December 19, 2013 Matt Landreman

Technical Documentation for SFINCS with multiple species

Introduction

In this document, we detail the equations implemented in SFINCS: the Stellarator Fokker-Planck Iterative Neoclassical Conservative Solver. The normalizations and input and output quantities are also defined.

Kinetic equation

We begin with the following drift-kinetic equation:

$$\left(\upsilon_{\|}\mathbf{b}+\mathbf{v}_E+\mathbf{v}_{ms}\right)\cdot\nabla_{\mu,W_s} f_{s1} - C_s\left\{f_{s1}\right\} = -\mathbf{v}_{ms}\cdot\nabla_{W_s} f_{sM} + \frac{Z_s e}{T_s}\upsilon_{\|}\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_{sM} \tag{1}$$

where s denotes species, $\mu = \upsilon_\perp^2/(2B)$,

$$W_s = \frac{\upsilon^2}{2} + \frac{Z_s e\Phi}{m_s} \tag{2}$$

is the total energy, Z_s is the charge in units of the proton charge e, T_s is the temperature, m_s is the mass, $\mathbf{v}_E$ is the $\mathbf{E}\times\mathbf{B}$ drift,

$$\mathbf{v}_{ms} = \left(\upsilon_{\|}/\Omega\right)\nabla_{\mu,\upsilon}\times\left(\upsilon_{\|}\mathbf{b}\right) = \frac{\upsilon_\perp^2}{2\Omega_s B^2}\mathbf{B}\times\nabla B + \frac{\upsilon_{\|}^2}{\Omega_s}\nabla\times\mathbf{b} \tag{3}$$

is the magnetic drift, $\Omega_s = Z_s eB/(m_s c)$ is the gyrofrequency (which is negative for electrons with $Z=-1$), and c is the speed of light. Subscripts on partial derivatives indicate quantities held fixed in differentiation. We assume the electrostatic potential Φ is a flux function to the order of interest. The total distribution function is $f_s = f_{sM} + f_{s1}$ where

$$f_{sM} = n_s(\psi)\left[\frac{m_s}{2\pi T_s(\psi)}\right]^{3/2}\exp\left(-\frac{m_s\upsilon^2}{2T_s(\psi)}\right). \tag{4}$$

In (1), C_s is the collision operator linearized about the Maxwellian f_{sM} for each species. We neglect contributions from the inductive electric field to $\mathbf{v}_E$, writing $\mathbf{v}_E = \left(c/B^2\right)\left(d\Phi/d\psi\right)\mathbf{B}\times\nabla\psi$ where $2\pi\psi$ is the toroidal flux. Let $\upsilon_s = \sqrt{2T_s/m_s}$ be the thermal speed, and let $x_s = \upsilon/\upsilon_s$.

The independent variables used in SFINCS are (θ,ζ,x_s,ξ) where $\xi = \upsilon_{\|}/\upsilon$. Changing velocity variables to (x_s,ξ) on the left side of (1),

$$\dot{\mathbf{r}}_s\cdot\nabla_{x_s,\xi} f_{s1} + \dot{x}_s\left(\frac{\partial f_{s1}}{\partial x_s}\right)_{\mathbf{r},\xi} + \dot{\xi}_s\left(\frac{\partial f_{s1}}{\partial \xi}\right)_{\mathbf{r},x_s} - C_s\left\{f_{s1}\right\} = -\mathbf{v}_{ms}\cdot\nabla_{W_s} f_{sM} + \frac{Z_s e}{T_s}\upsilon_{\|}\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_{sM} \tag{5}$$

where

$$\dot{\mathbf{r}}_s = \upsilon_{\|}\mathbf{b} + \mathbf{v}_E + \mathbf{v}_{ms}, \tag{6}$$

$$\dot{x}_s = \left(\upsilon_{\|}\mathbf{b} + \mathbf{v}_E + \mathbf{v}_{ms}\right)\cdot\left(\nabla_{\mu,W_s} x_s\right), \tag{7}$$

and

$$\dot{\xi}_s = \left(\upsilon_\| \mathbf{b} + \mathbf{v}_E + \mathbf{v}_{ms}\right) \cdot \left(\nabla_{\mu,W_s} \xi\right). \tag{8}$$

Applying ∇_{W_s} to (2) we find

$$\nabla_W x_s = -\frac{x_s}{m_s \upsilon_s^2} \nabla T - \frac{Z_s e}{2 T_s x_s} \nabla \Phi , \tag{9}$$

so (7) simplifies to

$$\dot{x}_s = \left(\mathbf{v}_{ms} \cdot \nabla \psi\right) \left(-\frac{x_s}{2T_s} \frac{dT_s}{d\psi} - \frac{Z_s e}{2 T_s x_s} \frac{d\Phi}{d\psi} \right). \tag{10}$$

Similarly, applying ∇_{μ,W_s} to $\mu = \upsilon_s^2 x_s^2 \left(1-\xi^2\right)/\left(2B\right)$, we find

$$\nabla_{\mu,W_s} \xi = -\frac{Z_s e}{2 T_s x_s^2 \xi} \left(1-\xi^2\right) \nabla \Phi - \frac{\left(1-\xi^2\right)}{\xi} \frac{1}{2B} \nabla B . \tag{11}$$

Thus, (8) may be written

$$\dot{\xi} = -\frac{Z_s e}{2 T_s x_s^2 \xi} \left(1-\xi^2\right) \frac{d\Phi}{d\psi} \mathbf{v}_{ms} \cdot \nabla \psi - \frac{\left(1-\xi^2\right)}{\xi} \frac{1}{2B} \left(\upsilon_\| \mathbf{b} + \mathbf{v}_E + \mathbf{v}_{ms}\right) \cdot \nabla B . \tag{12}$$

Noting

$$\mathbf{v}_{ms} \cdot \nabla \psi = -\frac{T_s c}{Z_s e B^3} x_s^2 \left(1+\xi^2\right) \mathbf{B} \times \nabla \psi \cdot \nabla B \tag{13}$$

then the two electric field terms in (12) may be combined to give

$$\dot{\xi}_s = -\frac{\left(1-\xi^2\right)}{\xi} \frac{1}{2B} \upsilon_\| \mathbf{b} \cdot \nabla B + \xi \left(1-\xi^2\right) \frac{c}{2B^3} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \cdot \nabla B - \frac{\left(1-\xi^2\right)}{\xi} \frac{1}{2B} \mathbf{v}_{ms} \cdot \nabla B . \tag{14}$$

In the present implementation of SFINCS, the $\mathbf{v}_{ms}$ terms in (6) and (14) are neglected, as is the $dT_s / d\psi$ term in (10). (This last term must be dropped in order to maintain conservation of μ .) We are then left with

$$\dot{\mathbf{r}}_s = \upsilon_\| \mathbf{b} + \frac{c}{B^2} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi , \tag{15}$$

$$\dot{x}_s = \frac{c}{2B^3} \frac{d\Phi}{d\psi} x_s \left(1+\xi^2\right) \mathbf{B} \times \nabla \psi \cdot \nabla B , \tag{16}$$

$$\dot{\xi}_s = -x_s \left(1-\xi^2\right) \frac{\upsilon_s}{2B^2} \mathbf{B} \cdot \nabla B + \xi \left(1-\xi^2\right) \frac{c}{2B^3} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \cdot \nabla B . \tag{17}$$

These are the same terms as in the last section of the appendix of Ref. [1].

We can verify that (15)-(17) still conserve μ :

$$\begin{aligned} \dot{\mu} &= \frac{d}{dt} \left(\frac{T_s x_s^2 \left(1-\xi^2\right)}{m_s B} \right) = \frac{T_s}{m_s} \frac{d}{dt} \left(\frac{x_s^2 \left(1-\xi^2\right)}{B} \right) \\ &= \frac{T_s}{m_s} \left\{ 2 \frac{1-\xi^2}{B} x_s \dot{x}_s - 2\xi \frac{x_s^2}{B} \dot{\xi} - \frac{x_s^2}{B^2} \left(1-\xi^2\right) \dot{\mathbf{r}}_s \cdot \nabla B \right\} \\ &= 0. \end{aligned} \tag{18}$$

As shown in the appendix of Ref. [1], (15)-(17) do not conserve W because the radial magnetic drift has been dropped. However, in an axisymmetric or quasisymmetric field, (15)-(17) do conserve a combination of energy and canonical momentum.

To compare various effective particle trajectories, the code allows the $d\Phi / d\psi$ terms in (16) and (17) to be turned off, in which case

$$\dot{x}_s = 0 , \tag{19}$$

$$\dot{\xi}_s = -x_s \left(1-\xi^2\right) \frac{\upsilon_s}{2B^2} \mathbf{B}\cdot\nabla B . \tag{20}$$

For comparison with DKES, SFINCS allows the option of using

$$\dot{\mathbf{r}}_s = \upsilon_\| \mathbf{b} + \frac{c}{\left\langle B^2 \right\rangle} \frac{d\Phi}{d\psi} \mathbf{B}\times\nabla\psi , \tag{21}$$

in place of (15).

One further option allowed in the code is to also include a term

$$-f_{s1} \frac{2c}{B^3} \frac{d\Phi}{d\psi} \mathbf{B}\times\nabla\psi\cdot\nabla B = f_{s1} \nabla\cdot\mathbf{v}_E \tag{22}$$

on the left-hand side of (5). The rationale for including this term is that it allows the left-hand side of (5) to be put into a conservative form when (19)-(20) are used:

$$\nabla_{x_s,\xi}\cdot\left(f_{s1}\dot{\mathbf{r}}_s\right) + \left(\frac{\partial}{\partial\xi}\right)_{\mathbf{r},x_s} \left[f_{s1}\dot{\xi}_s\right] - C_s\left\{f_{s1}\right\} = -\mathbf{v}_{ms}\cdot\nabla_{W_s} f_{sM} + \frac{Z_s e}{T_s} \upsilon_\| \frac{\left\langle E_\| B \right\rangle B}{\left\langle B^2 \right\rangle} f_{sM} . \tag{23}$$

For the rest of these notes, we will include the term (22) multiplied by α_{cons}, so α_{cons} will be either 0 or 1.

Now consider the magnetic field in Boozer coordinates:

$$\mathbf{B} = \nabla\psi\times\nabla\theta + \iota\nabla\zeta\times\nabla\psi , \tag{24}$$

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

$$\mathbf{B} = \beta\nabla\psi + G\nabla\zeta + I\nabla\theta , \tag{25}$$

where $G(\psi) = 2i_p / c$, $I(\psi) = 2i_t / c$, $i_p(\psi)$ is the poloidal current outside the flux surface, and $i_t(\psi)$ is the toroidal current inside the flux surface. Notice $\mathbf{B}\cdot\nabla\theta = \iota\mathbf{B}\cdot\nabla\zeta$. The product of (24) with (25) gives the Jacobian

$$\nabla\psi\times\nabla\theta\cdot\nabla\zeta = \frac{B^2}{G+\iota I} = \mathbf{B}\cdot\nabla\zeta . \tag{26}$$

Notice also that

$$\mathbf{B}\cdot\nabla X = \mathbf{B}\cdot\nabla\zeta\left[\iota\frac{\partial X}{\partial\theta} + \frac{\partial X}{\partial\zeta}\right] \tag{27}$$

for any quantity X , and

$$\mathbf{B}\times\nabla\psi\cdot\nabla B = \mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial\theta} - I\frac{\partial B}{\partial\zeta}\right]. \tag{28}$$

The kinetic equation (5) with (15)-(17) is thus equivalent to

$$\dot{\theta}_s \frac{\partial f_{s1}}{\partial \theta} + \dot{\zeta}_s \frac{\partial f_{s1}}{\partial \zeta} + \dot{x}_s \frac{\partial f_{s1}}{\partial x_s} + \dot{\xi}_s \frac{\partial f_{s1}}{\partial \xi} - C_s\{f_{s1}\} - \alpha_{cons} f_{s1} \frac{2c}{B^3}\frac{d\Phi}{d\psi}\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial \theta} - I\frac{\partial B}{\partial \zeta}\right]$$
$$= \frac{T_s c}{Z_s e B^3} x_s^2 \left(1+\xi^2\right)\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial \theta} - I\frac{\partial B}{\partial \zeta}\right] f_{sM}\left[\frac{1}{n_s}\frac{dn_s}{d\psi} + \frac{Z_s e}{T_s}\frac{d\Phi}{d\psi} + \left(x_s^2 - \frac{3}{2}\right)\frac{1}{T_s}\frac{dT_s}{d\psi}\right] + \frac{Z_s e}{T_s}\upsilon_\parallel \frac{\langle E_\parallel B\rangle B}{\langle B^2\rangle} f_{sM} \quad (29)$$

where

$$\dot{\theta}_s = \left[\frac{\upsilon_s x_s \xi}{B}\iota + \frac{cG}{B^2}\frac{d\Phi}{d\psi}\right]\mathbf{B}\cdot\nabla\zeta\,, \quad (30)$$

$$\dot{\zeta}_s = \left[\frac{\upsilon_s x_s \xi}{B} - \frac{Ic}{B^2}\frac{d\Phi}{d\psi}\right]\mathbf{B}\cdot\nabla\zeta\,, \quad (31)$$

$$\dot{x}_s = \frac{c}{2B^3}\frac{d\Phi}{d\psi} x_s \left(1+\xi^2\right)\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial \theta} - I\frac{\partial B}{\partial \zeta}\right], \quad (32)$$

$$\dot{\xi}_s = -x_s\left(1-\xi^2\right)\frac{\upsilon_s}{2B^2}\mathbf{B}\cdot\nabla\zeta\left[\iota\frac{\partial B}{\partial \theta} + \frac{\partial B}{\partial \zeta}\right] + \xi\left(1-\xi^2\right)\frac{c}{2B^3}\frac{d\Phi}{d\psi}\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial \theta} - I\frac{\partial B}{\partial \zeta}\right]. \quad (33)$$

Normalizations

Let's suppose we are given T_s, $dT_s/d\psi_N$, n_s, $dn_s/d\psi_N$, $d\Phi/d\psi_N$, $B(\theta,\zeta)$, ι, G, I, $\psi_a = \psi(\psi_N = 1)$, and $\langle E_\parallel B\rangle$ where ψ_N is the normalized toroidal flux. The flux at the last closed flux surface is ψ_a, so the dimensional flux ψ is related to ψ_N by $\psi = \psi_N \psi_a$. The input quantities are specified in terms of some species-independent dimensions $\bar{T}$ (e.g. eV), $\bar{n}$ (e.g. $10^{20}/m^3$), $\bar{\Phi}$ (e.g. kV), $\bar{B}$ (e.g. T), $\bar{R}$ (e.g. m), and $\bar{m}$ (typically the proton or deuteron mass). In other words, the quantities we are actually given are

$$\hat{m}_s = m_s / \bar{m}\,, \quad (34)$$

$$\hat{T}_s = T_s / \bar{T}\,, \quad (35)$$

$$\hat{n}_s = n_s / \bar{n}\,, \quad (36)$$

$$d\hat{T}_s / d\psi_N = \left(dT_s / d\psi_N\right) / \bar{T}\,, \quad (37)$$

$$d\hat{n}_s / d\psi_N = \left(dn_s / d\psi_N\right) / \bar{n}\,, \quad (38)$$

$$d\hat{\Phi} / d\psi_N = \left(d\Phi / d\psi_N\right) / \bar{\Phi}\,, \quad (39)$$

$$\hat{B} = B / \bar{B}\,, \quad (40)$$

$$\hat{G} = G / \left(\bar{R}\bar{B}\right), \quad (41)$$

$$\hat{I} = I / \left(\bar{R}\bar{B}\right), \quad (42)$$

$$\hat{\psi}_a = \psi_a / \left(\bar{B}\bar{R}^2\right), \quad (43)$$

and

$$\hat{E} = \langle E_\parallel B\rangle \frac{\bar{R}}{\bar{\Phi}\bar{B}}\,. \quad (44)$$

Notice $\psi = \psi_N \hat{\psi}_a \bar{R}^2 \bar{B}$, and so

$$\frac{dX}{d\psi} = \frac{1}{\hat{\psi}_a \bar{R}^2 \bar{B}} \frac{dX}{d\psi_N} \tag{45}$$

for any flux function X.

It will be useful to define the following combinations of normalization constants:

$$\bar{\upsilon} = \sqrt{2\bar{T} / \bar{m}}\,, \tag{46}$$

$$\Delta = \frac{\bar{m}c\bar{\upsilon}}{e\bar{B}\bar{R}} \tag{47}$$

(which resembles $\rho_* = \rho / R$),

$$\alpha = \frac{e\bar{\Phi}}{\bar{T}}, \tag{48}$$

$$\omega = \frac{c\bar{\Phi}}{\bar{\upsilon}\bar{R}\bar{B}} = \frac{\Delta\alpha}{2}, \tag{49}$$

and a normalized collisionality

$$\nu_n = \bar{\nu}\bar{R} / \bar{\upsilon} \tag{50}$$

where $\bar{\nu}$ is the dimensional collisionality at the reference parameters:

$$\bar{\nu} = \frac{4\sqrt{2\pi}\bar{n}e^4 \ln\Lambda}{3\bar{m}^{1/2}\bar{T}^{3/2}}. \tag{51}$$

We assume $\ln\Lambda$ has the same value for all species. It will be useful to notice

$$\mathbf{B}\cdot\nabla\zeta = \frac{\bar{B}}{\bar{R}} \frac{\hat{B}^2}{\hat{G} + \iota\hat{I}}. \tag{52}$$

We define a normalized distribution function $\hat{f}_s$ as follows:

$$f_{s1} = \frac{\bar{n}}{\bar{\upsilon}^3} \hat{f}_s. \tag{53}$$

Notice the normalization is the same for each species. Also notice that the normalization is different than in the original 1-species version of SFINCS.

The kinetic equation (29) for each species is made dimensionless by multiplying through by

$$\frac{\bar{\upsilon}^3}{\bar{n}} \frac{\bar{B}}{\bar{\upsilon}\mathbf{B}\cdot\nabla\zeta}. \tag{54}$$

(this normalization too is slightly different than in the 1-species version of SFINCS.) We then obtain

$$
\begin{aligned}
&\left[\frac{\hat{T}_s^{1/2} x_s \xi}{\hat{m}_s^{1/2}\hat{B}}\iota + \frac{\alpha\Delta\hat{G}}{2\hat{\psi}_a\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\right]\frac{\partial\hat{f}_s}{\partial\theta}\\
&\left[\frac{\hat{T}_s^{1/2} x_s \xi}{\hat{m}_s^{1/2}\hat{B}} - \frac{\alpha\Delta\hat{I}}{2\hat{\psi}_a\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\right]\frac{\partial\hat{f}_s}{\partial\zeta}\\
&+\frac{\alpha\Delta}{4\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}x_s\left(1+\xi^2\right)\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\frac{\partial\hat{f}_s}{\partial x_s}\\
&+\left\{-x_s\left(1-\xi^2\right)\frac{\hat{T}_s^{1/2}}{2\hat{m}_s^{1/2}\hat{B}^2}\left[\iota\frac{\partial\hat{B}}{\partial\theta}+\frac{\partial\hat{B}}{\partial\zeta}\right]+\xi\left(1-\xi^2\right)\frac{\alpha\Delta}{4\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\right\}\frac{\partial\hat{f}_s}{\partial\xi}\\
&-\frac{\hat{G}+\iota\hat{I}}{\hat{B}^2}\nu_n\frac{1}{\bar{\nu}}C_s\left\{\hat{f}_s\right\}-\alpha_{cons}\frac{d\hat{\Phi}}{d\psi_N}\frac{\Delta\alpha}{\hat{\psi}_a\hat{B}^3}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\hat{f}_s\\
&=\frac{\Delta\hat{n}_s\hat{T}_s}{2\pi^{3/2}\hat{\psi}_a Z_s\hat{B}^3}\left(\frac{\hat{m}_s}{\hat{T}_s}\right)^{3/2}x_s^2\left(1+\xi^2\right)\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]e^{-x_s^2}\left[\frac{1}{\hat{n}_s}\frac{d\hat{n}_s}{d\psi_N}+\frac{\alpha Z_s}{\hat{T}_s}\frac{d\hat{\Phi}}{d\psi_N}+\left(x_s^2-\frac{3}{2}\right)\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\psi_N}\right]\\
&+\alpha\frac{\hat{G}+\iota\hat{I}}{\hat{B}}\frac{Z_s}{\hat{T}_s^2}x_s\xi\hat{E}\frac{1}{\left\langle\hat{B}^2\right\rangle}\frac{\hat{n}_s\hat{m}_s}{\pi^{3/2}}e^{-x_s^2} \qquad (55)
\end{aligned}
$$

where $\hat{C}_s\left\{\hat{f}_s\right\} = \bar{\nu}^{-1}C_s\left\{\hat{f}_s\right\}$.

Legendre discretization

SFINCS uses a collocation discretization in the x_s, θ, and ζ coordinates, but a modal discretization in the ξ coordinate. In other words, the distribution function is known at certain grid points in x_s, θ, and ζ, but it is expanded as modes in ξ. We employ the following modal expansion in terms of Legendre polynomials $P_\ell\left(\xi\right)$:

$$\hat{f}_s = \sum_\ell f_{s,\ell}P_\ell\left(\xi\right). \qquad (56)$$

We discretize the kinetic equation (55) by applying

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\; P_L\left(\xi\right)\left(\quad\cdot\quad\right). \qquad (57)$$

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

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\xi P_L\left(\xi\right)P_\ell\left(\xi\right) = \frac{L+1}{2L+3}\delta_{L+1,\ell}+\frac{L}{2L-1}\delta_{L-1,\ell}, \qquad (58)$$

$$
\begin{aligned}
\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\left(1+\xi^2\right)P_L\left(\xi\right)P_\ell\left(\xi\right) = &\frac{2\left[3L^2+3L-2\right]}{\left(2L+3\right)\left(2L-1\right)}\delta_{L,\ell}\\
&+\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell}+\frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell},
\end{aligned} \qquad (59)
$$

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\left(1-\xi^2\right)P_L\left(\xi\right)\frac{dP_\ell}{d\xi} = \frac{\left(L+1\right)\left(L+2\right)}{2L+3}\delta_{L+1,\ell}-\frac{\left(L-1\right)L}{2L-1}\delta_{L-1,\ell}, \qquad (60)$$

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ \left(1-\xi^2\right)\xi P_L\left(\xi\right)\frac{dP_\ell}{d\xi} = \frac{\left(L+1\right)L}{\left(2L-1\right)\left(2L+3\right)}\delta_{L,\ell} + \frac{\left(L+3\right)\left(L+2\right)\left(L+1\right)}{\left(2L+5\right)\left(2L+3\right)}\delta_{L+2,\ell} - \frac{L\left(L-1\right)\left(L-2\right)}{\left(2L-3\right)\left(2L-1\right)}\delta_{L-2,\ell}, \tag{61}$$

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\xi = \delta_{L,1}, \tag{62}$$

and

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\left(1+\xi^2\right) = \frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}. \tag{63}$$

As a result, (55) may be written

$$\sum_\ell M_{s,L,\ell}\hat{f}_{s,\ell} = R_{s,L} \tag{64}$$

where

$$M_{s,L,\ell} = \dot{\theta}_{s,L,\ell}\frac{\partial}{\partial\theta} + \dot{\zeta}_{s,L,\ell}\frac{\partial}{\partial\zeta} + M^{(\xi)}_{s,L,\ell} + \dot{x}_{s,L,\ell}\frac{\partial}{\partial x_s} - \nu_n\frac{\left(\hat{G}+\iota\hat{I}\right)}{\hat{B}^2}\hat{C}_{s,L}\delta_{L,\ell} + \alpha_{cons}\delta_{L,\ell}Y, \tag{65}$$

$$\dot{\theta}_{s,L,\ell} = \frac{\hat{T}_s^{1/2}x_s}{\hat{m}_s^{1/2}\hat{B}}\iota\left[\frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}\right] + \frac{\alpha\Delta\hat{G}}{2\hat{\psi}_a\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\delta_{L,\ell} \tag{66}$$

$$\dot{\zeta}_{s,L,\ell} = \frac{\hat{T}_s^{1/2}x_s}{\hat{m}_s^{1/2}\hat{B}}\left[\frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}\right] - \frac{\alpha\Delta\hat{I}}{2\hat{\psi}_a\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\delta_{L,\ell} \tag{67}$$

$$\begin{aligned} M^{(\xi)}_{s,L,\ell} = &-x_s\frac{\hat{T}_s^{1/2}}{2\hat{m}_s^{1/2}\hat{B}^2}\left[\iota\frac{\partial\hat{B}}{\partial\theta} + \frac{\partial\hat{B}}{\partial\zeta}\right]\left[\frac{\left(L+1\right)\left(L+2\right)}{2L+3}\delta_{L+1,\ell} - \frac{\left(L-1\right)L}{2L-1}\delta_{L-1,\ell}\right] \\ &+\frac{\alpha\Delta}{4\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\begin{array}{l}\frac{\left(L+1\right)L}{\left(2L-1\right)\left(2L+3\right)}\delta_{L,\ell} \\ +\frac{\left(L+3\right)\left(L+2\right)\left(L+1\right)}{\left(2L+5\right)\left(2L+3\right)}\delta_{L+2,\ell} - \frac{L\left(L-1\right)\left(L-2\right)}{\left(2L-3\right)\left(2L-1\right)}\delta_{L-2,\ell}\end{array}\right] \end{aligned} \tag{68}$$

$$\dot{x}_{s,L,\ell} = \frac{\alpha\Delta}{4\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}x_s\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\begin{array}{l}\frac{2\left[3L^2+3L-2\right]}{\left(2L+3\right)\left(2L-1\right)}\delta_{L,\ell} \\ +\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell} + \frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell}\end{array}\right], \tag{69}$$

$$Y = -\frac{d\hat{\Phi}}{d\psi_N}\frac{\Delta\alpha}{\hat{\psi}_a\hat{B}^3}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right], \tag{70}$$

and

$$R_{s,L} = \frac{\Delta \hat{n}_s \hat{T}_s}{2\pi^{3/2}\hat{\psi}_a Z_s \hat{B}^3}\left(\frac{\hat{m}_s}{\hat{T}_s}\right)^{3/2} x_s^2 \left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right] e^{-x_s^2}\left[\frac{1}{\hat{n}_s}\frac{d\hat{n}_s}{d\psi_N} + \frac{\alpha Z_s}{\hat{T}_s}\frac{d\hat{\Phi}}{d\psi_N} + \left(x_s^2 - \frac{3}{2}\right)\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\psi_N}\right]\left[\frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}\right] \tag{71}$$

$$+\alpha \frac{\hat{G}+\iota \hat{I}}{\hat{B}}\frac{Z_s}{\hat{T}_s^2} x_s \xi \hat{E}\frac{1}{\langle \hat{B}^2\rangle}\frac{\hat{n}_s \hat{m}_s}{\pi^{3/2}} e^{-x_s^2}\delta_{L,1}$$

Collision operator

The total collision operator for species a is a sum of collision operators with each species:

$$C_a = \sum_b C_{ab} \,. \tag{72}$$

The linearized Fokker-Planck collision operator for each pair of species may be written

$$C_{ab} = C_{ab}^L + C_{ab}^E + C_{ab}^F , \tag{73}$$

where the Lorentz part of the collision term is

$$C_{ab}^L = \frac{\nu_{Dab}}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial f_{a1}}{\partial \xi} \tag{74}$$

with

$$\nu_{Dab} = \frac{\Gamma_{ab} n_b}{\upsilon^3}\left[\operatorname{erf}\left(x_b\right) - \Psi\left(x_b\right)\right], \tag{75}$$

$$\Gamma_{ab} = \frac{4\pi Z_a^2 Z_b^2 e^4 \ln \Lambda}{m_a^2}, \tag{76}$$

$$\Psi\left(x_b\right) = \frac{\operatorname{erf}\left(x_b\right) - x_b \operatorname{erf}'\left(x_b\right)}{2x_b^2}. \tag{77}$$

The energy scattering contribution is

$$C_{ab}^E = \nu_{\|ab}\left[\frac{\upsilon^2}{2}\frac{\partial^2 f_{a1}}{\partial \upsilon^2} - x_b^2\left(1-\frac{m_a}{m_b}\right)\upsilon \frac{\partial f_{a1}}{\partial \upsilon}\right] + \nu_{Dab}\upsilon \frac{\partial f_{a1}}{\partial \upsilon} + 4\pi \Gamma_{ab}\frac{m_a}{m_b} f_{Mb} f_{a1} \tag{78}$$

where

$$\nu_{\|ab} = 2\frac{\Gamma_{ab} n_b}{\upsilon^3}\Psi\left(x_b\right). \tag{79}$$

The field term is

$$C_{ab}^F = \Gamma_{ab} f_{Ma}\left[\frac{2\upsilon^2}{\upsilon_a^4}\frac{\partial^2 G_{b1}}{\partial \upsilon^2} - \frac{2\upsilon}{\upsilon_a^2}\left(1-\frac{m_a}{m_b}\right)\frac{\partial H_{b1}}{\partial \upsilon} - \frac{2}{\upsilon_a^2}H_{b1} + 4\pi \frac{m_a}{m_b} f_{b1}\right] \tag{80}$$

where the potentials are defined by

$$\nabla_\upsilon^2 H_{b1} = -4\pi f_{b1} \tag{81}$$

and

$$\nabla_\upsilon^2 G_{b1} = 2H_{b1}. \tag{82}$$

We write the field term as

$$C_{ab}^F = C_{ab}^H + C_{ab}^G + C_{ab}^D \tag{83}$$

where

$$C_{ab}^{G} = \Gamma_{ab} f_{Ma} \frac{2\upsilon^2}{\upsilon_a^4} \frac{\partial^2 G_{b1}}{\partial \upsilon^2} \tag{84}$$

$$C_{ab}^{H} = \Gamma_{ab} f_{Ma} \left[-\frac{2\upsilon}{\upsilon_a^2} \left(1 - \frac{m_a}{m_b} \right) \frac{\partial H_{b1}}{\partial \upsilon} - \frac{2}{\upsilon_a^2} H_{b1} \right] \tag{85}$$

$$C_{ab}^{D} = \Gamma_{ab} f_{Ma} 4\pi \frac{m_a}{m_b} f_{b1} = \frac{\Gamma_{ab} n_a}{\upsilon_a^3} \exp\left(-x_a^2\right) \frac{4}{\pi^{1/2}} \frac{m_a}{m_b} f_{b1} \tag{86}$$

The Poisson equations that define the potentials are (for Legendre mode $P_\ell\left(\xi\right)$)

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial H_{b1}}{\partial x_b} - \ell\left(\ell+1\right) H_{b1} = -4\pi\upsilon^2 f_{b1} \tag{87}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial G_{b1}}{\partial x_b} - \ell\left(\ell+1\right) G_{b1} = 2\upsilon^2 H_{b1}. \tag{88}$$

Let us define

$$\hat{H}_{b1} = H_{b1} / \upsilon_b^2 \tag{89}$$

$$\hat{G}_{b1} = G_{b1} / \upsilon_b^4 \tag{90}$$

so the defining equations for the potentials become

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{H}_{b1}}{\partial x_b} - \ell\left(\ell+1\right) \hat{H}_{b1} = -4\pi x_b^2 f_{b1} \tag{91}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{G}_{b1}}{\partial x_b} - \ell\left(\ell+1\right) \hat{G}_{b1} = 2x_b^2 \hat{H}_{b1}. \tag{92}$$

Next, recall that in the kinetic equation (65), we need to evaluate

$$\hat{C}_{ab} = \frac{1}{\bar{\nu}} C_{ab} \tag{93}$$

where $\bar{\nu}$ is defined in (51). It is convenient to note

$$\frac{\Gamma_{ab}}{\bar{\nu}} = \frac{3\sqrt{\pi}}{4} \frac{1}{\bar{n}} \frac{Z_a^2 Z_b^2}{\hat{T}_a^{3/2} \hat{m}_a^{1/2}} \upsilon_a^3 \tag{94}$$

Expanding $\hat{C}_{ab} = \hat{C}_{ab}^{L} + \hat{C}_{ab}^{E} + \hat{C}_{ab}^{F}$ as before,

$$\hat{C}_{ab}^{L} = \frac{\hat{\nu}_{Dab}}{2} \frac{\partial}{\partial \xi} \left(1 - \xi^2\right) \frac{\partial f_{a1}}{\partial \xi} \tag{95}$$

where

$$\hat{\nu}_{Dab} = \frac{3\sqrt{\pi}}{4} \frac{\hat{n}_b Z_a^2 Z_b^2}{\hat{T}_a^{3/2} \hat{m}_a^{1/2}} \frac{1}{x_a^3} \left[\operatorname{erf}\left(x_b\right) - \Psi\left(x_b\right) \right] \tag{96}$$

The energy scattering component is

$$\hat{C}_{ab}^{E}\left\{f_{a1}\right\} = \frac{3\sqrt{\pi}}{4}\frac{\hat{n}_b Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left[\begin{array}{l} \frac{1}{x_a}\Psi\left(x_b\right)\frac{\partial^2 f_{a1}}{\partial x_a^2} \\ +\left\{-2\frac{\hat{T}_a}{\hat{T}_b}\frac{\hat{m}_b}{\hat{m}_a}\Psi\left(x_b\right)\left(1-\frac{\hat{m}_a}{\hat{m}_b}\right)+\frac{1}{x_a^2}\left[\mathrm{erf}\left(x_b\right)-\Psi\left(x_b\right)\right]\right\}\frac{\partial f_{a1}}{\partial x_a} \\ +\frac{4}{\sqrt{\pi}}\left(\frac{\hat{T}_a}{\hat{T}_b}\right)^{3/2}\left(\frac{\hat{m}_b}{\hat{m}_a}\right)^{1/2} e^{-x_b^2} f_{a1} \end{array}\right] \tag{97}$$

The diagonal term is

$$\hat{C}_{ab}^{D} = 3\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\frac{\hat{m}_a}{\hat{m}_b}\exp\left(-x_a^2\right) f_{b1} \tag{98}$$

In the cross-species case, this term is no longer identical to the f_{a1} term in energy scattering (as it is in the same-species case).

The G term in the collision operator is

$$\begin{aligned} \hat{C}_{ab}^{G} &= \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right)^2 e^{-x_a^2} x_b^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_b^2} \\ &= \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right) e^{-x_a^2} x_a^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_b^2}. \end{aligned} \tag{99}$$

Although in principle we would also be free to write

$$\hat{C}_{ab}^{G} = \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right)^2 e^{-x_a^2} x_a^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_a^2} \tag{100}$$

(i.e. replacing $x_b \to x_a$ in two places), the resulting expression is less convenient because we compute $\hat{G}_{b1}$ on the x_b grid, and so it is easier to differentiate with respect to x_b.

The H collision term is

$$\hat{C}_{ab}^{H} = -\frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b} e^{-x_a^2}\left[\left(1-\frac{\hat{m}_a}{\hat{m}_b}\right) x_b \frac{\partial \hat{H}_{b1}}{\partial x_b} + \hat{H}_{b1}\right] \tag{101}$$

Output quantities

Flux surface average:

For any quantity X, the flux surface average can be computed from

$$\left\langle X\right\rangle = \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{X}{\hat{B}^2} \tag{102}$$

where

$$\texttt{VPrimeHat} = \hat{V}' = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^2}. \tag{103}$$

Notice

$$\texttt{FSABHat2} = \left\langle \hat{B}^2 \right\rangle = \frac{4\pi^2}{\hat{V}'}. \tag{104}$$

Density perturbation

SFINCS returns the density carried in $\hat{f}_{s1}$:

$$\texttt{densityPerturbation} = \frac{1}{\bar{n}} \int d^3\upsilon\, f_{s1} = 4\pi \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{3/2} \int_0^\infty dx_s x_s^2 \hat{f}_{s,L=0}. \tag{105}$$

Upon flux surface averaging, we obtain

$$\begin{aligned} \texttt{FSADensityPerturbation} &= \left\langle \frac{1}{\bar{n}} \int d^3\upsilon\, f_{s1} \right\rangle \\ &= \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{\texttt{densityPerturbation}}{\hat{B}^2}. \end{aligned} \tag{106}$$

Pressure perturbation

SFINCS also returns the pressure in $\hat{f}_{s1}$, normalized to the reference pressure $\bar{n}\bar{T}$:

$$\begin{aligned} \texttt{pressurePerturbation} &= \frac{1}{\bar{n}\bar{T}} \frac{m_s}{3} \int d^3\upsilon\, \upsilon^2 f_{s1} \\ &= \frac{8\pi \hat{m}_s}{3} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \int_0^\infty dx_s x_s^4 \hat{f}_{s,L=0}. \end{aligned} \tag{107}$$

Upon flux surface averaging, we obtain

$$\begin{aligned} \texttt{FSAPressurePerturbation} &= \left\langle \frac{1}{\bar{n}\bar{T}} \frac{m_s}{3} \int d^3\upsilon \upsilon^2 f_{s1} \right\rangle \\ &= \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{\texttt{pressurePerturbation}}{\hat{B}^2}. \end{aligned} \tag{108}$$

Flow

We choose to normalize the parallel flow at each point as follows:

$$\texttt{flow} = \frac{1}{\bar{n}\bar{\upsilon}} \int d^3\upsilon\, \upsilon_\| f_{s1} = \frac{4\pi}{3} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^2 \int_0^\infty dx_s x_s^3 \hat{f}_{s,L=1}. \tag{109}$$

Both numerical and analytic calculations often employ the weights average flow $\left\langle V_\| B \right\rangle$. In SFINCS, this quantity is normalized in the following way:

$$\texttt{FSABFlow} = \frac{1}{\bar{n}\bar{\upsilon}\bar{B}} \left\langle B \int d^3\upsilon\, \upsilon_\| f \right\rangle = \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{\texttt{flow}}{\hat{B}}. \tag{110}$$

Particle flux

The following expression is useful for evaluating the radial fluxes:

$$\mathbf{v}_{ms} \cdot \nabla\psi = -\bar{\upsilon}\bar{R}\bar{B} \frac{\Delta \hat{T}_s}{2 Z_s \hat{B}} x_s^2 \left(1+\xi^2\right) \frac{1}{\hat{G}+\iota\hat{I}} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right]. \tag{111}$$

We may write the radial particle flux as

$$\left\langle \int d^3\upsilon f_{s1} \mathbf{v}_{ms} \cdot \nabla\psi \right\rangle = -\bar{n}\bar{\upsilon}\bar{R}\bar{B} \frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \frac{1}{\hat{G}+\iota\hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G}\frac{\partial \hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right] \times \int_{-1}^{1} d\xi \int_0^\infty dx_s \hat{f}_s x_s^4 \left(1+\xi^2\right). \tag{112}$$

Using

$$\int_{-1}^{1} d\xi\, P_L(\xi)\left(1+\xi^2\right) = \frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{113}$$

then

$$\left\langle \int d^3\upsilon f_{s1} \mathbf{v}_{ms} \cdot \nabla\psi \right\rangle = \bar{n}\bar{\upsilon}\bar{R}\bar{B}\left(\texttt{particleFlux}\right) \tag{114}$$

where

$$\texttt{particleFlux} = -\frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \frac{1}{\hat{G}+\iota\hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G}\frac{\partial \hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right] \times \int_0^\infty dx_s x_s^4 \left[\frac{8}{3}\hat{f}_{s,L=0} + \frac{4}{15}\hat{f}_{s,L=2}\right]. \tag{115}$$

Momentum flux

We may write a radial momentum flux as

$$\left\langle \int d^3\upsilon f_{s1} m_s \upsilon_\parallel \mathbf{v}_{ms} \cdot \nabla\psi \right\rangle = -\bar{n}\bar{m}\bar{\upsilon}^2\bar{R}\bar{B} \frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{2} \frac{\hat{m}_s}{\hat{G}+\iota\hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G}\frac{\partial \hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right] \times \int_{-1}^{1} d\xi \int_0^\infty dx_s \hat{f}_s x_s^5 \xi \left(1+\xi^2\right). \tag{116}$$

Using

$$\int_{-1}^{1} d\xi\, P_L(\xi)\,\xi\left(1+\xi^2\right) = \frac{16}{15}\delta_{L,1} + \frac{4}{35}\delta_{L,3} \tag{117}$$

then

$$\left\langle \int d^3\upsilon f_{s1} \upsilon_\parallel \mathbf{v}_{ms} \cdot \nabla\psi \right\rangle = \bar{n}\bar{m}\bar{\upsilon}^2\bar{R}\bar{B}\left(\texttt{momentumFlux}\right) \tag{118}$$

where

$$\texttt{momentumFlux} = -\frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{2} \frac{\hat{m}_s}{\hat{G}+\iota\hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G}\frac{\partial \hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right] \times \int_0^\infty dx_s x_s^5 \left[\frac{16}{15}\hat{f}_{s,L=1} + \frac{4}{35}\hat{f}_{s,L=3}\right]. \tag{119}$$

Heat flux

We may write the radial energy flux as

$$\left\langle \int d^3\upsilon f_{s1} \frac{m_s\upsilon^2}{2} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = -\bar{n}\bar{m}\bar{\upsilon}^3 \bar{R}\bar{B} \frac{\pi \Delta \hat{T}_s \hat{m}_s}{2 Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \frac{1}{\hat{G} + \iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_{-1}^{1} d\xi \int_0^\infty dx_s \hat{f}_s x_s^6 \left(1 + \xi^2\right). \tag{120}$$

Using (113), then

$$\left\langle \int d^3\upsilon f_{s1} \frac{m_s\upsilon^2}{2} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = \bar{n}\bar{m}\bar{\upsilon}^3 \bar{R}\bar{B} \left(\texttt{heatFlux}\right) \tag{121}$$

where

$$\texttt{heatFlux} = -\frac{\pi \Delta \hat{T}_s \hat{m}_s}{2 Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \frac{1}{\hat{G} + \iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_0^\infty dx_s \hat{f}_s x_s^6 \left[\frac{8}{3} \hat{f}_{s,L=0} + \frac{4}{15} \hat{f}_{s,L=2} \right]. \tag{122}$$

Parallel current

The current is normalized as follows:

$$j_\parallel = \sum_s Z_s e n_s V_{\parallel s} = \sum_s Z_s e \int d^3\upsilon f_{s1} \upsilon_\parallel = e\bar{n}\bar{\upsilon} \left(\texttt{jHat}\right) \tag{123}$$

so

$$\texttt{jHat} = \frac{1}{e\bar{n}\bar{\upsilon}} \sum_s Z_s e \int d^3\upsilon f_{s1} \upsilon_\parallel = \sum_s Z_s \left(\texttt{flow}_s\right). \tag{124}$$

We also form the average $\langle \mathbf{B} \cdot \mathbf{j} \rangle$ which is associated with the bootstrap current:

$$\langle \mathbf{B} \cdot \mathbf{j} \rangle = \left\langle \sum_s Z_s e n_s B V_{\parallel s} \right\rangle = \left\langle B \sum_s Z_s e \int d^3\upsilon f_{s1} \upsilon_\parallel \right\rangle = e\bar{n}\bar{\upsilon}\bar{B} \left(\texttt{FSABjHat}\right) \tag{125}$$

where

$$\texttt{FSABjHat} = \frac{1}{e\bar{n}\bar{\upsilon}\bar{B}} \left\langle B \sum_s Z_s e \int d^3\upsilon f_{s1} \upsilon_\parallel \right\rangle = \sum_s Z_s \left(\texttt{FSABFlow}_s\right). \tag{126}$$

Perturbed electrostatic potential

From eq (21) in the Physics of Plasmas paper, the variation of the electrostatic potential on a flux surface, Φ_1, may be found from

$$e\Phi_1 \sum_a \frac{Z_a^2 n_a}{T_a} = \sum_a Z_a \int d^3\upsilon f_{a1}. \tag{127}$$

We define the normalized perturbed potential to be $\hat{\Phi}_1 = \Phi_1 / \bar{\Phi}$, and so

$$\hat{\Phi}_1 = \frac{\sum_a Z_a \frac{1}{\bar{n}} \int d^3\upsilon f_{a1}}{\alpha \sum_a \frac{Z_a^2 \hat{n}_a}{\hat{T}_a}} = \frac{\sum_a Z_a \left(\texttt{densityPerturbation}\right)}{\alpha \sum_a \frac{Z_a^2 \hat{n}_a}{\hat{T}_a}}. \tag{128}$$