The Fokker-Planck collision operator in `Gkeyll`

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1 The multi-species Fokker-Planck operator

The Fokker-Planck operator in a multi-species plasma can be written as (see NRL Plasma Formulary and the original Rosenbluth, MacDonald and Judd (RMJ) paper[2][1])

$$\frac{\partial f_s}{\partial t} = -\nabla \cdot \left[\mathbf{a}_s f_s - \frac{1}{2} \nabla \cdot (\mathbf{D}_s f_s) \right] \tag{1}$$

where the ∇ operator is the gradient operator in *velocity space*. The drag velocity and diffusion tensor are given by

$$\mathbf{a}_s = \nabla h_s \tag{2}$$

$$\mathbf{D}_s = \nabla \nabla g_s \tag{3}$$

where

$$h_s = \sum_b \Gamma_{sb} \left(1 + \frac{m_s}{m_b} \right) H_b \tag{4}$$

$$g_s = \sum_b \Gamma_{sb} G_b. \tag{5}$$

are scalar potentials. Here

$$\Gamma_{ab} = 4\pi \lambda_{ab} \frac{q_a^2 q_b^2}{m_a^2} \tag{6}$$

where λ_{ab} is the Coulomb logarithm and q_a and m_a are the charge and mass of the species respectively. The potentials H_s and G_s are the Rosenbluth potentials and are determined from

$$H_s(\mathbf{v}) = \int \frac{f_s(\mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|} \, d^3\mathbf{v}', \tag{7}$$

$$G_s(\mathbf{v}) = \int f_s(\mathbf{v}')|\mathbf{v} - \mathbf{v}'| \, d^3\mathbf{v}'. \tag{8}$$

Using the identity

$$\nabla^2 |\mathbf{v} - \mathbf{v}'|^{-1} = -4\pi \delta^3(\mathbf{v} - \mathbf{v}') \tag{9}$$

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[1]Historically, the first derivation of the FPO in the case of Coulomb (inverse square law) was by Lev Landau in 1936[1]. Landau, however, writes the equation in an integral form and does not introduce the potentials as RMJ did. Curiously, the 1957 paper by RMJ does not mention Landau's work at all. As is usually the case, the original papers by these Masters of the field remain highly readable and still provide the best derivations of the equations.

and as $\nabla^2|\mathbf{v}| = 2/|\mathbf{v}|$ we can derive alternate expressions for the Rosenbluth potentials as

$$\nabla^2 H_s = -4\pi f_s \tag{10}$$

$$\nabla^2 G_s = 2H_s. \tag{11}$$

As is clear from these equations, the FPO is a complicated 3D (in velocity space) nonlinear integro-differential equation, coupling all species via the Rosenbluth potentials. Its solutions display rich structure, specially when combined with the particle motion in self-consistent electromagnetic fields. Designing a general production solver for the case of multi-species FPO poses a formidable challenge.

I should mention that this is not the *exact* form of the FPO as given in the RMJ paper. There they assume that all species have the *same* absolute value of charge $|e|$, allowing them to write $\Gamma_a = \Gamma_{aa}$. With this assumption a little algebra shows that the equations listed above are indeed identical to the ones in the RMJ paper.

We can easily derive the following two relations:

$$\mathrm{Tr}(\mathbf{D}_s) = \nabla^2 g_s = 2\sum_b \Gamma_{sb} H_b \tag{12}$$

and

$$\nabla \cdot \mathbf{D}_s = \nabla \cdot (\nabla\nabla g_s) = \nabla\nabla^2 g_s = 2\sum_b \Gamma_{sb} \nabla H_b. \tag{13}$$

The latter expression allows us to write the FPO as

$$\frac{\partial f_s}{\partial t} = -\frac{1}{2}\nabla \cdot \Big[\underbrace{\mathbf{a}'_s f_s}_{\text{drag}} - \underbrace{\mathbf{D}_s \cdot \nabla f_s}_{\text{diffusion}}\Big] \tag{14}$$

where

$$\frac{1}{2}\mathbf{a}'_s = \mathbf{a}_s - \sum_b \Gamma_{sb} \nabla H_b = \sum_b \Gamma_{sb}\frac{m_s}{m_b}\nabla H_b. \tag{15}$$

Written in the form Eq. (14) the FPO clearly has two competing terms: the first *drag* term and the second the *diffusion* term. For the special case of a single species we have $h_s = 2\Gamma_s H_s$ and rather elegantly, $\mathbf{a}'_s = \mathbf{a}_s$.

1.1 The case of a Maxwellian

The Rosenbluth potentials given by Eq. (7) and Eq. (8) can be explicitly computed for the case of the Maxwellian

$$f_M(\mathbf{v}) = \frac{n}{(2\pi v_{th}^2)^{3/2}} e^{-v^2/2v_{th}^2} \tag{16}$$

where n and v_{th} are the number density and thermal-speed respectively. We can show that

$$H_M(\mathbf{v}) = \frac{n}{v}\,\mathrm{erf}\left(\frac{v}{\sqrt{2}v_{th}}\right) \tag{17}$$

and

$$G_M(\mathbf{v}) = \sqrt{2}n v_{th}\left[\frac{e^{-v^2/2v_{th}^2}}{\sqrt{\pi}} + \mathrm{erf}\left(\frac{v}{\sqrt{2}v_{th}}\right)\left(\frac{v_{th}}{\sqrt{2}v} + \frac{v}{\sqrt{2}v_{th}}\right)\right] \tag{18}$$

where $\mathrm{erf}(x)$ is the error function. For a drifting Maxwellian shift the velocity to be centered at the drift velocity (i.e. replace $v \to |\mathbf{v} - \mathbf{u}|$).

2 Conservation properties and constraints

The FPO conserves the particle count, total momentum and total energy. Starting from Eq. (1) we can derive the constraints to ensure momentum and energy by taking $m_s \mathbf{v}$ and $m_s v^2 / 2$ moments to arrive at the following constraint

$$\sum_s \int_{-\infty}^{\infty} m_s \mathbf{a}_s f_s \, d^3 \mathbf{v} = 0 \tag{19}$$

for momentum conservation, and

$$\sum_s \int_{-\infty}^{\infty} m_s \left[\mathbf{v} \cdot \mathbf{a}_s + \frac{1}{2} \operatorname{Tr}(\mathbf{D}_s) \right] f_s \, d^3 \mathbf{v} = 0 \tag{20}$$

for energy conservation.

Remark 1. *These constraints depend only on the form of Eq. (1) and not on the details of how $\mathbf{a}$ and $\mathbf{D}$ are computed. Hence, we must show that for the* specific case *of FPO in which the drag and diffusion terms are computed from Rosenbluth potentials, they are indeed satisfied.*

Remark 2. *An approximate model for the drag velocity and diffusion tensor is provided by Lenard-Bernstein or Dougherty collision operator. In this case the advection velocity and diffusion matrix are computed from the local drift-velocity and thermal speeds as follows*

$$\mathbf{a}_s = -\nu_{ss}(\mathbf{v} - \mathbf{u}_s) - \sum_{r \neq s} \nu_{sr}(\mathbf{v} - \mathbf{u}_{sr}) \tag{21}$$

$$\mathbf{D}_s = 2\nu_{ss} v_{th,s}^2 \mathbf{I} + \sum_{r \neq s} 2\nu_{sr} v_{th,sr}^2 \mathbf{I} \tag{22}$$

Here ν_{sr} is the collision frequency between particles of species s and r, and $\mathbf{u}_s$ and $v_{th,s} = \sqrt{T_s/m_s}$ are the mean (drift) velocity and thermal speed of particles of species s respectively, and the quantities with subscript sr are intermediate quantities that need to be determined (partly) from momentum and energy conservation, that is choosen to satisfy Eq. (19) and Eq. (20).

3 The single-species Fokker-Planck operator

The Fokker-Planck operator in a single-species plasma can be written as

$$\frac{1}{\Gamma} \frac{\partial f}{\partial t} = -\nabla \cdot \left[\mathbf{a} f - \frac{1}{2} \nabla \cdot (\mathbf{D} f) \right] \tag{23}$$

where the ∇ operator is the gradient operator in *velocity space* and $\Gamma = 4\pi e^4 \lambda / m^2$ where λ is the Coulomb logarithm. The drag velocity and diffusion tensor are given by

$$\mathbf{a} = \nabla h \tag{24}$$

$$\mathbf{D} = \nabla \nabla g \tag{25}$$

where the potentials h and g are the Rosenbluth potentials and are determined from

$$h(\mathbf{v}) = 2 \int \frac{f(\mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|} \, d^3 \mathbf{v}', \tag{26}$$

$$g(\mathbf{v}) = \int f(\mathbf{v}') |\mathbf{v} - \mathbf{v}'| \, d^3 \mathbf{v}'. \tag{27}$$

Alternatively,

$$\nabla^2 h = -8\pi f \tag{28}$$

$$\nabla^2 g = h. \tag{29}$$

We can easily derive the following two relations:

$$\text{Tr}(\mathbf{D}) = \nabla^2 g = h \tag{30}$$

and

$$\nabla \cdot \mathbf{D} = \nabla \cdot (\nabla \nabla g) = \nabla \nabla^2 g = \mathbf{a}. \tag{31}$$

The latter expression allows us to write the FPO as

$$\frac{1}{\Gamma} \frac{\partial f}{\partial t} = -\frac{1}{2} \nabla \cdot \big[\underbrace{\mathbf{a} f}_{\text{drag}} - \underbrace{\mathbf{D} \cdot \nabla f}_{\text{diffusion}} \big] \tag{32}$$

Below I present finite-volume schemes to solve the FPO written as Eq. (23) called **Form I** and written as Eq. (32), called **Form II**.

4   Solving the Poisson equations

To discretize the Poisson equations that determine the Rosenbluth potentials we use a central scheme to write

$$\sum_{d=1}^{m} \frac{V_d}{\Delta v_d^2} (\Delta_p - 2I + \Delta_m) h = -8\pi f \tag{33}$$

and

$$\sum_{d=1}^{m} \frac{V_d}{\Delta v_d^2} (\Delta_p - 2I + \Delta_m) g = h. \tag{34}$$

Here I am using the symbol V_d, $d = 1, \ldots, 3$ to represent the directional modifer operators in velocity space.

5   A finite-volume scheme for Form II

We will first construct a finite-volume scheme for Form II Eq. (32). For this we will construct a scheme in which the Rosenbluth potentials are directly used in the update stencil, without explicit computation of $\mathbf{a}$ and $\mathbf{D}$ (though these need to be computed at the appropriate interfaces). Start by writing

$$\frac{\partial f}{\partial t} = -\frac{1}{2} \frac{\partial}{\partial v_1} \underbrace{\left(a_1 f - D_{11} \frac{\partial f}{\partial v_1} - D_{12} \frac{\partial f}{\partial v_2} - D_{12} \frac{\partial f}{\partial v_3} \right)}_{G} + \ldots \tag{35}$$

where G is the flux. We will discretize this using a finite-volume scheme as

$$\frac{\partial f}{\partial t} = -\frac{1}{2} \frac{G_{i+1/2} - G_{i-1/2}}{\Delta v_1} + \ldots \tag{36}$$

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where $G_{i\pm 1/2}$ are the numerical fluxes which we need to determine. We will do this in steps. Note that in the following we are assuming we have *cell-average* values of f, h and g in each cell.

Advective Flux. First, let us deal with the advection term (the edge index is now dropped)

$$a_1 f = \frac{(d_p - d_m)h}{\Delta v_1} \hat{f} \tag{37}$$

where we have used central difference to compute $a_1 = \partial h / \partial v_1$ and $\hat{f}$ is the distribution function evaluated at the cell edge. Several approximations can be used to compute $\hat{f}$, for example upwind value ($\hat{f} = d_m f$ if $a_1 > 0$ or $\hat{f} = d_p f$ if if $a_1 < 0$) or plain averages. For example, if we use averages then we would write the advection flux as

$$a_1 f = \frac{(d_p - d_m)h}{\Delta v_1} \frac{(d_p + d_m)f}{2}. \tag{38}$$

A third-order recovery based upwind value is described later in this document.

Diagonal diffusive flux. Next consider the diffusive term with the diagonal diffusion coefficient D_{11}. As there is no preferred direction for diffusion we can use central differences for computing gradient of f and hence write

$$D_{11} \frac{\partial f}{\partial v_1} = D_{11} \frac{(d_p - d_m)f}{\Delta v_1} \tag{39}$$

where now D_{11} is the diffusion coefficient on the *cell face* and must be computed from $\partial^2 g / \partial v_1^2$ evaluated at the interface. To do this recover a polynomial across four cells (two to the left and two to the right) by matching cell averages in those cells and evaluate its second derivative at the interface. This leads to the expression

$$D_{11} = \frac{\partial^2 g}{\partial v_1^2} = \frac{(d_{2p} - d_p - d_m + d_{2m})g}{2\Delta v_1^2}. \tag{40}$$

Note to compute D_{11} we have to use a four-point stencil in X.

Transverse diffusive fluxes. Finally consider the transverse diffusive fluxes. To discretize this we need to deal with two types of terms: first, the derivative of f in transverse direction and the cross-diffusion coefficient at the interface, which itself is a cross-derivative of g. For both of these we will use central differences to get

$$D_{12} \frac{\partial f}{\partial v_2} + D_{13} \frac{\partial f}{\partial v_3} = D_{12} \frac{(T_p^1 - T_m^1)}{2\Delta v_2} \frac{(d_p + d_m)}{2} f + D_{13} \frac{(T_p^2 - T_m^2)}{2\Delta v_3} \frac{(d_p + d_m)}{2} f \tag{41}$$

and

$$D_{12} = \frac{\partial}{\partial v_1} \frac{\partial g}{\partial v_2} = \frac{(d_p - d_m)}{\Delta v_1} \frac{(T_p^1 - T_m^1)}{2\Delta v_2} g \tag{42}$$

and

$$D_{13} = \frac{\partial}{\partial v_1} \frac{\partial g}{\partial v_3} = \frac{(d_p - d_m)}{\Delta v_1} \frac{(T_p^2 - T_m^2)}{2\Delta v_3} g \tag{43}$$

This completes the scheme as the same formulas can be used for the flux in Y and Z directions by inserting the appropriate modifier operators at various places.

6 Computing interface value $\hat{f}$

The first thing to notice is that the stencil for the FPO in 3D is rather complicated. In each direction to update cell we need a 5-point 1D stencil (to compute D_{11} at each interface we need 4 cells, two to the right and two to the left) and we also need a 2×3-point stencil $(d_p, d_m, d_p T_p, d_p T_m, d_m T_p, d_m T_m)$ for each transverse direction to compute the cross-derivative terms at each face. Hence, we need $3^3 - 8$ cells (i.e. the corners of the 3D cube $(T_p^1 T_p^2$ etc) do not appear in the stencil) and need to add a cell on each face of the 3D cube to enable computing D_{11}, leading to a $3^3 - 8 + 6 = 25$ point stencil.

As we already need cells $(d_{2m}, d_m, d_p, d_{2p})$ to compute D_{11} at an interface we can use these to also compute $\hat{f}$ needed in the advective flux. We have two choices here: first we can use all four cells to compute a high-order non-dissipative value (which however may have overshoots when there are sharp gradients) or use an upwind biased recovery, i.e. use (d_{2m}, d_m, d_p) if $a_1 > 0$ or (d_m, d_p, d_{2p}) if $a_1 < 0$. Fitting the appropriate polynomials to the known cell averages we get expressions

$$\hat{f} = \frac{1}{12}(-d_{2p} + 7d_p + 7d_m - d_{2m})f \tag{44}$$

for the non-dissipative interface value, and

$$\hat{f} = \frac{1}{6}(2d_p + 5d_m - d_{2m})f \qquad \text{if } a_1 > 0 \tag{45}$$

or

$$\hat{f} = \frac{1}{6}(-d_{2p} + 5d_p + 2d_m)f \qquad \text{if } a_1 < 0 \tag{46}$$

when using upwinding. Further limiting may be required to ensure monotonicity.

References

[1] L. Landau. The transport equations in the case of Coulomb interactions. *Phys. Z. Sowjet*, 10:154, 1936.

[2] M. N. Rosenbluth, W. M. MacDonald, and D. L. Judd. Fokker-Planck equation for an inverse-square force. *Phys. Rev.*, 107(1):1–6, 1957.