

Nonrandom collision method for delta-f PIC simulations

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Abstract

In delta-f simulations of tokamak physics, the distribution function is written as a background plus a small perturbation, where the background is usually taken to be Maxwellian. A Canonical Maxwellian is a function of particle constants of motion which reduces to a Maxwellian in the limit of zero orbit width. If the background is taken to be a Canonical Maxwellian in PIC simulations, the large orbit contribution to the rapid growth of the particle weights, and the associated statistical noise, would be eliminated. Another important contributor to statistical noise in turbulence simulations is the phase-space filamentation which develops over long times. This should be reduced by including Coulomb collisions as a velocity diffusion process. A linearized collision operator for simulating ion-ion collisions has been developed, which consists of a diffusive test-particle part plus a field-particle part constructed to maintain conservation laws and have the correct null space. The friction and diffusion coefficients in the test-particle operator are evaluated using a shifted Maxwellian with a parallel flow velocity consistent with a Canonical Maxwellian to second order in poloidal gyroradius. A Langevin method for use in delta-f PIC codes has also been developed, which is equivalent to the linearized collision operator.

It provides update equations for the components of particle velocity parallel and perpendicular to the magnetic field, in the form of acceleration contributions from the collisional friction and field-particle drag, plus diffusive contributions modeled by sampling velocity increments in a way consistent with the diffusion coefficients in the test-particle collision operator. This method uses deterministic sampling as described in recent work[1], in which the samples are chosen as quadrature points in approximate evaluations of moments of the Fokker-Planck Green's function. This should eliminate the sampling noise which occurs in random sampling (Monte-Carlo) collision methods.

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[1] Fred L. Hinton, submitted to Physics of Plasmas
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Canonical Maxwellian

A Canonical Maxwellian is defined by

$$f(v_{\perp}, v_{\parallel}, \vec{x}) = \exp[\alpha(\psi^*) - \beta(\psi^*)\mathcal{E}] \quad (1)$$

which is a function of the particle constants of motion ψ^* and \mathcal{E} . The Canonical angular momentum (gyroaveraged) is

$$\psi^* = \psi - \frac{I}{\Omega_i} v_{\parallel} \quad (2)$$

where ψ is the poloidal flux function, $I = RB_T$, with B_T is the toroidal magnetic field, and $\Omega_i = eB/m_i c$, the ion gyrofrequency. The total particle energy is

$$\mathcal{E} = \frac{1}{2}(v_{\perp}^2 + v_{\parallel}^2) + \frac{e_i}{m_i} \Phi(\vec{x}) \quad (3)$$

where Φ is the electrostatic potential energy.

A shifted Maxwellian is defined by

$$f_{sm}(v_{\perp}, v_{\parallel}, \vec{x}) = n_i(\vec{x}) \left[\frac{m_i}{2\pi T_i(\psi)} \right]^{3/2} \exp\left\{ -\frac{m_i}{2T_i(\psi)} [v_{\perp}^2 + (v_{\parallel} - u_{\parallel}(\vec{x}))^2] \right\} \quad (4)$$

where n_i is the ion density, T_i is the ion temperature, and u_{\parallel} is the parallel ion flow velocity.

The functions $\alpha(\psi^*)$ and $\beta(\psi^*)$ can be identified by considering the limit of zero orbit width, $\psi^* - \psi \rightarrow \mathbf{0}$, when the Canonical Maxwellian must reduce to a Maxwellian. Since the flow velocity must go to zero for zero orbit width,

$$\alpha(\psi) = \ln N(\psi) - \frac{3}{2} \ln T_i(\psi) + \frac{3}{2} \ln \left(\frac{m_i}{2\pi} \right) \quad (5)$$

where $N(\psi) = n_i(\vec{x}) \exp[e\Phi(\vec{x})/T_i(\psi)]$ and $\beta(\psi) = m_i/T_i(\psi)$.

Then we have

$$\ln f - \ln f_{sm} = \alpha(\psi_*) - \alpha(\psi) - [\beta(\psi_*) - \beta(\psi)]\mathcal{E} + \beta(\psi) \left(-v_{\parallel} u_{\parallel} + \frac{1}{2} u_{\parallel}^2 \right) \quad (6)$$

Small orbit width approximation

If the orbit width is small but not zero, we can expand $\alpha(\psi_*)$ and $\beta(\psi_*)$ in Taylor series; to second order, we have

$$\alpha(\psi_*) \simeq \alpha(\psi) + \alpha'(\psi)(\psi_* - \psi) + \frac{1}{2}\alpha''(\psi)(\psi_* - \psi)^2 \quad (7)$$

and

$$\beta(\psi_*) \simeq \beta(\psi) + \beta'(\psi)(\psi_* - \psi) + \frac{1}{2}\beta''(\psi)(\psi_* - \psi)^2 \quad (8)$$

Then, using $\psi_* - \psi = -(I/\Omega_i)v_{\parallel}$, we have

$$\begin{aligned} \ln f - \ln f_{sm} &\simeq -\frac{I}{\Omega_i}\alpha'v_{\parallel} + \frac{1}{2}\frac{I^2}{\Omega_i^2}\alpha''v_{\parallel}^2 \\ &+ \left(\frac{I}{\Omega_i}\beta'v_{\parallel} - \frac{1}{2}\frac{I^2}{\Omega_i^2}\beta''v_{\parallel}^2 \right) \varepsilon + \beta \left(-v_{\parallel}u_{\parallel} + \frac{1}{2}u_{\parallel}^2 \right) \quad (9) \end{aligned}$$

Parallel Flow

We shall determine the parallel flow by maximizing an entropy expression defined by

$$S \equiv \frac{1}{n_i} \int d^3v f_{sm} (\ln f - \ln f_{sm}) \quad (10)$$

where f is the Canonical Maxwellian. We use the small orbit width approximation. After substituting Eq.(9) and carrying out the velocity integrals, we have

$$\begin{aligned} S &= -\frac{I}{\Omega_i} \alpha' u_{\parallel} - \beta \frac{u_{\parallel}^2}{2} + \frac{I}{\Omega_i} \beta' \left(\frac{5 T_i}{2 m_i} + \frac{u_{\parallel}^2}{2} \right) u_{\parallel} + \frac{I}{\Omega_i} \beta' \frac{e_i}{m_i} \Phi u_{\parallel} \\ &+ \frac{1}{2} \frac{I^2}{\Omega_i^2} \left(\frac{T_i}{m_i} + u_{\parallel}^2 \right) \alpha'' \\ &- \frac{1}{2} \frac{I^2}{\Omega_i^2} \left[\frac{5 T_i^2}{2 m_i^2} + \left(\frac{4 T_i}{m_i} + \frac{1}{2} u_{\parallel}^2 \right) u_{\parallel}^2 + \left(\frac{T_i}{m_i} + u_{\parallel}^2 \right) \frac{e_i}{m_i} \Phi \right] \beta'' \quad (11) \end{aligned}$$

We assume the flow velocity is much smaller than the ion thermal speed, and neglect the terms cubic and quartic in u_{\parallel} , so that

$$\begin{aligned}
 S = & -\frac{I}{\Omega_i} \alpha' u_{\parallel} - \beta \frac{u_{\parallel}^2}{2} + \frac{5}{2} \frac{I}{\Omega_i} \beta' \frac{T_i}{m_i} u_{\parallel} + \frac{I}{\Omega_i} \beta' \frac{e_i}{m_i} \Phi u_{\parallel} \\
 & + \frac{1}{2} \frac{I^2}{\Omega_i^2} \left(\frac{T_i}{m_i} + u_{\parallel}^2 \right) \alpha'' - \frac{1}{2} \frac{I^2}{\Omega_i^2} \left[\frac{5}{2} \frac{T_i^2}{m_i^2} + \frac{4T_i}{m_i} u_{\parallel}^2 + \left(\frac{T_i}{m_i} + u_{\parallel}^2 \right) \frac{e_i}{m_i} \Phi \right] \beta''
 \end{aligned}
 \tag{12}$$

We now determine u_{\parallel} by maximizing \mathcal{S} . By taking the derivative with respect to u_{\parallel} and setting it to zero, we find

$$u_{\parallel} = \frac{I}{\Omega_i \beta} \left[-\alpha' + \left(\frac{5}{2} \frac{T_i}{m_i} + \frac{e_i}{m_i} \Phi \right) \beta' \right] \frac{1}{D} \quad (13)$$

where

$$D = 1 - \frac{I^2}{\Omega_i^2 \beta} \alpha'' + \frac{I^2}{\Omega_i^2 \beta} \left(4 \frac{T_i}{m_i} + \frac{e_i}{m_i} \Phi \right) \beta'' \quad (14)$$

Using the definitions of $\alpha(\psi)$ and $\beta(\psi)$, this can be written

$$u_{\parallel} = -\frac{IT_i}{m_i \Omega_i} \left[\frac{\partial}{\partial \psi} \ln \left(\frac{N}{T_i^{3/2}} \right) + \left(\frac{5}{2} + \frac{e_i}{T_i} \Phi \right) \frac{\partial}{\partial \psi} \ln T_i \right] \frac{1}{D} \quad (15)$$

where

$$D = 1 - \frac{I^2 T_i}{m_i \Omega_i^2} \left\{ \frac{\partial^2}{\partial \psi^2} \ln N + \left(\frac{5}{2} + \frac{e \Phi}{T_i} \right) \frac{\partial^2}{\partial \psi^2} \ln T_i - \left(4 + \frac{e \Phi}{T_i} \right) \left(\frac{\partial}{\partial \psi} \ln T_i \right)^2 \right\} \quad (16)$$

Poloidal Flow

The poloidal flow is given by

$$\mathbf{u}_p = \vec{\mathbf{u}} \cdot \vec{\mathbf{B}}_p / B_p = (\vec{\mathbf{u}}_{\perp} + \hat{\mathbf{b}}u_{\parallel}) \cdot \vec{\mathbf{B}}_p / B_p \quad (17)$$

where $\vec{\mathbf{B}}_p$ is the poloidal magnetic field, u_{\parallel} is the parallel component of the flow velocity, and $\hat{\mathbf{b}} = \vec{\mathbf{B}}/B$ is a unit vector parallel to $\vec{\mathbf{B}}$.

The perpendicular component of the flow velocity is

$$\vec{\mathbf{u}}_{\perp} = \frac{c}{n_i e B} \hat{\mathbf{b}} \times (\nabla(n_i T_i) + n_i e \nabla \Phi) \quad (18)$$

whose poloidal component is

$$\vec{\mathbf{u}}_{\perp} \cdot \vec{\mathbf{B}}_p / B_p = \frac{c I B_p T_i}{e B^2} \left[\frac{N'}{N} + \left(1 + \frac{e \Phi}{T_i} \right) \frac{T'_i}{T_i} \right] \quad (19)$$

Also, from Eq.(20) we have

$$u_{\parallel} \hat{\mathbf{b}} \cdot \vec{\mathbf{B}}_p / B_p = - \frac{c I B_p T_i}{e B^2} \left[\frac{N'}{N} + \left(1 + \frac{e \Phi}{T_i} \right) \frac{T'_i}{T_i} \right] \frac{1}{D} \quad (20)$$

so the poloidal flow velocity is

$$u_p = \frac{cIB_p T_i}{eB^2} \left[\frac{N'}{N} + \left(1 + \frac{e\Phi}{T_i} \right) \frac{T_i'}{T_i} \right] \left(1 - \frac{1}{D} \right) \quad (21)$$

By using the definition of $N(\psi)$, the poloidal flow velocity can be written as

$$u_p = \frac{cIB_p T_i}{eB^2} \left[\frac{\partial}{\partial \psi} \ln(n_i T_i) + \frac{e}{T_i} \frac{\partial \Phi}{\partial \psi} \right] \left(1 - \frac{1}{D} \right) \quad (22)$$

where

$$D = 1 - \frac{I^2 T_i}{m_i \Omega_i^2} \left\{ \frac{\partial^2}{\partial \psi^2} \ln n_i + \frac{e}{T_i} \frac{\partial^2 \Phi}{\partial \psi^2} - 2 \frac{e}{T_i} \frac{\partial \Phi}{\partial \psi} \frac{\partial}{\partial \psi} \ln T_i \right. \\ \left. + \frac{5}{2} \frac{\partial^2}{\partial \psi^2} \ln T_i - 4 \left(\frac{\partial}{\partial \psi} \ln T_i \right)^2 \right\} \quad (23)$$

The isothermal case; effect of orbit squeezing

If the temperature gradient is zero, the above expressions simplify:

$$u_{\parallel} \simeq -\frac{IT_i}{m_i\Omega_i} \frac{N'}{N} \frac{1}{D} \quad \text{where } D \simeq 1 + \frac{I}{\Omega_i} \frac{\partial u_{\parallel}}{\partial \psi} \quad (24)$$

Therefore, the poloidal flow velocity is

$$u_p \simeq \frac{I^2 T_i B_p}{m_i \Omega_i^2 B} \left(\frac{\partial}{\partial \psi} \ln n_i + \frac{e_i}{T_i} \frac{\partial \Phi}{\partial \psi} \right) \frac{\partial u_{\parallel}}{\partial \psi} \quad (25)$$

If, in addition, $|(\partial^2 / \partial \psi^2) \ln n_i| \ll (e_i / T_i) |\partial^2 \Phi / \partial \psi^2|$, then

$$u_p \simeq \frac{IT_i B_p}{m_i \Omega_i B} \left(\frac{\partial}{\partial \psi} \ln n_i + \frac{e_i}{T_i} \frac{\partial \Phi}{\partial \psi} \right) \left(1 - \frac{1}{D} \right) \quad (26)$$

where

$$D \simeq 1 - \frac{cI^2}{\Omega_i B} \frac{\partial^2 \Phi}{\partial \psi^2} \quad (27)$$

which may be recognized as the orbit-squeezing factor.

Nonlinear Collision Term

The distribution function f is assumed to be independent of gyrophase, and only a function of $\vec{x}, v_{\perp}, v_{\parallel}$. The nonlinear Fokker-Planck ion-ion collision term is given by

$$C[f, f] = -\frac{1}{2} \left\{ \frac{1}{v_{\perp}} \frac{\partial}{\partial v_{\perp}} \left[v_{\perp} A_{\perp}[f] f - v_{\perp} \left(D_{\perp}[f] \frac{\partial f}{\partial v_{\perp}} + D_{\times}[f] \frac{\partial f}{\partial v_{\parallel}} \right) \right] + \frac{\partial}{\partial v_{\parallel}} \left[A_{\parallel}[f] f - \left(D_{\times}[f] \frac{\partial f}{\partial v_{\perp}} + D_{\parallel}[f] \frac{\partial f}{\partial v_{\parallel}} \right) \right] \right\} \quad (28)$$

The Fokker-Planck coefficients A_{\perp} , A_{\parallel} , D_{\perp} , D_{\times} , and D_{\parallel} are integrals containing f . The friction coefficients are

$$A_{\perp}[f] = \Gamma \frac{\partial h}{\partial v_{\perp}} \quad (29)$$

$$A_{\parallel}[f] = \Gamma \frac{\partial h}{\partial v_{\parallel}} \quad (30)$$

The diffusion coefficients are

$$D_{\perp}[f] = \frac{\Gamma}{2} \frac{\partial^2 g}{\partial v_{\perp}^2} \quad (31)$$

$$D_{\times}[f] = \frac{\Gamma}{2} \frac{\partial^2 g}{\partial v_{\perp} \partial v_{\parallel}} \quad (32)$$

$$D_{\parallel}[f] = \frac{\Gamma}{2} \frac{\partial^2 g}{\partial v_{\parallel}^2} \quad (33)$$

where $\Gamma = (8\pi e_i^4 / m_i^2) \ln \Lambda$, with $\ln \Lambda$ the Coulomb logarithm, and h and g are the Rosenbluth potentials:

$$h(\vec{v}) = \int d^3 v' \frac{f(\vec{v}')}{u} \quad (34)$$

$$g(\vec{v}) = \int d^3 v' f(\vec{v}') u \quad (35)$$

where $u = |\vec{v}' - \vec{v}|$.

Test-particle Operator

The linearized collision operator is obtained by substituting $f = F + \delta f$ into $C[f, f]$, where F is a known function, expanding in δf , and neglecting the term quadratic in δf :

$$C[f, f] \simeq C[F, F] + C[F, \delta f] + C[\delta f, F] \quad (36)$$

The first linear term is the test-particle operator on δf : $C[F, \delta f] \equiv C^{TP} \delta f$, where

$$C^{TP} \delta f = -\frac{1}{2} \left\{ \frac{1}{v_{\perp}} \frac{\partial}{\partial v_{\perp}} \left[v_{\perp} A_{\perp}[F] \delta f - v_{\perp} \left(D_{\perp}[F] \frac{\partial \delta f}{\partial v_{\perp}} + D_{\times}[F] \frac{\partial \delta f}{\partial v_{\parallel}} \right) \right] + \frac{\partial}{\partial v_{\parallel}} \left[A_{\parallel}[F] \delta f - \left(D_{\times}[F] \frac{\partial \delta f}{\partial v_{\perp}} + D_{\parallel}[F] \frac{\partial \delta f}{\partial v_{\parallel}} \right) \right] \right\} \quad (37)$$

Since C^{TP} is a divergence in velocity space, it conserves particles:

$$\int d^3 v C^{TP} = 0 \quad (38)$$

We shall take F to be a shifted Maxwellian:

$$F(\vec{v}) = n(\vec{x}) \left(\frac{m}{2\pi T(\vec{x})} \right)^{3/2} \exp \left[-\frac{m}{2T(\vec{x})} (v_{\perp}^2 + (v_{\parallel} - u_{\parallel})^2) \right] \quad (39)$$

where u_{\parallel} is the parallel flow velocity. The Fokker-Planck coefficients evaluated as above, using F , where the Rosenbluth potentials are given as follows. Using spherical coordinates w, μ , where $w = [v_{\perp}^2 + (v_{\parallel} - u_{\parallel})^2]^{1/2}$, $\mu = \cos \theta$ and θ is the angle between \vec{v}' and \vec{v} , we have

$$h(w) = 2\pi \int_0^{\infty} dw' (w')^2 F(w') \int_{-1}^1 \frac{d\mu'}{u} \quad (40)$$

$$g(w) = 2\pi \int_0^{\infty} dw' (w')^2 F(w') \int_{-1}^1 d\mu' u \quad (41)$$

After changing from integration variable μ' to u , with $u^2 = (v')^2 - 2v'\mu'v + v^2$, the last integrals can be easily evaluated and we obtain single integrals over w' , the particle speed in a frame with the parallel flow speed u_{\parallel} . Using a Maxwellian in this frame, we obtain the same integrals as given by Chandrasekhar and Spitzer.

Field-particle Operator

The second linear term in Eq.(36) is the field-particle operator on δf . Rather than use the exact form, which is an integral operator, we follow the procedure of Lin, Tang and Lee [PoP 1995], which results in a linearized collision operator which conserves particles, momentum and energy, and has the correct null space, i.e. gives zero when acting on a shifted Maxwellian or a shifted Maxwellian with a perturbation in density or temperature.

We write the field-particle operator in the form

$$C[\delta f, F] \equiv C^{FP}[\delta f] \simeq (r(v_{\perp}, v'_{\parallel})v'_{\parallel}P[\delta f] + q(v_{\perp}, v'_{\parallel})E[\delta f]) F \quad (42)$$

where

$$P[\delta f] = - \int d^3v v'_{\parallel} C^{TP} \delta f \quad (43)$$

$$E[\delta f] = - \int d^3v (v'^2/2) C^{TP} \delta f \quad (44)$$

where $v'_{\parallel} = v_{\parallel} - u_{\parallel}$ and $v'^2 = v_{\perp}^2 + v'_{\parallel}{}^2$.

Here $\mathbf{r}(\mathbf{v}_\perp, v'_\parallel)$ and $\mathbf{q}(\mathbf{v}_\perp, v'_\parallel)$ are functions to be determined; we take \mathbf{r} and \mathbf{q} to be even functions of v'_\parallel , like \mathbf{F} .

Momentum and energy conservation,

$$\int d^3v v'_\parallel \{C^{TP} \delta f + C^{FP} [\delta f]\} = 0 \quad (45)$$

$$\int d^3v (v'^2/2) \{C^{TP} \delta f + C^{FP} [\delta f]\} = 0 \quad (46)$$

are satisfied, assuming \mathbf{r} and \mathbf{q} satisfy the equations

$$\int d^3v v'^2_\parallel \mathbf{r}(\mathbf{v}_\perp, v'_\parallel) \mathbf{F} = \mathbf{1} \quad (47)$$

$$\int d^3v (v'^2/2) \mathbf{q}(\mathbf{v}_\perp, v'_\parallel) \mathbf{F} = \mathbf{1} \quad (48)$$

In order for the linearized collision operator to have the correct null space, we require

$$C^{TP} \delta f + C^{FP}[\delta f] = 0 \quad (49)$$

for $\delta f = v'_{\parallel} F$ or $\delta f = (v'^2/2)F$. These conditions determine the functions $r(v_{\perp}, v'_{\parallel})$ and $q(v_{\perp}, v'_{\parallel})$. We need to use the following property of the test-particle operator: it preserves parity in v'_{\parallel} , i.e. $C^{TP}(v'_{\parallel} F)$ is odd in v'_{\parallel} , and $C^{TP}(v'^2 F)$ is even in v'_{\parallel} .

Then we find that r and q are determined by

$$r(v_{\perp}, v'_{\parallel})v'_{\parallel} F = C^{TP}(v'_{\parallel} F)/I_1 \quad (50)$$

$$q(v_{\perp}, v'_{\parallel})F = C^{TP}(v'^2 F)/I_2 \quad (51)$$

where

$$I_1 = \int d^3v v'_{\parallel} C^{TP}(v'_{\parallel} F) \quad \text{and} \quad I_2 = \int d^3v (v'^2/2) C^{TP}(v'^2 F) \quad (52)$$

Langevin Equations Equivalent to the Test-particle Operator

The Langevin equations for \mathbf{v}_\perp and v_\parallel are

$$d\mathbf{v}_\perp = \mathbf{A}_\perp dt + \beta_\perp \boldsymbol{\xi}_1 dt^{1/2} \quad (53)$$

$$dv_\parallel = A_\parallel dt + (\beta_\times \xi_1 + \beta_\parallel \xi_3) dt^{1/2} \quad (54)$$

The β s are given in terms of the diffusion coefficients by

$$\beta_\perp = D_\perp^{1/2} \quad (55)$$

$$\beta_\times = D_\times / \beta_\perp \quad (56)$$

and

$$\beta_\parallel = \left(D_\parallel - D_\times^2 / D_\perp \right)^{1/2} \quad (57)$$

Samples

The ξ s are components of sample vectors, which are required to satisfy

$$\langle \xi_1 \rangle = 0, \quad \langle \xi_3 \rangle = 0, \quad \langle \xi_1^2 \rangle = 1, \quad \langle \xi_1 \xi_3 \rangle = 0, \quad \langle \xi_3^2 \rangle = 1 \quad (58)$$

The brackets would denote statistical averages in the conventional Monte-Carlo method. In the deterministic sampling method, the brackets denote integrals using numerical quadratures, with the sample points taken to be the quadrature points [Albright, et al., 2003]. The numerical quadratures are defined as those which would be used to evaluate moments of the Fokker-Planck Green's function:

$$\int d^3 \vec{w} G(\vec{w}, \tau) F(\vec{w}) = (2\pi)^{-3/2} \int d^3 \xi e^{-\frac{1}{2} |\vec{\xi}|^2} \hat{F}(\vec{\xi}) \quad (59)$$

$$\simeq \sum_j C_j \hat{F}(\vec{\xi}_j) \quad (60)$$

where $F(\vec{w})$ is a polynomial, $\hat{F}(\vec{\xi}) = F(\vec{w})$,
and the $\vec{\xi}_j$ s and C_j s are the quadrature points and weights.

Summary

Topics discussed:

Canonical Maxwellian

Shifted Maxwellian

Parallel and Poloidal Flows

Effect of Orbit Squeezing

Linearized Collision Operator

Test-particle and Field-particle Operators

Langevin Equations

Samples