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MONTE CARLO COLLISION OPERATOR FOR δf GYROKINETIC PARTICLE SIMULATION CODES

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ABSTRACT

A δf-weighting scheme is proposed for investigating the gyrokinetic Fokker Planck equation describing the dynamics of e.m. perturbations in a multi-species toroidal magnetoplasma. It is shown that Monte Carlo collision operators can be consistently defined to describe Coulomb binary collisions in such a way to assure conservation of collisional invariants as well as to take into account the full nonlinear particle charactertistics.

Promising current areas of research in the physics of magnetically confined plasmas are related to the development of gyrokinetic simulation codes as well as the adoption, in such codes, of Monte Carlo methods to describe both Coulomb binary interactions as well as collective interactions produced by plasma turbulence. A significant deficiency of previous numerical simulation techniques [1-3] for plasma dynamics, which has been recently recognized [4-7], concerns the use of Monte Carlo collision operators which are inconsistent from the viewpoint of conservation laws, namely do not allow the fulfillment of the exact conservation laws characterizing the Fokker-Planck operator [i.e., particle number, total linear momentum and total kinetic energy conservation in a multi-species plasma]. In particular, Tessarotto et al.[4-6,9] have recently proposed Monte Carlo collision operators which exhibit the correct conservation laws (collisional invariants) and simulate accurately the Fokker-Planck collision operators. These operators can, in principle, be used in gyrokinetic particle simulation codes to describe consistently the influence of Coulomb binary collisions on the transport dynamics.

The purpose of this paper is to construct a discretization approach for the gyrokinetic distribution function based on a **δf-weighting scheme** [3,7,8,11-13] adopting a Monte Carlo approach to describe Coulomb binary collisions [as well as, possibly, particle-wave interactions]. This implies that Coulomb collisions are described in terms of a stochastic evolution operator, defining suitable Monte Carlo collision operators advancing in time each gyrokinetic variable. defining the gyrokinetic state of a set of test particles. In particular, such an operator is constructed in such a way to conserve the collisional invariants (particle number, total linear momentum and kinetic energy). Furthermore, since the Fokker-Planck operator fulfills the property of Galileian invariance as well as the condition of

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This is a preprint of a paper intended for presentation at a scientific meeting. Because of the provisional nature of its

self-adjointness (i.e., symmetry with respect to the customary definition of scalar product), one expects that the Monte Carlo operators reflect these symmetry properties [12,13].

Basic feature of Monte Carlo collision operators here adopted is that they can be expressed in terms of momentum, energy (and possibly higher moments), restoring coefficients; hence, they can be determined at each time step in terms of particle averages over suitable spatial cells [9]. In addition, it is possible to retain the full non-linear particle characteristics, as appropriate for the investigation of the nonlinear evolution of collisional eletromagnetic perturbations in a multispecies plasma [10,11].

We are interested here in describing the dynamics of a magnetoplasma described by a non-linear gyrokinetic equation of the form:

$$\mathscr{L}_s f_{1,s} = S_s f_{M_s} + C_s(f_M | f_1) \tag{1}$$

where the distribution function is assumed of the form

$$f_s = f_{M_s} + f_{1,s} \tag{2}$$

with f_{M_s} and $f_{1,s}$, respectively, suitable "explicit" and "implicit" parts. Here, in particular, f_{M_s} will be required to be a local Maxwellian distribution. Furthermore, $\mathscr{L}_s$ is the gyrokinetic Vlasov operator in the conservation form expressed in terms of an arbitrary set of v-space gyrokinetic coordinates z_i (for example, i=1,2); thus denoting as J the Jacobian of the transformation $(\underline{r},\underline{v}) \to (\underline{r},z_1,z_2,\varphi)$ [with φ a suitable gyrophase], $\mathscr{L}_s$ may be assumed of the form:

$$\mathscr{L}_s f_{1,s} = \frac{1}{J}\frac{\partial}{\partial t}\left[J f_{1,s}\right] + \frac{1}{J}\nabla\cdot\left[J(u\underline{b}+\underline{v}_D+\underline{v}_E) f_{1,s}\right] + \\ + \frac{1}{J}\frac{\partial}{\partial z_i}\left[J \langle \dot{z}_i \rangle_\phi f_{1,s}\right] \tag{3}$$

with $\underline{v}_D$ and $\underline{v}_E$, respectively, the diamagnetic and ExB drift velocities; the source term $S_s f_{M_s}$ reads

$$S_s f_{M_s} \equiv \mathscr{L}_s f_{M_s} = \frac{1}{J}\frac{\partial}{\partial t}\left[J f_{M_s}\right] + \frac{1}{J}\nabla\cdot\left[J(u\underline{b}+\underline{v}_D+\underline{v}_E) f_{M_s}\right] + \\ + \frac{1}{J}\frac{\partial}{\partial z_i}\left[J \langle \dot{z}_i \rangle_\phi f_{M_s}\right] \tag{4}$$

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For definitess, we shall require in the sequel that both $\underline{v}_E$ and $\langle \dot{z}_i \rangle_\phi$ are functionals of the perturbed distribution $f_{1,s}$ and hence Eq.(1) is nonlinear in $f_{1,s}$. More precisely, $\underline{v}_E$ and $\langle \dot{z}_i \rangle_\phi$ will be assumed as functionals of suitable moments of $f_{1,s}$, i.e., $I_s = \int d^3v\, X_s f_{1,s}$, with appropriate $X_s = X_s(\underline{r},\underline{v},t)$.

Similarly, the linearized Fokker-Planck collision operator reads, assuming that the gyrokinetic variables z_i (i=1,2) are normal, i.e., that the Coulomb diffusion tensor is diagonal in terms of them:

$$C_s(f_M | f_1) = \frac{1}{2}\frac{1}{J}\frac{\partial^2}{\partial z_i^2}\left[J \frac{\langle \Delta z_i^2 \rangle}{\Delta t} f_{1,s}\right] - \frac{1}{J}\frac{\partial}{\partial z_i}\left[J \frac{\langle \Delta z_i \rangle^{(o)}}{\Delta t} f_{1,s}\right] + \tag{5}$$

$$- \frac{1}{J}\frac{\partial}{\partial z_i}\left[J \frac{\langle \Delta z_i \rangle^{(1)}}{\Delta t} f_{M_s}\right]$$

where $\frac{\langle \Delta z_i^2 \rangle}{\Delta t}$ is the (diagonal) Coulomb diffusion tensor and $\frac{\langle \Delta z_i \rangle}{\Delta t} = \frac{\langle \Delta z_i \rangle^{(o)}}{\Delta t} + \frac{\langle \Delta z_i \rangle^{(1)}}{\Delta t}$ is the corresponding (Coulomb) friction vector [5].

A non-linear particle simulation approach for Eq.(1), based on a δf-weighting scheme [10,11], can be obtained adopting an extension of the approach recently pointed out by the present authors [5,6], based, instead, on a full discretization scheme for the kinetic distribution function. To construct a discretization scheme of this type for Eq.(1), we represent both $f_{M,s}(y,t)$ and $f_{1,s}(y,t)$ in the form:

$$f_{M,s}(y,t) \cong \sum_{j=1,N_s} N_{j,s}(\underline{y},t) f_{j,s}(\underline{y},t) \tag{6}$$

$$f_{1,s}(y,t) \cong \sum_{j=1,N_s} \eta_{j,s}(\psi,t) N_{j,s}(\underline{y},t) f_{j,s}(\underline{y},t) \tag{7}$$

with $N_{j,s}(\underline{y},t)$ and $\bar{\eta}_s(\psi,t) \equiv \eta_{j,s}(\psi,t) N_{j,s}(\underline{y},t)$ suitable particle weights and where the "discretized" distribution functions, $f_{j,s}(\underline{y},t)$, are assumed to fulfill at the (initial) time

t_o the initial (deterministic) condition [in the sequel the index j will be understood, when necessary]:

$$f_{j,s}(\underline{y},t=t_o) = \frac{1}{2\pi J}\,\delta^{(3)}(\underline{r}-\underline{r}_{o,j})\delta(z_1-z_{1o,j})\delta(z_2-z_{2o,j}) \tag{8}$$

The particle weights $\eta_{j,s}$ and the distribution $f_{j,s}$ at an arbitrary time t are here required to fulfill an appropriate "stochastic Liouville equation" [which, however, does **not** determine uniquely $\eta_{j,s}$ nor $f_{j,s}$] of the form:

$$\mathscr{L}\bar{\eta}_s f_{j,s}(\underline{y},t) + \frac{1}{J}\frac{\partial}{\partial z_m}\left[J\{\langle\!\langle a_m^{(0)}\rangle\!\rangle + a_m^{(S)}\}\bar{\eta}_s f_{j,s} + \right.$$
$$\left. + \langle\!\langle a_m^{(1)}\rangle\!\rangle N_{j,s} f_{j,s}\right] = S_s N_{j,s}(\underline{y},t) f_{j,s} \tag{9}$$

Here, $a_m \equiv \langle\!\langle a_m\rangle\!\rangle + a_m^{(S)}$, with $\langle\!\langle a_m\rangle\!\rangle = \langle\!\langle a_m^{(0)}\rangle\!\rangle + \langle\!\langle a_m^{(1)}\rangle\!\rangle$ is an appropriate generalized acceleration. More precisely, denoting with the brackets "$\langle\!\langle\ \rangle\!\rangle$" a suitable stochastic average to be defined, $\langle\!\langle a_m\rangle\!\rangle$ and $a_m^{(S)}$ are, respectively, the average and the stochastic $[a_m^{(S)}]$ part of the generalized acceleration. In particular, $\langle\!\langle a_m^{(0)}\rangle\!\rangle$ and $\langle\!\langle a_m^{(1)}\rangle\!\rangle$ denote to first two order [in a Larmor radius expansion] the leading-order contributions to $\langle\!\langle a_m\rangle\!\rangle$.

The phase-space trajectories of the test particles, i.e., $\underline{y}(t)=\{\underline{r}(t),z_1(t),z_2(t)\}$, are then solutions of the stochastic equations of motion:

$$\frac{d}{dt}\underline{r} = u\underline{b} + \underline{V} + \underline{v}_D + \underline{v}_E$$
$$\frac{d}{dt}z_i = \langle\!\langle a_i\rangle\!\rangle + a_i^{(S)} \quad (i=1,2) \tag{10}$$

with initial conditions $\underline{y}(t_o)=\{\underline{r}_o,z_{1o},z_{2o}\}$. These equations can be cast in the form of a stochastic evolution operators advancing in time the gyrokinetic varia- bles for z_i (i=1,2). It follows that the stochastic average can be defined so that, in particular, the average of $a_m(\underline{y}(t),t)$ is indeed $\langle\!\langle a_m(\underline{y}(t),t)\rangle\!\rangle$. Moreover, it can be shown that the accelerations $a_m^{(S)}$,$\langle\!\langle a_m^{(0)}\rangle\!\rangle$ and $\langle\!\langle a_m^{(1)}\rangle\!\rangle$ must be defined, for consistency with the gyrokinetic equation, Eq.(1), in terms of the Coulomb diffusion coefficients, i.e., respectively, as follows:

$$\langle\langle a_m^{(0)} \rangle\rangle = \frac{\langle \Delta z_m \rangle^{(o)}}{\Delta t} \tag{11}$$

$$\langle\langle a_m^{(1)} \rangle\rangle = \frac{\langle \Delta z_m \rangle^{(1)}}{\Delta t} \tag{12}$$

$$\hat{a}_m^{(S)} = \frac{d}{dt}\left[3 \int_{t_n}^{t} d\tau \frac{\langle \Delta z_m^2 \rangle}{\Delta t} \right]^{1/2} \tag{13}$$

We stress that a significant aspect of the present Monte Carlo operators is that, indipendently of the particle weights [$N_{j,s}(\underline{v},t)$ and $\eta_{j,s}(\psi,t)$], they can be proven to fulfill the conservation laws (collisional invariants) charac- teristic of the Fokker-Planck collision operator, i.e., the conservation of particle number, total linear momentum as well as total kinetic energy [5]. This corrects the deficiency of previous numerical simulation techniques for plasma dynamics [1-3], based on inconsistent Monte Carlo operators.

The discretization scheme here proposed, in contrast to previous approaches due to Dimits and Cohen [7], exhibits the significant feature that the particle weight [$\eta_{j,s}(\underline{r},\underline{v},t)$, with j and s the particle and species index] is **not** used to implement the conservation of momentum or energy; hence, it can be used to satisfy additional constraints, to be suitably defined. Notice that the particle weight $\eta_{j,s}(\underline{r},\underline{v},t)$ can always be represented as: $\eta_{j,s}(\underline{r},\underline{v},t) = \langle \eta_s(\underline{r},t) \rangle + \hat{\eta}_{j,s}(\underline{r},\underline{v},t)$, with $\langle \eta_s(\underline{r},t) \rangle$ some suitable local average [on test particles of species s]. As an example, for transport calculations in neoclassical theory (as well as to turbulence) the average weight $\langle \eta_s(\underline{r},t) \rangle$ can be determined in such a way to obtain particle flux ambipolarity, and Onsager symmetry, independently of the number of test particles used in the discretization [12,13]. An application, which deserves particular attention by itself, concerns toroidal magnetoplasmas with finite aspect-ratio and exhibiting rotation shear as well as, possibly, strong rotation speeds [14].

However, in gyrokinetic particle-simulation codes, more generally, particle weights could be determined to fit experimental data or higher-order symmetries.

We stress that for the numerical implementation of the previous stochastic differential equations, Eqs.(10), suitable ODE solvers (particle pushers) should be used. In particular, expecially implementing a split-time algorithm, only ODE solvers having only one initial condition (state) should preferably be used. In fact multiple-states predictor-corrector pushers require that the Monte Carlo operastor be applied several times at each time step, i.e.,for example, twice for a two-state predictor-corrector, an approach [7] which appears, therefore, inconvenient from the viewpoint of code speed optimization.

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