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Equations for a minimal stellarator drift-kinetic code for obtaining monoenergetic coefficients

Let's try to solve the kinetic equation

$$\upsilon_{\|}\left(\nabla_{\|} f_1\right)_{\mu} - C\left[f_1\right] - S = -\mathbf{v}_d \cdot \nabla\psi \frac{\partial f_M}{\partial \psi} + \frac{Ze}{T}\upsilon_{\|}\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_M \tag{1}$$

where I will consider only $E_r = 0$ for simplicity. In (1), S represents a "source" that is independent of all 3 independent variables $\left(\theta,\zeta,\xi\right)$. As in Beidler 2011, let's take the collision operator to be

$$C\left[f_1\right] = \nu\frac{1}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_1}{\partial\xi}. \tag{2}$$

We will use Boozer coordinates, so

$$\mathbf{B} = \nabla\psi\times\nabla\theta + \iota\nabla\zeta\times\nabla\psi, \tag{3}$$

where $\iota = 1/q$ is the rotational transform with q the safety factor, and

$$\mathbf{B} = \beta\left(\psi,\theta,\zeta\right)\nabla\psi + I\left(\psi\right)\nabla\theta + G\left(\psi\right)\nabla\zeta. \tag{4}$$

where $G\left(\psi\right) = 2i_p/c$, $I\left(\psi\right) = 2i_t/c$, $i_p\left(\psi\right)$ is the poloidal current outside the flux surface, and $i_t\left(\psi\right)$ is the toroidal current inside the flux surface. The product of (3) with (4) gives

$$\mathbf{B}\cdot\nabla\zeta = \nabla\psi\cdot\nabla\theta\times\nabla\zeta = \frac{B^2}{G+\iota I}. \tag{5}$$

From the documentation for multispecies SFINCS, we know

$$\dot{\xi} = -\left(1-\xi^2\right)\frac{\upsilon}{2B^2}\left(\iota\frac{\partial B}{\partial\theta} + \frac{\partial B}{\partial\zeta}\right)\mathbf{B}\cdot\nabla\zeta \tag{6}$$

and

$$\mathbf{v}_m\cdot\nabla\psi = -\frac{Tc}{ZeB^3}x^2\left(1+\xi^2\right)\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial\theta} - I\frac{\partial B}{\partial\zeta}\right]. \tag{7}$$

Then (1) becomes

$$\begin{aligned}&\frac{\upsilon\xi}{B}\mathbf{B}\cdot\nabla\zeta\left[\iota\frac{\partial f_1}{\partial\theta}+\frac{\partial f_1}{\partial\zeta}\right] - \left(1-\xi^2\right)\frac{\upsilon}{2B^2}\left(\iota\frac{\partial B}{\partial\theta}+\frac{\partial B}{\partial\zeta}\right)\mathbf{B}\cdot\nabla\zeta\frac{\partial f_1}{\partial\xi} - \nu\frac{1}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_1}{\partial\xi} - S \\ &= \frac{Tc}{Ze}x^2\left(1+\xi^2\right)\frac{\mathbf{B}\cdot\nabla\zeta}{B^3}\left[G\frac{\partial B}{\partial\theta} - I\frac{\partial B}{\partial\zeta}\right]\frac{\partial f_M}{\partial\psi} + \frac{Ze}{T}\upsilon\xi\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_M.\end{aligned} \tag{8}$$

For normalizations, we introduce reference values of magnetic field and length, $\bar{R}$ and $\bar{B}$. We introduce normalized quantities

$$\hat{B} = B/\bar{B} \tag{9}$$

$$\hat{G} = G/\left(\bar{R}\bar{B}\right) \tag{10}$$

$$\hat{I} = I/\left(\bar{R}\bar{B}\right) \tag{11}$$

We normalize everything in the usual way, except for the normalization of f_1. We multiply (8) through by

$$\frac{\bar{R}}{\upsilon}\left(\hat{G}+\iota\hat{I}\right) \tag{12}$$

and define the normalized collisionality

$$\nu' = \frac{\nu\left(G+\iota I\right)}{\upsilon\bar{B}}. \tag{13}$$

We let the normalized source be

$$\hat{S} = \frac{\bar{R}}{\upsilon}\left(\hat{G}+\iota\hat{I}\right)S. \tag{14}$$

Then (8) becomes

$$\begin{aligned}&\xi\hat{B}\left[\iota\frac{\partial f_1}{\partial\theta}+\frac{\partial f_1}{\partial\zeta}\right]-\left(1-\xi^2\right)\frac{1}{2}\left(\iota\frac{\partial\hat{B}}{\partial\theta}+\frac{\partial\hat{B}}{\partial\zeta}\right)\frac{\partial f_1}{\partial\xi}-\frac{\nu'}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_1}{\partial\xi}-\hat{S}\\&=\frac{\bar{R}}{\upsilon}\frac{Tc}{Ze}x^2\left(1+\xi^2\right)\frac{1}{\hat{B}}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\frac{\partial f_M}{\partial\psi}+\bar{R}\left(\hat{G}+\iota\hat{I}\right)\frac{Ze}{T}\xi\frac{\left\langle E_\parallel B\right\rangle\bar{B}\hat{B}}{\left\langle B^2\right\rangle}f_M\end{aligned} \tag{15}$$

We then define 2 normalized versions of f_1, one for each gradient drive term:

$$f_1 = f_\nabla\frac{\bar{R}}{\upsilon}\frac{Tc}{Ze}x^2\frac{\partial f_M}{\partial\psi}, \tag{16}$$

$$f_1 = f_E\bar{R}\left(\hat{G}+\iota\hat{I}\right)\frac{Ze}{T}\frac{\left\langle E_\parallel B\right\rangle\bar{B}}{\left\langle B^2\right\rangle}f_M, \tag{17}$$

where f_∇ and f_E are the solutions of

$$\begin{aligned}&\xi\hat{B}\left[\iota\frac{\partial f_\nabla}{\partial\theta}+\frac{\partial f_\nabla}{\partial\zeta}\right]-\left(1-\xi^2\right)\frac{1}{2}\left(\iota\frac{\partial\hat{B}}{\partial\theta}+\frac{\partial\hat{B}}{\partial\zeta}\right)\frac{\partial f_\nabla}{\partial\xi}-\frac{\nu'}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_\nabla}{\partial\xi}-\hat{S}\\&=\left(1+\xi^2\right)\frac{1}{\hat{B}}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\end{aligned} \tag{18}$$

$$\xi\hat{B}\left[\iota\frac{\partial f_E}{\partial\theta}+\frac{\partial f_E}{\partial\zeta}\right]-\left(1-\xi^2\right)\frac{1}{2}\left(\iota\frac{\partial\hat{B}}{\partial\theta}+\frac{\partial\hat{B}}{\partial\zeta}\right)\frac{\partial f_E}{\partial\xi}-\frac{\nu'}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_E}{\partial\xi}-\hat{S}=\xi\hat{B} \tag{19}$$

Legendre modal discretization

We employ the following modal expansion in terms of Legendre polynomials $P_\ell\left(\xi\right)$:

$$f = \sum_\ell f_\ell P_\ell\left(\xi\right). \tag{20}$$

We discretize the kinetic equations (18)-(19) by applying

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\; P_L\left(\xi\right)(\quad\cdot\quad). \tag{21}$$

To evaluate the various integrals that result, the following identities may be used:

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\xi P_L\left(\xi\right)P_\ell\left(\xi\right)=\frac{L+1}{2L+3}\delta_{L+1,\ell}+\frac{L}{2L-1}\delta_{L-1,\ell}, \tag{22}$$

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ \left(1-\xi^2\right) P_L\left(\xi\right)\frac{dP_\ell}{d\xi} = \frac{\left(L+1\right)\left(L+2\right)}{2L+3}\delta_{L+1,\ell} - \frac{\left(L-1\right)L}{2L-1}\delta_{L-1,\ell}, \tag{23}$$

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\xi = \delta_{L,1}, \tag{24}$$

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\left(1+\xi^2\right) = \frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}, \tag{25}$$

and

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\frac{d}{d\xi}\left(1-\xi^2\right)\frac{dP_\ell}{d\xi} = -\left(L+1\right)L\delta_{L,\ell}. \tag{26}$$

As a result, we get

$$\sum_L M_{L,\ell}\, f_{\nabla,\ell} = R_{\nabla,L} \tag{27}$$

and

$$\sum_L M_{L,\ell}\, f_{E,\ell} = R_{E,L} \tag{28}$$

where

$$\begin{aligned} M_{L,\ell} = &\left(\frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}\right)\hat{B}\left[\iota\frac{\partial}{\partial\theta} + \frac{\partial}{\partial\zeta}\right] \\ &-\frac{1}{2}\left(\iota\frac{\partial\hat{B}}{\partial\theta} + \frac{\partial\hat{B}}{\partial\zeta}\right)\left(\frac{\left(L+1\right)\left(L+2\right)}{2L+3}\delta_{L+1,\ell} - \frac{\left(L-1\right)L}{2L-1}\delta_{L-1,\ell}\right) \\ &+\frac{\nu'}{2}L\left(L+1\right)\delta_{L,\ell} \end{aligned} \tag{29}$$

$$R_{\nabla,L} = \frac{1}{\hat{B}}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left(\frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}\right), \tag{30}$$

$$R_{E,L} = \hat{B}\delta_{L,1} \tag{31}$$

Diagnostics

For computing outputs, we use the following Legendre identities:

$$\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\left(1+\xi^2\right) = \frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{32}$$

$$\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\xi = \frac{2}{3}\delta_{L,1} \tag{33}$$

One quantity we care about is the radial particle flux:

$$\texttt{flux} = \int d\theta \int d\zeta \int d\xi \frac{1}{\hat{B}} \left(1+\xi^2\right) \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] f_{\nabla} . \tag{34}$$

Using (32), we find

$$\texttt{flux} = \int d\theta \int d\zeta \frac{1}{\hat{B}} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \left[\frac{8}{3} f_0 + \frac{4}{15} f_2 \right] f_{\nabla} . \tag{35}$$

Another quantity we care about is the parallel flow:

$$\texttt{flow} = \left\langle \hat{B} \int_{-1}^{1} d\xi \; \xi f \right\rangle = \frac{2}{3} \left\langle \hat{B} f_1 \right\rangle \tag{36}$$

where the flux surface average of any quantity Y is

$$\left\langle Y \right\rangle = \frac{\int d\theta \int d\zeta \left(Y / \hat{B}^2 \right)}{\int d\theta \int d\zeta \left(1 / \hat{B}^2 \right)} . \tag{37}$$

Conversion to sfincs version 3

$$L_{11} = \frac{\dfrac{Ze\left(G+\iota I\right)}{ncTG} \left\langle \int d^3\upsilon f \mathbf{v}_m \cdot \nabla \psi \right\rangle}{\dfrac{GTc}{ZeB_0 \upsilon_i} \left(\dfrac{1}{n} \dfrac{dn}{d\psi} \right)} \tag{38}$$

Using (16),

$$L_{11} = \frac{Ze\left(G+\iota I\right)}{cTG^2} B_0 \frac{\bar{R}}{1} \frac{1}{\upsilon_{th}^3 \pi^{3/2}} \left\langle \int d^3\upsilon f_{\nabla} x^2 e^{-x^2} \mathbf{v}_m \cdot \nabla \psi \right\rangle \tag{39}$$

Using (7),

$$L_{11} = -\frac{1}{\hat{G}^2} \frac{B_0}{\bar{B}} \frac{1}{\upsilon_{th}^3 \pi^{3/2}} \left\langle \int d^3\upsilon f_{\nabla} x^4 e^{-x^2} \frac{1}{\hat{B}} \left(1+\xi^2\right) \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \right\rangle . \tag{40}$$

$$\int d^3\upsilon = 2\pi \upsilon_{th}^3 \int_0^\infty dx \int_{-1}^{1} d\xi \tag{41}$$

$$L_{11} = -\frac{1}{\hat{G}^2} \frac{B_0}{\bar{B}} \frac{2}{\pi^{1/2}} \left\langle \int_0^\infty dx \int_{-1}^{1} d\xi f_{\nabla} x^4 e^{-x^2} \frac{1}{\hat{B}} \left(1+\xi^2\right) \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \right\rangle . \tag{42}$$

Hakan's prescription is to set $x \to 1$ and xWeights=exp(1), so the integration weight cancels the Maxwelllian. Thus,

$$L_{11} = -\frac{1}{\hat{G}^2} \frac{B_0}{\bar{B}} \frac{2}{\pi^{1/2}} \left\langle \int_{-1}^{1} d\xi f_{\nabla} \frac{1}{\hat{B}} \left(1+\xi^2\right) \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \right\rangle . \tag{43}$$

Using (32),

$$L_{11} = -\frac{1}{\hat{G}^2} \frac{B_0}{\bar{B}} \frac{2}{\pi^{1/2}} \left\langle \frac{1}{\hat{B}} \left(\frac{8}{3} f_0 + \frac{4}{15} f_2 \right) \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \right\rangle . \tag{44}$$

$$L_{11} = -\frac{1}{\hat{G}^2}\frac{B_0}{\bar{B}}\frac{2}{\pi^{1/2}}\frac{\int d\theta \int d\zeta \frac{1}{\hat{B}^3}\left(\frac{8}{3}f_0 + \frac{4}{15}f_2\right)\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]}{\int d\theta \int d\zeta \frac{1}{\hat{B}^2}}. \tag{45}$$

$$L_{31} = \frac{\frac{1}{\upsilon_{th} B_0}\left\langle B V_\| \right\rangle}{\frac{GTc}{ZeB_0\upsilon_i}\frac{1}{n}\frac{dn}{d\psi}} = \frac{\frac{1}{n\upsilon_{th} B_0}\left\langle B \int d^3\upsilon\, f\, \upsilon \xi \right\rangle}{\frac{GTc}{ZeB_0\upsilon_i}\frac{1}{n}\frac{dn}{d\psi}} \tag{46}$$

Using (16) and (41),

$$L_{31} = \frac{2}{\hat{G}\pi^{1/2}}\left\langle \hat{B}\int_0^\infty dx \int_{-1}^1 d\xi \xi\, f_\nabla x^2 e^{-x^2} \right\rangle \tag{47}$$

The ξ integral gives

$$L_{31} = \frac{4}{\hat{G}3\pi^{1/2}}\left\langle \hat{B}\int_0^\infty dx\, f_1 x^2 e^{-x^2} \right\rangle. \tag{48}$$

Using Hakan's convention in which x=1 and xWeights = exp(1),

$$L_{31} = \frac{4}{3\pi^{1/2}\hat{G}}\left\langle \hat{B} f_1 \right\rangle = \frac{4}{3\pi^{1/2}\hat{G}}\frac{\int d\theta \int d\zeta \left(f_1 / \hat{B}\right)}{\int d\theta \int d\zeta \left(1/\hat{B}^2\right)}. \tag{49}$$

For comparison, the particle flux in sfincs version 3 is

$$\texttt{particleFlux\_vm\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{\upsilon}}\left\langle \int d^3\upsilon\, f_s \mathbf{v}_m \cdot \nabla \hat{\psi} \right\rangle. \tag{50}$$

Summary of equations:

In this section I will drop decorations wherever possible. Before the Legendre modal expansion, the kinetic equation is

$$\xi B\left[\iota \frac{\partial f}{\partial \theta} + \frac{\partial f}{\partial \zeta}\right] - \left(1-\xi^2\right)\frac{1}{2}\left(\iota \frac{\partial B}{\partial \theta} + \frac{\partial B}{\partial \zeta}\right)\frac{\partial f}{\partial \xi} - \frac{\nu}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial f}{\partial \xi} = \left(1+\xi^2\right)\frac{1}{B}\left[G\frac{\partial B}{\partial \theta} - I\frac{\partial B}{\partial \zeta}\right]. \tag{51}$$

After the Legendre expansion, the kinetic equation becomes

$$\sum_L M_{L,\ell} f_\ell = R_L \tag{52}$$

where

$$
\begin{aligned}
M_{L,\ell} = & \left(\frac{L+1}{2L+3} \delta_{L+1,\ell} + \frac{L}{2L-1} \delta_{L-1,\ell} \right) B \left[\iota \frac{\partial}{\partial \theta} + \frac{\partial}{\partial \zeta} \right] \\
& - \frac{1}{2} \left(\iota \frac{\partial B}{\partial \theta} + \frac{\partial B}{\partial \zeta} \right) \left(\frac{(L+1)(L+2)}{2L+3} \delta_{L+1,\ell} - \frac{(L-1)L}{2L-1} \delta_{L-1,\ell} \right) \\
& + \frac{\nu}{2} L(L+1) \delta_{L,\ell}
\end{aligned} \tag{53}
$$

and

$$
R_L = \frac{1}{B} \left[G \frac{\partial B}{\partial \theta} - I \frac{\partial B}{\partial \zeta} \right] \left(\frac{4}{3} \delta_{L,0} + \frac{2}{3} \delta_{L,2} \right). \tag{54}
$$