appendix B for precise formulas.

It can be shown that the dynamics preserves the total momentum and the total energy, sum of the mechanical energy H and of the internal energy:

$$\mathcal{E}(q,p,\varepsilon) = H(q,p) + \sum_{i=1}^N \varepsilon_i, \qquad H(q,p) = V(q) + \sum_{i=1}^N \frac{p_i^2}{2m_i}.$$

This is discussed more precisely in Section 2.3, where it is shown that the complete DPDE evolution can be separated into elementary dynamics which all preserve the total energy $\mathcal{E}$. Moreover, the friction is taken as