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Journal of Computational Physics 227 (2008) 2286–2292
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

A Monte-Carlo method for coulomb collisions in hybrid plasma models

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Received 3 May 2007; received in revised form 22 November 2007; accepted 27 November 2007
Available online 8 December 2007

Abstract

A procedure for implementing Coulomb collisions into hybrid (particle-fluid) plasma models is outlined which is rapid in execution due to the use of approximate expressions for the collision integrals and conserves energy and momentum exactly. Particles undergo dynamic friction and diffusion in velocity-space at rates consistent with the velocity-dependent Fokker–Planck diffusion coefficients and there are no assumptions made about the shape or size of the particle distribution function. The method is tested against the analytical theory of test particle slowing in a background plasma and the thermal equilibration of a Maxwellian distribution.

Keywords: Coulomb collision; Fokker–Planck; Hybrid model; Monte-Carlo simulation

1. Introduction

Many plasma models treat either the ions or the electrons as a fluid in local thermodynamic equilibrium while retaining the kinetic aspects of the other component [1,2]. Such models have been applied to a variety of physical systems: from fast electron transport in intense laser–plasma interactions [3] to fast ignition [4] and very recently to coronal mass ejections [5]. In these models, there often arises a need to simulate the Coulomb collisional interaction of the kinetic component with the fluid background.

The modelling of Coulomb interactions between two kinetic species of charged particle was pioneered by Takizuka and Abe in their seminal paper by [6]. Their method, which utilizes Monte-Carlo techniques, is based on the random pairing of particles in close proximity, the calculation of a scattering angle in the centre-of-mass frame and the subsequent acceleration of those particles due to the interaction. This model has been improved and commented on many times since its first publication, in, e.g. [7,8]. Indeed, there is a wealth

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doi:10.1016/j.jcp.2007.11.037

of information on the implementation of Coulomb collisions in particle–particle models [9–11] (e.g. Particle-In-Cell models) but relatively little on the subject for hybrid particle-fluid models.

In principle, it is straightforward to apply the model of [6] to the case in which one component is a background fluid. This can be achieved by generating the background particles at random (every time-step), consistent with a local Maxwellian distribution at the fluid temperature. However, in the case that the kinetic particle and background particle masses differ by a large factor, a prohibitively small time-step is required to model the scattering. This is because the scattering angle is calculated in the centre-of-mass frame, and the scattering angle in the laboratory frame may be much smaller (by a factor of the order of the mass ratio). Hence, in order to simulate, for example, the scattering of a particle through an angle of $\pi/2$ radians, it may be necessary to over-resolve the relevant collision time.

A model for colliding a particle species with a fluid background has been developed by Jones et al. [12] through the calculation of a grid-based particle force (as in [13]). This model conserves energy and momentum, is fast in execution and simple in implementation. However, while it does reproduce the multi-fluid momentum and energy transport equations on average, it does not necessarily evolve the particle distribution function in the correct way. It is essentially a low-order kinetic model, because only the first-(momentum) and second-(energy) order moment equations are considered. As in Manheimer et al.'s Langevin approach [14], the coefficients that determine particle scattering are not functions of the particle velocity and this may be too severe an approximation when a more exact description of transport is required (as opposed to, for example, the description of bulk properties such as the slowing of a fast beam of particles). Much analytic progress has also been made recently in the case of velocity-independent coefficients [15]. In this paper an alternative model is presented which evolves the particle distribution function according to the Fokker–Planck friction and diffusion coefficients for test particles scattering off a Maxwellian background fluid. These coefficients have been derived previously [16], and extended upon in a Langevin form by Cadjan and Ivanov [10], who consider the case in which both colliding species are represented by particles that undergo Langevin acceleration. The method described in this paper is an application of these ideas to hybrid plasma modelling in which at least one species is represented by a fluid (rather than by particles) and the rest of the plasma has a particle description. It is general in the sense that it applies to species of any given charge or mass (unlike [13,12,14]) and there is no assumption as to the velocity-distribution of the particle species (unlike and [15]). The method also conserves energy and momentum exactly.

In the next section, the reduction of the Fokker–Planck equation to a Langevin form appropriate to a particle-fluid description is outlined as well as how to expedite the calculation of the required background distribution integrals and enforce exact momentum and energy conservation through their transfer to the fluid. The final section describes some basic tests of the method.

2. Description of the method

Chandresekhar (as detailed in [16]) calculated the Fokker–Planck coefficients of dynamical friction and diffusion for a test particle incident on a (stationary) Maxwellian distribution of field particles. Here, this is extended to the case of a non-stationary background in which the only assumption is that the background can be represented by a Maxwellian distribution drifting at the background fluid velocity. Under these conditions, test particle motion is determined by three coefficients. The first represents a frictional force and is deterministic. For a test particle with velocity w, charge Z and mass m incident on a Maxwellian distribution of field particles with thermal speed $v_{\mathrm{th}} = \sqrt{2T/m_{\mathrm{f}}}$, charge Z_{f} and mass m_{f}, this friction is described by

$$\frac{\partial w_{\parallel}}{\partial t} = -A(1 + m/m_{\mathrm{f}})\frac{G(w/v_{\mathrm{th}})}{v_{\mathrm{th}}^2}, \tag{1}$$

where $A = Z^2 Z_{\mathrm{f}}^2 n_{\mathrm{f}} \ln\Lambda / 2\pi m^2 \epsilon_0^2$,

$$G(x) = \frac{\mathrm{Erf}(x) - x\frac{\partial \mathrm{Erf}(x)}{\partial x}}{2x^2}, \tag{2}$$

and $\mathrm{Erf}(x)$ is the standard error function. The other coefficients represent diffusion in velocity-space and as such are stochastic. They characterise particle diffusion in directions parallel ($\|$) and perpendicular ($\perp$) to w, which occurs at different rates according to

$$\frac{\partial w_\|^2}{\partial t} = A\frac{G(w/v_{\mathrm{th}})}{w}, \tag{3}$$

and

$$\frac{\partial w_\perp^2}{\partial t} = A\frac{\mathrm{Erf}(w/v_{\mathrm{th}}) - G(w/v_{\mathrm{th}})}{w}. \tag{4}$$

The above equations can be used to evolve the particle velocities in time, but they assume that the background fluid with which the particles interact is at rest. Thus it is first necessary to transform to the local fluid reference frame via the transformation $c = v - u$ where v is the particle velocity and u is the fluid velocity (both defined in the laboratory frame). The velocity c therefore represents the particle velocity in the fluid's frame of reference. It is then beneficial to transform to a frame of reference in which the particle velocity is directed along the w_z-axis. This is done by rotating the particle velocity vector in the following manner:

$$\begin{pmatrix} 0 \\ 0 \\ w_z \end{pmatrix} = \begin{pmatrix} \cos(\theta)\cos(\phi) & \cos(\theta)\sin(\phi) & -\sin(\theta) \\ -\sin(\phi) & \cos(\phi) & 0 \\ \cos(\phi)\sin(\theta) & \sin(\theta)\sin(\phi) & \cos(\theta) \end{pmatrix} \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix},$$

so that $w_z = c$. Note that the actual matrix multiplication need not be carried out because the evaluation of w is trivial, though it is necessary to pre-calculate the angles θ and ϕ for the reverse operation (see below) from the formulae:

$$\theta = a\cos\left(\frac{c_z}{c}\right), \tag{5}$$

$$\phi = a\cos\left(\frac{c_x}{c_\perp}\right), \tag{6}$$

and

$$c_\perp = \sqrt{c_x^2 + c_y^2}. \tag{7}$$

The inverse cosine should be appropriately defined in both half-planes of $v_\perp$ for the calculation of ϕ.

At this point the w_z component of the particle velocity can be evolved with Eq. (1) via

$$\Delta w_z = \Delta t\frac{\partial w_\|}{\partial t}, \tag{8}$$

where Δt is the time-step.

Next, the stochastic change in w during Δt can be simulated by first evaluating the standard deviations $\sigma_\| = \sqrt{\Delta t \partial w_\|^2/\partial t}$ and $\sigma_\perp = \sqrt{\Delta t \partial w_\perp^2/\partial t}$ from Eqs. (3) and (4), respectively.

The parallel diffusion is simulated by further updating w_z according to

$$\Delta w_z = \widehat{N}(\sigma_\|), \tag{9}$$

where the operator $\widehat{N}(\sigma)$ represents the act of choosing a random number from a normal distribution with standard deviation σ. The perpendicular diffusion is similarly obtained:

$$\Delta w_x = \Delta w_\perp \cos(\theta_\perp), \tag{10}$$

$$\Delta w_y = \Delta w_\perp \sin(\theta_\perp), \tag{11}$$

where $\Delta w_\perp = \widehat{N}(\sigma_\perp)$ and $\theta_\perp$ is an angle chosen at random from a uniform distribution between 0 and 2π. Upon completion of the above steps, the particle velocity vector must be rotated back to its original frame via the inverse operation:

$$\begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix} = \begin{pmatrix} \cos(\theta)\cos(\phi) & -\sin(\phi) & \cos(\phi)\sin(\theta) \\ \cos(\theta)\sin(\phi) & \cos(\phi) & \sin(\theta)\sin(\phi) \\ -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix},$$

followed by a translation to the laboratory frame ($v = c + u$).

As in the method of [6], the time-step may not always be less than the relevant relaxation time for every particle. In this case a limiting factor (f_{lim}) must multiply the change in velocity given by Eq. (8). An appropriate expression for f_{lim} is

$$f_{\text{lim}} = \min(1, \frac{\tau_s}{2\Delta t}, \frac{\tau_\parallel}{2\Delta t}, \frac{\tau_\perp}{2\Delta t}), \tag{12}$$

where

$$\tau_s = \frac{w}{(\partial w_\parallel/\partial t)}, \tag{13}$$

$$\tau_\parallel = \frac{w^2}{(\partial w_\parallel^2/\partial t)}, \tag{14}$$

$$\tau_\perp = \frac{w^2}{(\partial w_\perp^2/\partial t)}. \tag{15}$$

In order that the method remain accurate the time-step should be much shorter than the above scattering times for all relevant particles, though the slowing time is most important of all because if the time-step is too large then particles may gain energy from the fluid rather than lose it. The method can be expedited by using approximations to the velocity-dependent functions appearing in Eqs. (1)–(4). This avoids the need to numerically evaluate the integrals. The following approximations, which can be clearly identified in Eqs. (1), (3) and (4) for the diffusion coefficients, are suggested:

$$\frac{G(w/v_{\text{th}})}{v_{\text{th}}^2} \approx \frac{w}{2w^3 + \frac{3}{2\sqrt{\pi}} v_{\text{th}}^3}, \tag{16}$$

$$\frac{G(w/v_{\text{th}})}{w} \approx \frac{v_{\text{th}}^2}{2w^3 + \frac{3}{2\sqrt{\pi}} v_{\text{th}}^3}, \tag{17}$$

$$\frac{\text{Erf}(w/v_{\text{th}}) - G(w/v_{\text{th}})}{w} \approx \frac{\text{Erf}(w/v_{\text{th}})}{w} - \frac{v_{\text{th}}^2}{2w^3 + \frac{3}{2\sqrt{\pi}} v_{\text{th}}^3}. \tag{18}$$

A polynomial fit can be used to evaluate $\text{Erf}(x)$. The above expressions were found by ensuring $G(x)$ tends to the correct limits as $x \to 0$ and $x \to \infty$ and they have a maximum fractional error of 0.1 in the intermediate regime.

Finally, it is noted that conservation of energy and momentum can be easily ensured. Within each grid cell, the change in the total particle momentum ($= \mathbf{p}_{\text{part}}$) can be calculated by summing the individual particle momenta before and after the algorithm is executed:

$$\Delta\mathbf{p}_{\text{part}} = \sum \Delta\mathbf{p}_i, \tag{19}$$

where the summation is over the particle index i and $\Delta\mathbf{p}_i$ is the change in the particle momentum during a time-step. Momentum is balanced by ensuring the total particle momentum is transferred to the fluid ($n_{\text{fluid}}\Delta\mathbf{p}_{\text{fluid}} = -n_{\text{part}}\Delta\mathbf{p}_{\text{part}}$) by adding the corresponding force to the fluid's equation of motion. This allows the change in the kinetic energy of the fluid (ΔK_{fluid}) to be calculated:

$$\Delta K_{\text{fluid}} = \frac{(\mathbf{p}_{\text{fluid}} + \Delta\mathbf{p}_{\text{fluid}})^2}{2m} - \frac{(\mathbf{p}_{\text{fluid}})^2}{2m}, \tag{20}$$

where m is the fluid particle mass.

The change in the total energy of the particles can be calculated in a similar fashion to Eq. (19) and energy conservation requires that this is transferred to the fluid (i.e. $n_{\text{fluid}}\Delta E_{\text{fluid}} = -n_{\text{part}}\Delta E_{\text{part}}$). The fluid's thermal

energy gain (ΔU_{fluid}) will be the difference between its total energy gain (ΔE_{fluid}) and its kinetic energy gain (ΔK_{fluid}):

$$\Delta U_{\text{fluid}} = \Delta E_{\text{fluid}} - \Delta K_{\text{fluid}}. \tag{21}$$

3. Tests

The method has been implemented in the 2D hybrid plasma simulation code GEMINI. This code, the 2D extension of the model described in [17], treats two species of ion kinetically (i.e. as particles) with a background electron fluid. Two important tests have been carried out with the code for a homogeneous plasma (and an ion to electron mass ratio was chosen to correspond to aluminium ions). The first is the simulation of particle ion slowing in an electron fluid, which is theoretically described by the simple equation of motion:

$$\frac{\partial v_{\parallel}}{\partial t} = -v_{\parallel}/\tau_{\text{s}}, \tag{22}$$

with $\tau_{\text{s}} = w^2/(\partial w_{\parallel}/\partial t)$. Fig. 1 shows that a beam of test ions slows at the correct rate. For the simulation, 100 particle ions were initialised with the same arbitrary velocity (which was around twice the background electron thermal speed) and the velocity shown is the average over all ions. The ions had a charge state of one. Under these conditions, the ion-electron thermal exchange time is comparable to the ion-electron slowing time. The analytical slowing rate was calculated by numerically integrating Eq. (22) in time. Agreement is very good until around a time $t/\tau_{\text{s}} = 5$, when ion diffusion starts to become dynamically important and Eq. (22) is no longer the appropriate equation of motion. Diffusion starts to become important once the ion beam has slowed sufficiently so that its average speed becomes comparable to the size of the diffusive "knocks" that each of the particles suffer in velocity-space. During the slowing the ion beam distribution was observed to remain close to Maxwellian (in the rest frame of the beam).

The second test considered is the equilibration of a Maxwellian distribution of particle ions to an isothermal background electron fluid. This test is more demanding than the first in that all aspects of the method are simultaneously important because it relies on a relatively fine balance between dynamical friction and parallel and perpendicular diffusion. For this test, 1000 particle ions were initialised at a temperature 10 times that of the background electron fluid. The results are shown in Fig. 2 for three different time-steps. The theoretical

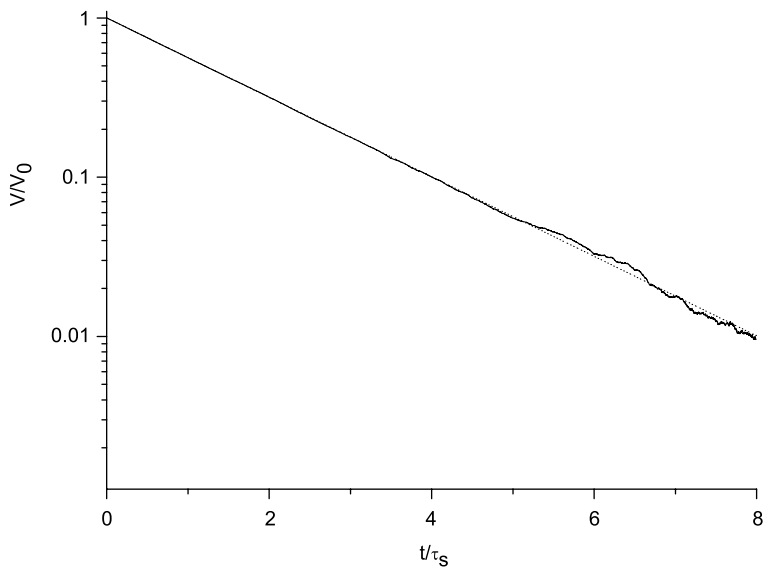

Fig. 1. The slowing of an ion beam by collisions with a background electron fluid. The average ion velocity is normalised to the initial velocity, while the time is normalised to the slowing timescale.

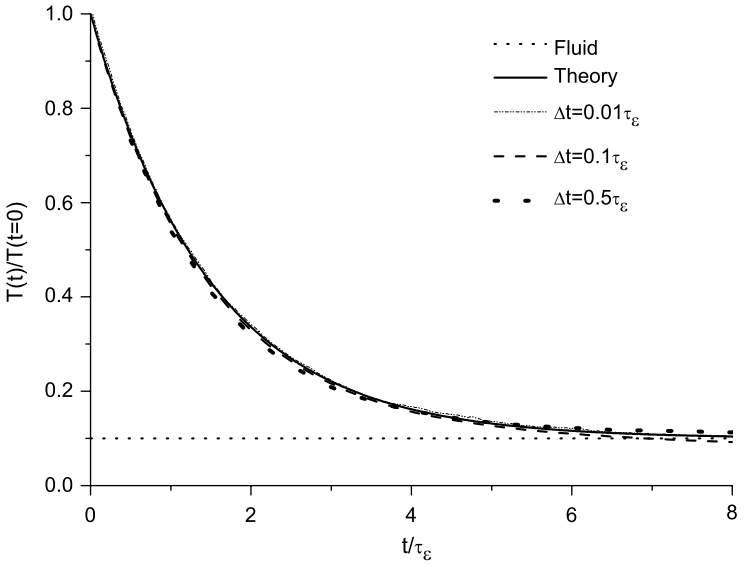

Fig. 2. The temperature of an initially Maxwellian ion particle distribution as it equilibrates with an isothermal background electron fluid for various timesteps. The theoretical prediction is shown as a solid line. The time is normalised to the equilibration timescale given in Eq. (24).

curve was calculated by solving the equation which describes the temperature evolution of two Maxwellian fluids [12]:

$$\frac{3}{2}\frac{\partial T_i}{\partial t} = -\nu_\epsilon (T_i - T_\mathrm{e}), \tag{23}$$

where

$$\nu_\epsilon = \frac{1}{\tau_\epsilon} = \frac{16\sqrt{\pi}Z^2\mathrm{e}^4 n_i \ln(\Lambda)}{m_\mathrm{e} m_i v_\mathrm{th}^3}, \tag{24}$$

and $v_\mathrm{th}^2 = 2(T_i/m_i + T_\mathrm{e}/m_\mathrm{e})$. Again, the agreement between theory and simulation is very good once the timestep (Δt) reaches one-hundredth of the equilibration time (τ_ϵ), while there is an acceptable error for $\Delta t = 0.1\tau_\epsilon$. When the equilibration is poorly resolved (i.e. for the case $\Delta t = 0.5\tau_\epsilon$), the rate of equilibration is relatively accurate but the equilibrium temperature is overestimated by a factor of about 1.11.

A point should be made regarding the practicality of the method: in many areas of high energy density physics the ion-electron collision time may well be shorter than hydrodynamical time-scales of interest but it is not so short so as to render the method computationally prohibitive. As an example consider the ion-electron collision frequency in Al wire-array Z-pinch precursor flow [18], where the typical electron density is 7×10^{17} cm^{-3} and the ion flow speed is 1.5×10^5 ms^{-1}. Taking an electron temperature of 20 (and $Z = 7$) results in a characteristic scattering time of ≈ 9 ns. By calling GEMINI's collision algorithm 10 times every scattering time, it is possible to simulate the precursor flow over hundreds of nanoseconds on a single CPU in a matter of hours, while still maintaining reasonable spatial ($\approx$80 μm) and particle-per-cell ($\approx$100) resolution in 2D.

References

[1] J.A. Byers et al., Hybrid simulations of quasineutral phenomena in magnetized plasma, J. Comput. Phys. 27 (1978) 363.
[2] D.W. Hewett, A global method of solving the electron-field equations in a zero-inertia-electron-hybrid plasma simulation code, J. Comput. Phys. 38 (1980) 378.
[3] J.R. Davies, A.R. Bell, M.G. Haines, Short-pulse high-intensity laser-generated fast electron transport into thick solid targets, Phys. Rev. E 56 (6) (1997).

[4] R.J. Mason, Heating mechanisms in short-pulse laser-driven cone targets, Phys. Rev. Lett. 96 (2006) 035001.
[5] L. Gargate et al., dHybrid: a massively parallel code for hybrid simulations of space plasmas, Comput. Phys. Commun. 176 (2007) 419.
[6] T. Takizuka, H. Abe, A binary collision model for plasma simulation with a particle code, J. Comput. Phys. 25 (1977) 205.
[7] R.H. Miller, M.R. Combi, A coulomb collision algorithm for weighted particle simulations, Geophys. Res. Lett. 21 (1994) 1735.
[8] K. Nanbu, Theory of cumulative small-angle collisions in plasmas, Phys. Rev. E 55 (1997) 4642.
[9] D.J. Larson, A coulomb collision model for pic plasma simulation, J. Comput. Phys. 188 (2003) 123.
[10] M.G. Cadjan, M.F. Ivanov, Langevin approach to plasma kinetics with coulomb collisions, J. Plasma Phys. 61 (1999) 89.
[11] N. Nakajima, W.X. Wang, M. Okamoto, S. Murakami, Vector implementation of nonlinear Monte-Carlo coulomb collisions, J. Comput. Phys. 128 (1996) 209.
[12] M.E. Jones et al., A grid-based coulomb collision model for pic codes, J. Comput. Phys. 123 (1996) 169.
[13] P.W. Rambo, R.J. Procassini, A comparison of kinetic and multi-fluid simulations of laser-produced colliding plasmas, Phys. Plasmas 2 (1995) 3130.
[14] W.M. Manheimer, M. Lampe, G. Joyce, Langevin representation of coulomb collisions in pic simulations, J. Comput. Phys. 138 (1997) 563.
[15] D.T. Gillespie, Exact numerical simulation of the Ornstein–Uhlenbeck process and its integral, Phys. Rev. E 54 (1996) 563.
[16] L. Spitzer, The Physics of Fully Ionized Gases, Interscience Publishers, 1956.
[17] M. Sherlock et al., Ion collisions and the z-pinch precursor column, Phys. Plasmas 11 (2004) 1609.
[18] S.V. Lebedev et al., Physics of wire array z-pinch implosions: experiments at imperial college, Plasma Phys. Control. Fusion 47 (2005) A91.