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Implementation of the Rosenbluth potential terms in the Fokker-Planck collision operator

In these notes, we describe how the field terms in the linearized Fokker-Planck collision operator is implemented in SFINCS for the preferred settings xGridScheme=5 or 6. (This method differs from the older xGridScheme=1 or 2 approach which is detailed in [1].) One part of the Fokker-Planck field term does not involve the perturbed Rosenbluth potentials, and it is implemented by a pseudospectral interpolation matrix. The rest of the field term involves the Rosenbluth potentials, which we evaluate as follows:

- First, a matrix multiplication is used to transform from the collocation speed grid (used for the speed coordinate everywhere else in the code) to the equivalent modal approach. We denote this transformation matrix by Y.

- Next, for each Legendre mode in pitch-angle, the Rosenbluth potentials can be written as a sum of indefinite integrals involving the polynomial mode in speed. The location at which the potential is evaluated becomes one endpoint of these integrals. Derivatives of the Rosenbluth potentials (which are needed for the Fokker-Planck operator) can be expressed by analytically differentiating these indefinite integrals.

- These integrals are evaluated by adaptive quadrature for a variety of integration endpoints, corresponding to the speed grid points for the other species. The number of integrals that need to be evaluated is $\propto NL \times Nspecies^2 \times Nx^2$, (independent of the large quantities Nxi, $Ntheta$, and $Nzeta$,) requiring a miniscule amount of time compared to solution of the main linear system. For each pair of species and each Legendre mode, the results for Nx polynomials and Nx evaluation points gives a $Nx \times Nx$ matrix we denote by R.

- Thus, the map from distribution function (for species b, on the usual speed collocation grid points) to Rosenbluth potentials (on the speed grid points for species a) is given by the matrix product RY.

The method described here has several advantages over the method described for treating the Rosenbluth potentials in Ref [1]. There is no need to introduce a separate grid for the potentials, along with interpolation matrices to transform between the two grids. Also, there is no need to specify the quantities xMax or NxPotentials needed in the old approach, and so there is no need to test for convergence with respect to these parameters. In many cases I find the two methods give results (for the neoclassical flows and fluxes) that are equivalent to >3 decimal places (i.e. far less of a change than other sources of discretization error). However I do find that the new method can give different results than the method of [1] at very high collisionality, with the new method yielding better convergence with respect to Nx.

Transformation from collocation to modal discretizations

Our speed discretization is based upon a set of polynomials M_n obeying the orthogonality relation

$$\int_0^\infty dx \; x^k e^{-x^2} M_n(x) M_m(x) = \delta_{n,m} A_n \tag{1}$$

where A_m is some normalization, and k is a constant corresponding to the namelist parameter `xGrid_k`. Suppose I know a function $f(x)$ on some grid points x_n. We can represent the function in a modal discretization by the vector of numbers F_n:

$$f(x) = \sum_n F_n M_n(x) e^{-x^2}. \tag{2}$$

(Notice that the x^k factor present in (1) is absent in (2), since we must be able to represent a Maxwellian in (2).) If we operate on (2) by

$$\int_0^\infty dx \; x^k M_m(x)(...) \tag{3}$$

we find

$$F_m = \frac{1}{A_m} \int_0^\infty dx \; x^k M_m(x) f(x). \tag{4}$$

Let us evaluate the integral in (4) using our Gaussian integration scheme. Assuming we have defined and computed weights w_n such that

$$\int_0^\infty dx \; y(x) \approx \sum_n w_n y(x_n) \tag{5}$$

for any function $y(x)$, then (4) becomes

$$F_m = \sum_n \left[\frac{1}{A_m} w_n x_n^k M_m(x_n) \right] f(x_n). \tag{6}$$

The quantity in square brackets in (6) thus is the matrix to transform from the collocation to modal representation:

$$Y_{m,n} = \frac{1}{A_m} w_n x_n^k M_m(x_n). \tag{7}$$

The matrix (7) corresponds to the 2D array `collocation2modal` constructed in xGrid.F90.

Collision operator

As discussed in the SFINCS technical manual, the field term in the Fokker-Planck operator has the form

$$C_{ab}\{f_{aM}, f_{b1}\} = C_{ab}^H + C_{ab}^G + C_{ab}^D \tag{8}$$

where

$$C_{ab}^G = \Gamma_{ab} f_{aM} \frac{2v^2}{v_a^4} \frac{\partial^2 G_b}{\partial v^2}, \tag{9}$$

$$C_{ab}^H = \Gamma_{ab} f_{aM} \left[-\frac{2v}{v_a^2}\left(1 - \frac{m_a}{m_b}\right)\frac{\partial H_b}{\partial v} - \frac{2}{v_a^2} H_b \right], \tag{10}$$

$$C_{ab}^D = \Gamma_{ab} f_{Ma} 4\pi \frac{m_a}{m_b} f_{b1} = \frac{\Gamma_{ab} n_a}{\upsilon_a^3} \exp\left(-x_a^2\right) \frac{4}{\pi^{1/2}} \frac{m_a}{m_b} f_{b1}, \tag{11}$$

$\upsilon_a = \sqrt{2T_a / m_a}$, and

$$\Gamma_{ab} = \frac{4\pi Z_a^2 Z_b^2 e^4 \ln \Lambda}{m_a^2}. \tag{12}$$

The term (11) does not involve the Rosenbluth potentials, and so we evaluate it by spectral interpolation. For (9)-(10), the Rosenbluth potentials H_{b1} and G_{b1} are defined by

$$\nabla_\upsilon^2 H_b = -4\pi f_{b1} \tag{13}$$

and

$$\nabla_\upsilon^2 G_b = 2H_b. \tag{14}$$

As usual, we decompose the distribution function for species b in Legendre polynomial modes:

$$f_{b1}(x_b, \xi) = \sum_\ell P_\ell(\xi) f_{b1,\ell}(x_b) \tag{15}$$

where $P_\ell(\xi)$ denotes a Legendre polynomial. The potentials are each expanded in the same Legendre modes:

$$H_b(x_b, \xi) = \sum_\ell P_\ell(\xi) H_{b\ell}(x_b). \tag{16}$$

$$G_b(x_b, \xi) = \sum_\ell P_\ell(\xi) G_{b\ell}(x_b). \tag{17}$$

Then, the Poisson equations that define the potentials become

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial H_b}{\partial x_b} - \ell(\ell+1) H_b = -4\pi\upsilon^2 f_{b1}, \tag{18}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial G_b}{\partial x_b} - \ell(\ell+1) G_b = 2\upsilon^2 H_{b1}, \tag{19}$$

where $x_a = \upsilon / \upsilon_a$. Let us define

$$\hat{H}_b = H_b / \upsilon_b^2 \tag{20}$$

$$\hat{G}_b = G_b / \upsilon_b^4 \tag{21}$$

so the defining equations for the potentials become

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{H}_b}{\partial x_b} - \ell(\ell+1) \hat{H}_b = -4\pi x_b^2 f_{b1} \tag{22}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{G}_b}{\partial x_b} - \ell(\ell+1) \hat{G}_b = 2x_b^2 \hat{H}_b. \tag{23}$$

For the next bit, we drop the species subscripts to minimize clutter.

1D integrals for potentials

Equations (40) and (45) in Ref [2] give expressions for the Rosenbluth potentials associated with each Legendre mode. (My notes 20110917-01 and 20111025-01 give a simpler derivation). These expressions are

$$H_\ell(x) = \frac{4\pi}{(2\ell+1)} \left[\frac{1}{x^{\ell+1}} \int_0^x dz \; z^{\ell+2} f_\ell(z) + x^\ell \int_x^\infty dz \; \frac{f_\ell(z)}{z^{\ell-1}} \right] \tag{24}$$

and

$$G_\ell = -\frac{4\pi}{(4\ell^2-1)} \left\{ \begin{array}{l} x^\ell \int_x^\infty dz \; z^{-\ell+3} f_\ell(z) + \alpha x^{\ell+2} \int_x^\infty dz \; z^{-\ell+1} f_\ell(z) \\[2mm] + \dfrac{\alpha}{x^{\ell+1}} \int_0^x dz \; z^{\ell+4} f_\ell(z) + \dfrac{1}{x^{\ell-1}} \int_0^x dz \; z^{\ell+2} f_\ell(z) \end{array} \right\} \tag{25}$$

where

$$\alpha = -(2\ell-1)/(2\ell+3). \tag{26}$$

To evaluate terms (9)-(10) in the Fokker-Planck operator, we actually need $\partial H_\ell / \partial x$ and $\partial^2 G_\ell / \partial x^2$. These quantities may be computed by analytically differentiating (24)-(25), with the following results:

$$\frac{dH_\ell}{dx} = \frac{4\pi}{(2\ell+1)} \left[-(\ell+1)\frac{1}{x^{\ell+2}} \int_0^x dz \; z^{\ell+2} f_\ell(z) + \ell x^{\ell-1} \int_x^\infty dz \; \frac{f_\ell(z)}{z^{\ell-1}} \right], \tag{27}$$

$$\frac{d^2 G_\ell}{dx^2} = -\frac{4\pi}{(4\ell^2-1)} \left\{ \begin{array}{l} \ell(\ell-1) x^{\ell-2} \int_x^\infty dz \; z^{-\ell+3} f_\ell(z) + \alpha(\ell+1)(\ell+2) x^\ell \int_x^\infty dz \; z^{-\ell+1} f_\ell(z) \\[2mm] + \dfrac{\alpha(\ell+1)(\ell+2)}{x^{\ell+3}} \int_0^x dz \; z^{\ell+4} f_\ell(z) + \dfrac{\ell(\ell-1)}{x^{\ell+1}} \int_0^x dz \; z^{\ell+2} f_\ell(z) \end{array} \right\}. \tag{28}$$

In performing the differentiations leading to (27)-(28), several cancellations have occurred.

In order to evaluate (24), (28), and (27) for a given function $f_\ell(y)$ and given ℓ, we need the following 4 integrals:

$$I_{\ell+2}(x) = \int_0^x dz \; z^{\ell+2} f_\ell(z) \tag{29}$$

$$I_{\ell+4}(x) = \int_0^x dz \; z^{\ell+4} f_\ell(z) \tag{30}$$

$$I_{-\ell+1}(x) = \int_x^\infty dz \; z^{-\ell+1} f_\ell(z) \tag{31}$$

$$I_{-\ell+3}(x) = \int_x^\infty dz \; z^{-\ell+3} f_\ell(z) \tag{32}$$

In the subroutine computeRosenbluthPotentialResponse of xGrid.F90, the integrals (29)-(32) are first computed by calling QUADPACK, and the results are used to evaluate (24), (27), and (28).

References

[1] Landreman & Ernst, Journal of Computational Physics 243, 130 (2013).
[2] Rosenbluth, MacDonald, & Judd, Physical Review 107, 1 (1957).