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A Monte Carlo method with negative particles for Coulomb collisions ☆

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ABSTRACT

In this work we propose a novel negative particle method for the general bilinear collision operators in the spatial homogeneous case and apply it to Coulomb collisions. This new method successfully reduces the growth of particle numbers from the numerical time scale to the physical time scale for Coulomb collisions. We also propose a particle resampling method which reduces the particle number to further improve the efficiency. Various numerical simulations are performed to demonstrate the accuracy and efficiency of the method.

1. Introduction

In the numerical study of non-equilibrium plasma physics, the simulation of long range Coulomb collisions between charged particles (electrons and ions) is of crucial importance. The particles are represented by a distribution $f(t, \mathbf{v})$ in phase space, at time t with velocity $\mathbf{v}$. Coulomb collisions can be modeled by a Landau–Fokker–Planck (LFP) equation as the grazing limit of the Boltzmann equation. Direct Simulation Monte Carlo (DSMC) [4] is the prevalent numerical method for solving LFP equations, since deterministic methods suffer from formidable computational costs due to the high dimensionality of the distribution function.

Two widely used DSMC methods are those of by Takizuka and Abe [21] (henceforth TA) and Nanbu [14], and recently studied extensively in, for example, [9,10,22]. Bobylev and Nanbu [5] derived a general formulation for the approximation of LFP equations. However, these (and all DSMC) methods become inefficient as the distribution approaches equilibrium, since most computation is spent on the collisions between particles sampled from the equilibrium part. A hybrid method is more favorable in this case, by evolving the equilibrium part according to a fluid equation and sampling particles from only the remaining part. Caflisch et al. [6] introduced thermalization/dethermalization (TD) methods by splitting the distribution into

$$f(\mathbf{v}) = m(\mathbf{v}) + f_p(\mathbf{v}), \tag{1.1}$$

i.e. an equilibrium part m and a *positive* deviation part $f_p(\mathbf{v}) \geq 0$. After performing collisions in each step, a thermalization/dethermalization step is applied as a reorganization of the splitting (1.1). Later Ricketson et al. [17] improved this method by associating each numerical particle with an entropy which provides more accurate information on whether thermalization/dethermalization is needed. Another hybrid method is proposed in [20].

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The splitting (1.1) is less efficient if defects exist in the equilibrium m, since one needs to take the equilibrium below the whole distribution (i.e. $m \le f$), leaving the large remaining part $(f - m)$ to be represented by particles. In this work we use "negative" particles, which represent the defects in equilibrium. More specifically, we write

$$f(\mathbf{v}) = m(\mathbf{v}) + f_p(\mathbf{v}) - f_n(\mathbf{v}),$$

with $f_p(\mathbf{v}) \ge 0$ and $f_n(\mathbf{v}) \ge 0$ the positive and negative parts of the deviation from equilibrium $m(\mathbf{v})$. Positive and negative particles are sampled from f_p and f_n respectively. Hadjiconstantinou and co-workers [2,3,11] studied the collisions involving negative particles in rarefied gas and developed the low-variance deviational simulation Monte Carlo (LVDSMC) method. Our work, described below, is the first use of negatives particles in a DSMC method for Coulomb collisions.

The major problem in a negative particle method is that the total number of positive and negative particles increases due to collisions involving a negative particle. In the DSMC method for rarefied gas, only a number of $\mathcal{O}(\Delta t)$ collisions are performed in one step, which makes $N(t)$, the total number of particles, grow exponentially on a *physical* time scale. To address this growth, [2] constructed a mesh with small grid size in phase space, and in each grid cell the particles with opposite signs are removed in pairs. Later a gridless method was developed for *linearized* variable hard sphere (VHS) type collisions in [12]. Besides, weighted particles have also been studied [8,1] in rarefied gas collisions for variance reduction. We refer the reader to a recent review [16] for more results.

However, a direct application of the negative particle method on Coulomb collisions leads to a much more severe problem in the growth of the number of particles. In the TA method and Nanbu's method for Coulomb collisions, every particle collides in every time step, which (more than) doubles $N(t)$ in every step. As a result the particle number grows in the *numerical* scale; i.e., $N(t)$ grows unbounded as time step $\Delta t \to 0$. We give more details in Section 2.2.

This work contains three main contributions.

- We propose a novel negative particle method for general bilinear collisions (including both RGD and Coulomb collisions), in which the particle number only grows in the *physical* time scale, i.e., independent of time step Δt. Two key ideas are:
  - We propose a new decomposition formulation for the collision operator. In each time step, the positive/negative particles undergo two processes: regular collisions with particles sampled from f; and particles sampled from a source term of size $\mathcal{O}(\Delta t)$. Hence only extra $\mathcal{O}(\Delta t)$ particles are created.
  - We propose to use a small number of independently evolved particles (called "F-particles" below) to represent the particles sampled from f in the first process.

  This is similar to a prediction–correction type method. The small number of independently evolved particles give a coarse solution to f. Then a finer solution is obtained by evolving the positive and negative particles. The applicability of this method is not restricted to the Coulomb collisions, but for the general bilinear operators. To the best knowledge of the authors these ideas have not been used before.
- We propose a particle resampling method to reduce the number of particles when it grows over some threshold.
- We apply this new method to Coulomb collisions. This method require sampling of particles from the source term $Q(f_p - f_n, m)$, the change in the Maxwellian component m due to collisions with positive and negative particles. We perform a detailed analysis of this source term and design an efficient sampling method when Q is the LFP operator.

These techniques lead to a new negative particle method which is much more accurate and efficient than the existing methods for Coulomb collisions. In this work we focus on the spatially homogeneous case. The extension to spatially inhomogeneous simulation deserves further investigation.

The remainder of this paper is organized as follows. In Section 2 the negative particle method for rarefied gas collisions is reviewed and then generalized to Coulomb collisions. We show that this method is not stable for Coulomb collisions due to the severe growth of the number of particles. Next in Section 3 we describe a new negative particle method for general binary collisions. A new particle reduction technique is also introduced in Section 3.5. Then in Section 4 we apply this method to the LFP equation, with details on how to sample from the source term. The whole algorithm is summarized in Section 5, with some discussions on acceleration techniques. Finally we give some numerical results in Section 6 to illustrate the high accuracy and efficiency. Conclusions are included in Section 7. Various details of the analysis are provided in four appendices.

2. Negative particle methods

In a negative particle method, the distribution f is split into

$$f(\mathbf{v}, t) = m(\mathbf{v}, t) + f_d(\mathbf{v}, t) = m(\mathbf{v}, t) + f_p(\mathbf{v}, t) - f_n(\mathbf{v}, t), \tag{2.1}$$

where m is a Maxwellian distribution which does not necessary have the same moments as f. $f_d(\mathbf{v})$ is the deviational distribution which might be negative for some $\mathbf{v}$. f_p and f_n are the positive and negative parts of f_d.

Denote the densities of each part as

$$\rho = \int f(\mathbf{v}, t)\,\mathrm{d}\mathbf{v}, \quad \rho_m = \int m(\mathbf{v}, t)\,\mathrm{d}\mathbf{v}, \quad \rho_p = \int f_p(\mathbf{v}, t)\,\mathrm{d}\mathbf{v}, \quad \rho_n = \int f_n(\mathbf{v}, t)\,\mathrm{d}\mathbf{v},$$