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A grid-based binary model for coulomb collisions in plasmas

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ABSTRACT

Both binary and grid-based Langevin equations models for Coulomb collisions are used in particle simulation of plasmas. We introduce a variant of the conventional binary collision algorithm for performing Coulomb collisions. In this algorithm particles in a configuration space cell are not paired for collisions. Instead, for every test particle in the cell, a unique field particle is defined by randomly sampling a velocity distribution defined on the grid by accumulating moments of the particle distribution function(s). The test and field particle pair then undergoes a collision using the standard methodology for binary collisions. The performance of the new algorithm is illustrated in example computations and compared to a drag-diffusion Langevin equations algorithm. The grid-based algorithms do not conserve momentum and energy, although with good particle statistics the non-conservation is relatively small. Conservation can be restored after collisions using a shift and scaling of the momenta. The comparative merits of the new algorithm are discussed.

1. Introduction

In this work we introduce a new variant of a well-known algorithm for including Coulomb collisions in particle simulations of plasmas using finite-sized particles and deposition of charge and current densities onto a grid (particle-in-cell simulation, i.e., PIC simulation). In the binary algorithm, particles in a sub-domain, e.g., a cell, are grouped into discrete pairs of interacting particles such that the relative velocity is scattered through an angle whose statistical variance is dictated by the theory of Coulomb collisions in a plasma, in the Fokker–Planck limit [1,2]. The post-collision velocities of the interacting pair conserve momentum and energy relative to the pre-collision velocities. In the second type of algorithm, the collisions are modeled by defining test and field particles; and the test-particle velocity is subject to drag and diffusion in three velocity dimensions using Langevin equations whose drag and diffusion coefficients depend jointly on the velocity of the test particle and the moments of the field-particle velocity distribution deposited on the configuration-space mesh [3–7]. The grid-based Langevin equations model conserves particle number trivially and conserves energy and momentum approximately in a statistical sense after averaging over many collisions and over the velocity distribution functions, although energy and momentum conservation can be repaired by scaling and shifting velocities after the Monte Carlo collisions occur on each time step [4,6]. The drag and diffusion coefficients are derived from the classical theory of screened Coulomb collisions in the Fokker–Planck limit [4,8–10].

Coulomb collisions are an important physics component of many plasma phenomena. Furthermore, computing collisions in particle-in-cell plasma simulation is a significant computational burden; and some collision algorithms are favored over others depending on considerations of the physics and the computational burden. Thus, it is of practical interest to assess the efficacy and performance of a new variant of the standard binary collision algorithm in which the field particle is created by

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random sampling from a velocity distribution that is computed from statistical moments of the particles accumulated onto the configuration-space grid. In particular, we introduce a grid-based variant of the algorithm of Takizuka and Abe (TA) [1]. We describe the algorithm in Section 2. We illustrate its performance in example calculations, examine how good the energy conservation is as a function of the particle statistics, discuss how momentum and energy conservation can be restored, and compare the new algorithm to the drag-diffusion Langevin equation algorithm of Lemons, et al. [6] in Section 3. We discuss the comparative merits of the new grid-based collision algorithm and its possible extension in Section 4. The merits of the grid-based TA algorithm are as follows: the grid-based TA algorithm is slightly more accurate than the Lemons, et al. algorithm in our example simulations, allows a $\sim 10\times$ larger time step for accurate electron–ion collisions, and tolerates the rare large Monte Carlo kick much better than does the Lemons, et al. algorithm; in situations where the ions and electrons may have unequal weights but share a common charge-to-mass ratio for each respective species so that application of the traditional TA algorithm becomes problematic, the grid-based TA scheme is a natural alternative and energy/momentum conservation can be restored; the grid-based TA scheme, like other grid-based collision algorithms, is well suited for including Coulomb collisions in a particle–fluid hybrid plasma simulation; the grid-based TA scheme can accommodate some of the self-consistent evolution of the field-particle velocity distribution without having to solve for the Rosenbluth potentials (an elliptic equation in velocity space) to update the drag-diffusion coefficients in the Langevin equations approach of [4], [5], and [6]; the grid-based collision algorithms in [4], [5], and [6] can be subject to a noise-induced instability, while the grid-based TA scheme is not; and the grid-based or traditional TA collision algorithm can be extended straightforwardly to different collision models subject to some restrictions.

2. Grid-based Takizuka and Abe collision algorithm

Ref. [11] gives an overview of some of the fundamentals of two Langevin equations collision algorithms and Takizuka and Abe's binary collision algorithm. In the Langevin equation models [3–7,10], Langevin equations in three velocity dimensions containing drag and diffusion terms are integrated, typically with a simple first-order, forward Euler integration [3–7,10,11,14]. The algorithms are based on the theory describing screened Coulomb collisions in the Fokker–Planck limit [8,9,15].

In the classic work of Takizuka and Abe [1] a binary algorithm for Coulomb collisions was introduced. In the binary algorithm, equally weighted particles in a cell are paired; and then the relative velocity vector of the two particles is scattered through a random angle with variance dictated by the theory of screened Coulomb collisions in a plasma [8,9]. After the relative velocity vector is scattered, the two scattered particle velocities are reconstructed such that particle momentum and energy are conserved algebraically. Particle number is conserved identically. Nanbu [2] extended the algorithm of Takizuka and Abe [1] to allow for a larger time step by aggregating multiple collisions. In Takizuka and Abe [1], the relative velocity of a pair is scattered through an angle Θ related to an angle δ by $\delta = \tan(\Theta/2)$ with variance given by

$$\begin{aligned} &\langle \delta^2 \rangle = 2\pi q_1^2 q_2^2 n_{(1,2)<} \ln \Lambda \Delta t / m_{12}^2 u^3 \\ &\mathbf{u} = \mathbf{v}_1 - \mathbf{v}_2, \quad m_{12} = m_1 m_2/(m_1 + m_2) \end{aligned} \tag{1a}$$

$$\mathbf{v}_1^{t+\Delta t} = \mathbf{v}_1^t + \frac{m_{12}}{m_1}\Delta \mathbf{u}, \quad \mathbf{v}_2^{t+\Delta t} = \mathbf{v}_2^t - \frac{m_{12}}{m_2}\Delta \mathbf{u}, \tag{1b}$$

and through a random angle ϕ about the axis of the relative velocity before the scattering event, where $\ln\Lambda$ is the Coulomb logarithm [8,9], $q_{1,2}$ and $m_{1,2}$ are the charges and masses of the two colliding particles, $\mathbf{u}$ is the relative velocity of the two particles, $\Delta\mathbf{u}$ is the change in the relative velocity vector due to the rotation, and $n_{(1,2)<}$ is the smaller of the densities $n_{1,2}$. The post-collision velocity vectors of the scattered pair are constructed from the scattered relative velocity vector. There is no separation of test and field particles in the binary scheme, and there is no assumption that the velocity distribution is isotropic and Maxwellian (ignoring corrections to $\ln\Lambda$). This method conserves particle number, energy and momentum.

In the work of Wang et al. [12] the convergence properties of the Takizuka and Abe, and the Nanbu binary collision operators with respect to particle number and time step were studied. It was found that the Nanbu collision algorithm achieved a factor of two improvement in relative accuracy over the Takizuka and Abe basic algorithm for the same time step for like-species collisions and an improvement for unlike-species collisions depending on the mass ratio. The underlying properties of the Nanbu algorithm were studied analytically in the work of Dimits et al. [13].

Both the grid-based Langevin equations and binary collision algorithms can be generalized to semi-relativistic collisions [16,17]. To accommodate a minority component of relativistic particles in a plasma that is otherwise non-relativistic, the binary algorithm Eq. (1a) is modified by replacing $n_{(1,2)<}$ with n_2 and replacing the denominator $m_{12}{}^2u^3$ with $p^2\mathrm{v}$ where p and v are the momentum and velocity of the test particle in the rest frame of the field particle before the collision [18]. Then

$$\langle \Delta\theta^2 \rangle = 8\pi q_1^2 q_2^2 n_2 \ln\Lambda \Delta t / p_1^2 \mathrm{v}_1 \tag{2}$$

is the variance of the polar scattering angle of the relative velocity in the rest frame of the field particle. Lorentz transformations are used between the laboratory and rest frames of the field particle as in Chapter 12 of Jackson's book [18]. We note that n_2 (the density of the field particles) is not computed relativistically here, which restricts the applicability of the model. The field particles on average must be nonrelativistic in their motion with respect to the laboratory frame. In addition, there