December 20, 2013 Matt Landreman

Technical Documentation for SFINCS - single species version

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:

$$\left(\upsilon_{\|}\mathbf{b}+\mathbf{v}_{E}+\mathbf{v}_{m}\right)\cdot\nabla_{\mu,W} f_1 - C\left\{f_1\right\} = -\mathbf{v}_m\cdot\nabla_W f_M + \frac{Ze}{T}\upsilon_{\|}\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_M \tag{1}$$

where $\mu = \upsilon_{\perp}^2/(2B)$,

$$W = \frac{\upsilon^2}{2} + \frac{Ze\Phi}{m} \tag{2}$$

is the total energy, Z is the ion charge in units of the proton charge e, T is the temperature, m is the ion mass, $\mathbf{v}_E$ is the $\mathbf{E}\times\mathbf{B}$ drift,

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

is the magnetic drift, $\Omega = ZeB/(mc)$ is the gyrofrequency, 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 $f = f_M + f_1$ where

$$f_M = n(\psi)\left[\frac{m}{2\pi T(\psi)}\right]^{3/2}\exp\left(-\frac{m\upsilon^2}{2T(\psi)}\right). \tag{4}$$

In (1), C is the collision operator linearized about f_M. 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 $\upsilon_{th} = \sqrt{2T/m}$ be the thermal speed, and let $x = \upsilon/\upsilon_{th}$.

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

$$\dot{\mathbf{r}}\cdot\nabla_{x,\xi} f_1 + \dot{x}\left(\frac{\partial f_1}{\partial x}\right)_{\mathbf{r},\xi} + \dot{\xi}\left(\frac{\partial f_1}{\partial \xi}\right)_{\mathbf{r},x} - C\left\{f_1\right\} = -\mathbf{v}_m\cdot\nabla_W f_M + \frac{Ze}{T}\upsilon_{\|}\frac{\left\langle E_{\|}B\right\rangle B}{\left\langle B^2\right\rangle} f_M \tag{5}$$

where

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

$$\dot{x} = \left(\upsilon_{\|}\mathbf{b} + \mathbf{v}_E + \mathbf{v}_m\right)\cdot\left(\nabla_{\mu,W} x\right), \tag{7}$$

and

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

Applying ∇_W to (2) we find

$$\nabla_W x = -\frac{x}{m\upsilon_{th}^2}\nabla T - \frac{Ze}{2Tx}\nabla\Phi , \tag{9}$$

so (7) simplifies to

$$\dot{x} = \left(\mathbf{v}_m\cdot\nabla\psi\right)\left(-\frac{x}{2T}\frac{dT}{d\psi} - \frac{Ze}{2Tx}\frac{d\Phi}{d\psi}\right). \tag{10}$$

Similarly, applying $\nabla_{\mu,W}$ to $\mu = \upsilon_{th}^2 x^2\left(1-\xi^2\right)/\left(2B\right)$, we find

$$\nabla_{\mu,W}\xi = -\frac{Ze}{2Tx^2\xi}\left(1-\xi^2\right)\nabla\Phi - \frac{\left(1-\xi^2\right)}{\xi}\frac{1}{2B}\nabla B . \tag{11}$$

Thus, (8) may be written

$$\dot{\xi} = -\frac{Ze}{2Tx^2\xi}\left(1-\xi^2\right)\frac{d\Phi}{d\psi}\mathbf{v}_m\cdot\nabla\psi - \frac{\left(1-\xi^2\right)}{\xi}\frac{1}{2B}\left(\upsilon_{\|}\mathbf{b} + \mathbf{v}_E + \mathbf{v}_m\right)\cdot\nabla B . \tag{12}$$

Noting

$$\mathbf{v}_m\cdot\nabla\psi = -\frac{Tc}{ZeB^3}x^2\left(1+\xi^2\right)\mathbf{B}\times\nabla\psi\cdot\nabla B \tag{13}$$

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

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

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

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

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

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

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:

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

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

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

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

For comparison with DKES, SFINCS allows the option of using

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

in place of (15).

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

$$-f_1\frac{2c}{B^3}\frac{d\Phi}{d\psi}\mathbf{B}\times\nabla\psi\cdot\nabla B = f_1\nabla\cdot\mathbf{v}_E \tag{22}$$

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:

$$\nabla_{x,\xi}\cdot\left(f_1\dot{\mathbf{r}}\right)+\left(\frac{\partial}{\partial\xi}\right)_{\mathbf{r},x}\left[f_1\dot{\xi}\right]-C\left\{f_1\right\} = -\mathbf{v}_m\cdot\nabla_W f_M + \frac{Ze}{T}\upsilon_{\|}\frac{\langle E_{\|}B\rangle B}{\langle B^2\rangle}f_M . \tag{23}$$

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

$$
\dot{\theta}\frac{\partial f_1}{\partial \theta}+\dot{\zeta}\frac{\partial f_1}{\partial \zeta}+\dot{x}\frac{\partial f_1}{\partial x}+\dot{\xi}\frac{\partial f_1}{\partial \xi}-C\{f_1\}-\alpha_{cons}f_1\frac{2c}{B^3}\frac{d\Phi}{d\psi}\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial\theta}-I\frac{\partial B}{\partial\zeta}\right]
$$

$$
=\frac{Tc}{ZeB^3}x^2\left(1+\xi^2\right)\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial\theta}-I\frac{\partial B}{\partial\zeta}\right]f_M\left[\frac{1}{n}\frac{dn}{d\psi}+\frac{Ze}{T}\frac{d\Phi}{d\psi}+\left(x^2-\frac{3}{2}\right)\frac{1}{T}\frac{dT}{d\psi}\right]+\frac{Ze}{T}\upsilon_\parallel\frac{\left\langle E_\parallel B\right\rangle B}{\left\langle B^2\right\rangle}f_M \tag{29}
$$

where

$$
\dot{\theta}=\left[\frac{\upsilon_{th}x\xi}{B}\iota+\frac{cG}{B^2}\frac{d\Phi}{d\psi}\right]\mathbf{B}\cdot\nabla\zeta\,, \tag{30}
$$

$$
\dot{\zeta}=\left[\frac{\upsilon_{th}x\xi}{B}-\frac{Ic}{B^2}\frac{d\Phi}{d\psi}\right]\mathbf{B}\cdot\nabla\zeta\,, \tag{31}
$$

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

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

Normalizations

Let's suppose we are given T, $dT/d\psi_N$, n, $dn/d\psi_N$, $d\Phi/d\psi_N$, $B(\theta,\zeta)$, 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 dimensions $\bar{T}$ (e.g. eV), $\bar{n}$ (e.g. $10^{20}/\mathrm{m}^3$), $\bar{\Phi}$ (e.g. kV), $\bar{B}$ (e.g. T), and $\bar{R}$ (e.g. m). In other words, the quantities we are actually given are

$$
\hat{T}=T/\bar{T}\,, \tag{34}
$$

$$
\hat{n}=n/\bar{n}\,, \tag{35}
$$

$$
d\hat{T}/d\psi_N=\left(dT/d\psi_N\right)/\bar{T}\,, \tag{36}
$$

$$
d\hat{n}/d\psi_N=\left(dn/d\psi_N\right)/\bar{n}\,, \tag{37}
$$

$$
d\hat{\Phi}/d\psi_N=\left(d\Phi/d\psi_N\right)/\bar{\Phi}\,, \tag{38}
$$

$$
\hat{B}=B/\bar{B}\,, \tag{39}
$$

$$
\hat{G}=G/\left(\bar{R}\bar{B}\right), \tag{40}
$$

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

$$
\hat{\psi}_a=\psi_a/\left(\bar{B}\bar{R}^2\right), \tag{42}
$$

and

$$
\hat{E}=\left\langle E_\parallel B\right\rangle\frac{\bar{R}}{\bar{\Phi}\bar{B}}\,. \tag{43}
$$

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

$$
\frac{dX}{d\psi}=\frac{1}{\hat{\psi}_a\bar{R}^2\bar{B}}\frac{dX}{d\psi_N} \tag{44}
$$

for any flux function X.

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

$$\bar{\upsilon} = \sqrt{2\bar{T} / m}\,, \tag{45}$$

$$\Delta = \frac{mc\bar{\upsilon}}{Ze\bar{B}\bar{R}}\,, \tag{46}$$

$$\omega = \frac{c\bar{\Phi}}{\bar{R}\bar{B}\bar{\upsilon}}\,. \tag{47}$$

and a normalized collisionality

$$\nu_n = \nu_{ii}\bar{R} / \bar{\upsilon} \tag{48}$$

where

$$\nu_{ii} = \frac{4\sqrt{2\pi}ne^4 \ln\Lambda}{3m^{1/2}T^{3/2}}\,. \tag{49}$$

Notice that (45)-(46) use the actual particle mass m, not a reference mass. Notice also that (49) uses the actual n and T, not the reference values $\bar{n}$ and $\bar{T}$. It will be useful to notice

$$\mathbf{B}\cdot\nabla\zeta = \frac{\bar{B}}{\bar{R}}\frac{\hat{B}^2}{\hat{G}+\iota\hat{I}}\,. \tag{50}$$

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

$$f_1 = \frac{\Delta n}{\pi^{3/2}\bar{\upsilon}^3\hat{\psi}_a}\,\hat{f}\,. \tag{51}$$

(Notice that we have normalized by the actual density, not by the reference density.)

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

$$\frac{\bar{B}\pi^{3/2}\bar{\upsilon}^3\hat{\psi}_a}{\bar{\upsilon}\Delta n\mathbf{B}\cdot\nabla\zeta}\,, \tag{52}$$

yielding

$$
\begin{aligned}
&\left[\frac{\hat{T}^{1/2}x\xi}{\hat{B}}\iota+\frac{\omega}{\hat{\psi}_a}\frac{\hat{G}}{\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\right]\frac{\partial\hat{f}}{\partial\theta}\\
&+\left[\frac{\hat{T}^{1/2}x\xi}{\hat{B}}-\frac{\omega}{\hat{\psi}_a}\frac{\hat{I}}{\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\right]\frac{\partial\hat{f}}{\partial\zeta}\\
&+\frac{\omega}{2\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}x\left(1+\xi^2\right)\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\frac{\partial\hat{f}}{\partial x}\\
&+\left\{-x\left(1-\xi^2\right)\frac{\hat{T}^{1/2}}{2\hat{B}^2}\left[\iota\frac{\partial\hat{B}}{\partial\theta}+\frac{\partial\hat{B}}{\partial\zeta}\right]+\xi\left(1-\xi^2\right)\frac{\omega}{2\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\right\}\frac{\partial\hat{f}}{\partial\xi}\\
&-\nu_n\frac{\left(\hat{G}+\iota\hat{I}\right)}{\hat{B}^2}\hat{C}\left\{\hat{f}\right\}-\alpha_{cons}\hat{f}\,\frac{2\omega}{\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\\
&=\frac{1}{2\hat{B}^3\hat{T}^{1/2}}x^2e^{-x^2}\left(1+\xi^2\right)\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta}-\hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\frac{1}{\hat{n}}\frac{d\hat{n}}{d\psi_N}+\frac{2\omega}{\Delta\hat{T}}\frac{d\hat{\Phi}}{d\psi_N}+\left(x^2-\frac{3}{2}\right)\frac{1}{\hat{T}}\frac{d\hat{T}}{d\psi_N}\right]\\
&+\frac{2\omega\hat{\psi}_a\hat{E}}{\Delta^2\hat{T}^2}\frac{\left(\hat{G}+\iota\hat{I}\right)}{\left\langle\hat{B}^2\right\rangle\hat{B}}x\xi e^{-x^2}
\end{aligned}
\tag{53}
$$

where $\hat{C}\left\{\hat{f}\right\}=\nu_{ii}^{-1}C\left\{\hat{f}\right\}$.

Legendre discretization

SFINCS uses a collocation discretization in the x, 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, θ, and ζ, but it is expanded as modes in ξ. We employ the following modal expansion in terms of Legendre polynomials $P_\ell\left(\xi\right)$:

$$\hat{f}=\sum_\ell f_\ell P_\ell\left(\xi\right). \tag{54}$$

We discretize the kinetic equation (53) by applying

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\;P_L\left(\xi\right)\left(\quad\cdot\quad\right). \tag{55}$$

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

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\xi P_L\left(\xi\right)P_\ell\left(\xi\right)=\frac{L+1}{2L+3}\delta_{L+1,\ell}+\frac{L}{2L-1}\delta_{L-1,\ell}, \tag{56}$$

$$
\begin{aligned}
\frac{2L+1}{2}\int_{-1}^{1}d\xi\;\left(1+\xi^2\right)P_L\left(\xi\right)P_\ell\left(\xi\right)=&\frac{2\left[3L^2+3L-2\right]}{\left(2L+3\right)\left(2L-1\right)}\delta_{L,\ell}\\
&+\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell}+\frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell},
\end{aligned}
\tag{57}
$$

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

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

and

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi \ P_L\left(\xi\right)\left(1+\xi^2\right) = \frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}. \tag{60}$$

As a result, (53) may be written

$$\sum_\ell M_{L,\ell}\hat{f}_\ell = R_L \tag{61}$$

where

$$M_{L,\ell} = \dot{\theta}_{L,\ell}\frac{\partial}{\partial\theta} + \dot{\zeta}_{L,\ell}\frac{\partial}{\partial\zeta} + M_{L,\ell}^{(\xi)} + \dot{x}_{L,\ell}\frac{\partial}{\partial x} - \nu_n\frac{\left(\hat{G}+\iota\hat{I}\right)}{\hat{B}^2}\hat{C}_L\delta_{L,\ell} + \alpha_{cons}\delta_{L,\ell}Y\ , \tag{62}$$

$$\dot{\theta}_{L,\ell} = \frac{\hat{T}^{1/2}x}{\hat{B}}\iota\left[\frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}\right] + \frac{\omega}{\hat{\psi}_a}\frac{\hat{G}}{\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\delta_{L,\ell}, \tag{63}$$

$$\dot{\zeta}_{L,\ell} = \frac{\hat{T}^{1/2}x}{\hat{B}}\left[\frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}\right] - \frac{\omega}{\hat{\psi}_a}\frac{\hat{I}}{\hat{B}^2}\frac{d\hat{\Phi}}{d\psi_N}\delta_{L,\ell}, \tag{64}$$

$$\begin{aligned}M_{L,\ell}^{(\xi)} &= -x\frac{\hat{T}^{1/2}}{2\hat{B}^2}\left[\iota\frac{\partial\hat{B}}{\partial\theta} + \frac{\partial\hat{B}}{\partial\zeta}\right]\left[\frac{\left(L+1\right)\left(L+2\right)}{2L+3}\delta_{L+1,\ell} - \frac{\left(L-1\right)L}{2L-1}\delta_{L-1,\ell}\right] \\ &+ \frac{\omega}{2\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\begin{aligned}&\frac{\left(L+1\right)L}{\left(2L-1\right)\left(2L+3\right)}\delta_{L,\ell} \\ &+ \frac{\left(L+3\right)\left(L+2\right)\left(L+1\right)}{\left(2L+5\right)\left(2L+3\right)}\delta_{L+2,\ell} - \frac{L\left(L-1\right)\left(L-2\right)}{\left(2L-3\right)\left(2L-1\right)}\delta_{L-2,\ell}\end{aligned}\right],\end{aligned} \tag{65}$$

$$\dot{x}_{L,\ell} = \frac{\omega}{2\hat{\psi}_a\hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N}x\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\begin{aligned}&\frac{2\left[3L^2+3L-2\right]}{\left(2L+3\right)\left(2L-1\right)}\delta_{L,\ell} \\ &+ \frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell} + \frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell}\end{aligned}\right], \tag{66}$$

$$Y = -\frac{d\hat{\Phi}}{d\psi_N}\frac{2\omega}{\hat{\psi}_a\hat{B}^3}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right], \tag{67}$$

and

$$
\begin{aligned}
R_L = {} & \frac{1}{2\hat{B}^3\hat{T}^{1/2}} x^2 e^{-x^2}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]\left[\frac{1}{\hat{n}}\frac{d\hat{n}}{d\psi_N} + \frac{2\omega}{\Delta\hat{T}}\frac{d\hat{\Phi}}{d\psi_N} + \left(x^2 - \frac{3}{2}\right)\frac{1}{\hat{T}}\frac{d\hat{T}}{d\psi_N}\right]\left[\frac{4}{3}\delta_{L,0} + \frac{2}{3}\delta_{L,2}\right] \\
& + \frac{2\omega\hat{\psi}_a\hat{E}}{\Delta^2\hat{T}^2}\frac{\left(\hat{G} + \iota\hat{I}\right)}{\left\langle \hat{B}^2\right\rangle \hat{B}} x e^{-x^2}\delta_{L,1}.
\end{aligned} \tag{68}
$$

Collision operator

At present, three options are available for the collision operator: pitch-angle scattering without momentum conservation, pitch-angle scattering with a model momentum conserving term, and the full linearized Fokker-Planck operator.

Pitch-angle scattering

This operator is defined by

$$
\hat{C}_{pas}\left\{\hat{f}\right\} = \nu_D \mathcal{L}\left\{\hat{f}\right\} \tag{69}
$$

where

$$
\mathcal{L} = \frac{1}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial}{\partial \xi}, \tag{70}
$$

$$
\nu_D = \frac{3\sqrt{\pi}}{4}\frac{\left[\operatorname{erf}(x) - \Psi(x)\right]}{x^3}, \tag{71}
$$

$$
\Psi(x) = \frac{1}{2x^2}\left[\operatorname{erf}(x) - \frac{2}{\sqrt{\pi}} x e^{-x^2}\right], \tag{72}
$$

and

$$
\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\, dt \tag{73}
$$

is the error function.

Applying the Legendre discretization,

$$
\frac{2L+1}{2}\int_{-1}^{1} d\xi\, P_L(\xi)\hat{C}_{pas}\left\{\hat{f}\right\} = -\frac{\nu_D}{2} L(L+1)\delta_{L,\ell}\hat{f}_\ell. \tag{74}
$$

Model momentum conserving operator

This model operator is defined by

$$
\hat{C}_{\mathrm{mod}}\left\{\hat{f}\right\} = \hat{C}_{pas}\left\{\hat{f}\right\} + \hat{C}_{mf}\left\{\hat{f}\right\} \tag{75}
$$

where $\hat{C}_{mf}$ is a model field term:

$$
\begin{aligned}
\hat{C}_{mf}\left\{\hat{f}\right\} &= \nu_D f_M \upsilon_{\|}\frac{m}{T}\frac{\int d^3\upsilon\ \hat{f}\nu_D\upsilon_{\|}}{\int d^3\upsilon \frac{m\upsilon^2}{3T} f_M \nu_D} \\
&= \nu_D x\xi e^{-x^2}\delta_{\ell,1}\frac{\int_0^\infty dx\ \hat{f}_\ell \nu_D x^3}{\int_0^\infty dx\, e^{-x^2} x^4 \nu_D}.
\end{aligned} \tag{76}
$$

Using the facts that $\mathcal{L}$ is self-adjoint and that $\mathcal{L}\left\{\upsilon_{\|}\right\}=-\upsilon_{\|}$, it can be verified that $\int d^3\upsilon\, \upsilon_{\|}\hat{C}_{\mathrm{mod}}\left\{\hat{f}\right\}=0$ for any $\hat{f}$, i.e. the operator conserves momentum. The integral in the denominator of (76) can be evaluated numerically:

$$\int_0^\infty dx\ x^4 e^{-x^2}\nu_D = 0.354162849836926\,. \tag{77}$$

Applying the Legendre discretization,

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\ P_L\left(\xi\right)\hat{C}_{mf}\left\{\hat{f}\right\}=\frac{\nu_D e^{-x^2}x\delta_{L,1}\delta_{\ell,1}}{0.354162849836926}\int_0^\infty dx\ f_\ell \nu_D x^3\,. \tag{78}$$

Full linearized Fokker-Planck operator

The full linearized Fokker-Planck operator (normalized by ν_{ii}) is

$$\hat{C}_{FP}\left\{\hat{f}\right\}=\hat{C}_{pas}\left\{\hat{f}\right\}+\hat{C}_{E}\left\{\hat{f}\right\}+\hat{C}_{D}\left\{\hat{f}\right\}+\hat{C}_{H}\left\{\hat{f}\right\}+\hat{C}_{G}\left\{\hat{f}\right\} \tag{79}$$

where

$$\hat{C}_E\left\{\hat{f}\right\}=\frac{3\sqrt{\pi}}{4}\frac{1}{x^2}\frac{\partial}{\partial x}\left\{e^{-x^2}\Psi\left(x\right)x\frac{\partial}{\partial x}\left(\frac{\hat{f}}{e^{-x^2}}\right)\right\} \tag{80}$$

is the energy scattering operator,

$$\hat{C}_D\left\{\hat{f}\right\}=3e^{-x^2}\hat{f}\,, \tag{81}$$

$$\hat{C}_H\left\{\hat{f}\right\}=-\frac{3}{2\pi}e^{-x^2}\hat{H}\,, \tag{82}$$

and

$$\hat{C}_G\left\{\hat{f}\right\}=\frac{3}{2\pi}e^{-x^2}x^2\frac{\partial^2\hat{G}}{\partial x^2}\,. \tag{83}$$

Here, $\hat{H}$ and $\hat{G}$ are normalized perturbed Rosenbluth potentials, related to the dimensional perturbed Rosenbluth potentials H and G by

$$H=\frac{\Delta n}{\pi^{3/2}\bar{\upsilon}^3\hat{\psi}_a}\upsilon_{th}^2\hat{H} \tag{84}$$

and

$$G=\frac{\Delta n}{\pi^{3/2}\bar{\upsilon}^3\hat{\psi}_a}\upsilon_{th}^4\hat{G}\,. \tag{85}$$

The Rosenbluth potentials are defined in terms of the distribution function by the following pair of Poisson equations:

$$\left[\frac{\partial}{\partial x}x^2\frac{\partial}{\partial x}+\mathcal{L}\right]\hat{H}=-4\pi x^2\hat{g} \tag{86}$$

and

$$\left[\frac{\partial}{\partial x}x^2\frac{\partial}{\partial x}+\mathcal{L}\right]\hat{G}=2x^2\hat{H}\,. \tag{87}$$

A clear derivation of the operator (79)-(87) may be found in Ref. [2], and it is identical to the linearized operator of Ref. [3].

To apply the Legendre discretization, $\hat{H}$ and $\hat{G}$ are expanded in the same way as $\hat{f}$:

$$\hat{H} = \sum_{\ell} \hat{H}_{\ell} P_{\ell}\left(\xi\right), \tag{88}$$

$$\hat{G} = \sum_{\ell} \hat{G}_{\ell} P_{\ell}\left(\xi\right), \tag{89}$$

and the operation (55) is applied to (86)-(87). As (80)-(83) contain no ξ dependence except through the unknowns, we may simply replace $\hat{f} \to f_{\ell}$, $\hat{H} \to \hat{H}_{\ell}$, and $\hat{G} \to \hat{G}_{\ell}$ in these equations. Finally, (86)-(87) become

$$\left[\frac{\partial}{\partial x} x^2 \frac{\partial}{\partial x} - \ell\left(\ell+1\right)\right] \hat{H}_{\ell} = -4\pi x^2 \hat{g}_{\ell} \tag{90}$$

and

$$\left[\frac{\partial}{\partial x} x^2 \frac{\partial}{\partial x} - \ell\left(\ell+1\right)\right] \hat{G}_{\ell} = 2x^2 \hat{H}_{\ell}. \tag{91}$$

The terms (82)-(83) and equations (90)-(91) are implemented in SFINCS using the method detailed in Ref. [4].

Output quantities

Flux surface average:

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

$$\left\langle X \right\rangle = \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{X}{\hat{B}^2} \tag{92}$$

where

$$\texttt{VPrimeHat} = \hat{V}' = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^2}. \tag{93}$$

Notice

$$\texttt{FSABHat2} = \left\langle \hat{B}^2 \right\rangle = \frac{4\pi^2}{\hat{V}'}. \tag{94}$$

Density perturbation

SFINCS returns the density in $\hat{f}$ normalized by the density in f_M :

$$\texttt{densityPerturbation} = \frac{1}{n}\int d^3 \upsilon\, f_1 = \frac{2\Delta \hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a} \int_{-1}^{1} d\xi \int_0^{\infty} dx x^2 \hat{f} = \frac{4\Delta \hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a} \int_0^{\infty} dx x^2 f_{L=0}. \tag{95}$$

Upon flux surface averaging, we obtain

$$\begin{aligned} \texttt{FSADensityPerturbation} &= \left\langle \frac{1}{n}\int d^3 \upsilon\, f_1 \right\rangle = \frac{1}{\hat{V}'} \frac{4\Delta \hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^2} \int_0^{\infty} dx x^2 f_{L=0} \\ &= \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{\texttt{densityPerturbation}}{\hat{B}^2}. \end{aligned} \tag{96}$$

Pressure perturbation

SFINCS also returns the pressure in $\hat{f}$ normalized by the pressure in f_M:

$$\begin{aligned}\texttt{pressurePerturbation} &= \frac{m}{3p}\int d^3\upsilon\,\upsilon^2 f_1 = \frac{4}{3}\frac{\Delta\hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a}\int_{-1}^{1} d\xi \int_0^\infty dx\; x^4 \hat{f} \\ &= \frac{8}{3}\frac{\Delta\hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a}\int_0^\infty dx\; x^4 f_{L=0}.\end{aligned} \tag{97}$$

Upon flux surface averaging, we obtain

$$\begin{aligned}\texttt{FSAPressurePerturbation} &= \left\langle \frac{m}{3p}\int d^3\upsilon\,\upsilon^2 f_1 \right\rangle \\ &= \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\, \frac{1}{\hat{B}^2}\frac{8}{3}\frac{\Delta\hat{T}^{3/2}}{\pi^{1/2}\hat{\psi}_a}\int_0^\infty dx\; x^4 f_{L=0} \\ &= \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\, \frac{\texttt{pressurePerturbation}}{\hat{B}^2}.\end{aligned} \tag{98}$$

Flow

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

$$\texttt{flow} = \frac{\hat{\psi}_a}{\Delta n\bar{\upsilon}}\int d^3\upsilon\,\upsilon_\parallel f = \frac{2\hat{T}^2}{\pi^{1/2}}\int_{-1}^{1} d\xi \int_0^\infty dx\; x^3 \xi \hat{f} = \frac{4\hat{T}^2}{3\pi^{1/2}}\int_0^\infty dx\; x^3 f_{L=1}. \tag{99}$$

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

$$\begin{aligned}\texttt{FSAFlow} &= \frac{\hat{\psi}_a}{\Delta n\bar{\upsilon}\bar{B}}\left\langle B\int d^3\upsilon\,\upsilon_\parallel f\right\rangle = \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\, \frac{1}{\hat{B}}\frac{4\hat{T}^2}{3\pi^{1/2}}\int_0^\infty dx\; x^3 f_{L=1} \\ &= \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\, \frac{\texttt{flow}}{\hat{B}}.\end{aligned} \tag{100}$$

Particle flux

We may write the radial particle flux as

$$\begin{aligned} V'\left\langle \int d^3\upsilon\, f\mathbf{v}_d\cdot\nabla\psi\right\rangle &= -\frac{\Delta n\bar{\upsilon}^2 cm\bar{R}\hat{T}^{5/2}}{Ze\bar{B}\hat{\psi}_a\pi^{1/2}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^\infty dx\,\hat{f}x^4\left(1+\xi^2\right)\frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right] \\ &= \frac{\Delta^2 n\bar{\upsilon}\bar{R}^2}{\hat{\psi}_a}[\texttt{particleFlux}]\end{aligned} \tag{101}$$

where

$$\texttt{particleFlux} = -\frac{\hat{T}^{5/2}}{\pi^{1/2}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^\infty dx\; \hat{f}x^4\left(1+\xi^2\right)\frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial\hat{B}}{\partial\theta} - \hat{I}\frac{\partial\hat{B}}{\partial\zeta}\right]. \tag{102}$$

Using

$$\int_{-1}^{1} d\xi\; P_L(\xi)\left(1+\xi^2\right) = \frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{103}$$

then

$$\texttt{particleFlux} = -\frac{\hat{T}^{5/2}}{\pi^{1/2}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_0^{\infty} dx \left[\frac{8}{3} f_{L=0} + \frac{4}{15} f_{L=2}\right] x^4 \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{104}$$

Momentum flux

We may write a radial momentum flux as

$$\begin{aligned} V'\left\langle \int d^3\upsilon\, f \upsilon_\parallel \mathbf{v}_d \cdot \nabla \psi \right\rangle &= -\frac{\Delta n \bar{\upsilon}^3 c m \bar{R}}{\bar{B}} \frac{\hat{T}^3}{\pi^{1/2}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^{\infty} dx\ \hat{f} x^5 \xi \left(1+\xi^2\right) \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right] \\ &= \frac{\Delta^2 n \bar{\upsilon}^2 \bar{R}^2}{\hat{\psi}_a} (\texttt{momentumFlux}) \end{aligned} \tag{105}$$

where

$$\texttt{momentumFlux} = -\frac{\hat{T}^3}{\pi^{1/2}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^{\infty} dx\ \hat{f} x^5 \xi \left(1+\xi^2\right) \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{106}$$

Using

$$\int_{-1}^{1} d\xi\ P_L(\xi)\, \xi \left(1+\xi^2\right) = \frac{16}{15}\delta_{L,1} + \frac{4}{35}\delta_{L,3} \tag{107}$$

then

$$\texttt{momentumFlux} = -\frac{\hat{T}^3}{\pi^{1/2}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_0^{\infty} dx \left[\frac{16}{15} f_{L=1} + \frac{4}{35} f_{L=3}\right] x^5 \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{108}$$

Heat flux

We may write the radial energy flux as

$$\begin{aligned} V'\left\langle \int d^3\upsilon\, f \frac{m\upsilon^2}{2} \mathbf{v}_d \cdot \nabla \psi \right\rangle &= -\frac{\Delta n \bar{\upsilon}^4 c m^2 \bar{R}}{Ze\bar{B}\hat{\psi}_a} \frac{\hat{T}^{7/2}}{2\pi^{1/2}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^{\infty} dx\ \hat{f} x^5 \left(1+\xi^2\right) \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right] \\ &= \frac{\Delta^2 n \bar{\upsilon}^3 m \bar{R}^2}{\hat{\psi}_a} (\texttt{heatFlux}) \end{aligned} \tag{109}$$

where

$$\texttt{heatFlux} = -\frac{\hat{T}^{7/2}}{2\pi^{1/2}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_{-1}^{1} d\xi \int_0^{\infty} dx\ \hat{f} x^6 \left(1+\xi^2\right) \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{110}$$

Using (103), then

$$\texttt{heatFlux} = -\frac{\hat{T}^{7/2}}{2\pi^{1/2}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \int_0^{\infty} dx \left[\frac{8}{3} f_{L=0} + \frac{4}{15} f_{L=2}\right] x^6 \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{111}$$

Test of quasisymmetry isomorphism

One useful test of any stellarator neoclassical code is to verify that it behaves correctly in the case of perfect quasisymmetry, meaning $B(\theta,\zeta) = B(M\theta - N\zeta)$. In this limit the ion particle flux should be zero (in the limit that ion-electron collisions are neglected in the ion kinetic equation.) Numerically, the flux will not be exactly zero, but it should be orders of magnitude smaller than the heat flux (in code units).

A second test may be formulated as follows. Suppose the helicity integers M and N are varied, at fixed effective collisionality

$$\nu_{*eff} = \frac{\nu_{ii}}{\upsilon_i \left\langle \left| \mathbf{b} \cdot \nabla \ln B \right| \right\rangle}, \tag{112}$$

(any average will do in the denominator) and holding fixed I, G, ι, $dn/d\psi$, $dT/d\psi$, and other input quantities. In this "helicity scan", the flow and heat flux should vary in the following way:

$$\left\langle V_{\|} B \right\rangle \frac{M - N/\iota}{NI + MG} = C_V \tag{113}$$

and

$$\left\langle \mathbf{q} \cdot \nabla \psi \right\rangle \frac{\left| N/\iota - M \right|}{\left(NI + MG \right)^2} = C_q \tag{114}$$

where C_V and C_q are independent of M and N. A derivation showing that the flow and heat flux scale as (113)-(114) is given in Ref. [5]. To hold (112) fixed while varying M and N, we set the normalized collision frequency to

$$\nu_n = \nu_{*s} \left| N/\iota - M \right| \tag{115}$$

where ν_{*s} is held fixed.

It was verified that SFINCS passed these tests. The Matlab version has a switch `testQuasisymmetryIsomorphism`, which if set, outputs the quantities on the left-hand side of (113)-(114) so you can verify they do not change when `helicity_l` and `helicity_n` are varied. (You must set `epsilon_t=0` for this test).

Transport matrix

For some applications, it may be useful to separate out the contributions to each flux and flow from the individual drive terms. To this end, we now develop the concept of a transport matrix. Our definitions will differ from those in e.g. Ref. [6] in order to make the matrix dimensionless and symmetric, to avoid introducing the unnecessary dimensional quantities r and R_0, and to clarify which quantities do and do not affect the matrix elements.

Thermodynamic forces

We begin by using the linearity of the kinetic equation (1) in f_1 to formally write its solution as

$$f_1 = \frac{n}{\pi^{3/2} \upsilon_{th}^3} \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) \tag{116}$$

where the A_j and $\hat{f}_j$ are all dimensionless, the $\hat{f}_j$ are unknown parts of the distribution function proportional to the individual drives A_j, and the A_j represent the three different inhomogeneous terms on the right-hand side of (53), distinguished by their velocity dependence:

$$A_1 \propto \frac{1}{n}\frac{dn}{d\psi} + \frac{Ze}{T}\frac{d\Phi}{d\psi} - \frac{3}{2}\frac{1}{T}\frac{dT}{d\psi}, \tag{117}$$

$$A_2 \propto \frac{1}{T}\frac{dT}{d\psi}, \tag{118}$$

$$A_3 \propto \left\langle E_\| B \right\rangle. \tag{119}$$

As dimensionless factors may always be absorbed into the A_j or $\hat{f}_j$, there is not a unique way to define the A_j and $\hat{f}_j$ quantities to satisfy our requirements. However, examination of (1) with

$$\mathbf{v}_m \cdot \nabla\psi = -\frac{Tc}{ZeB^3} x^2\left(1+\xi^2\right)\mathbf{B}\cdot\nabla\zeta\left[G\frac{\partial B}{\partial\theta} - I\frac{\partial B}{\partial\zeta}\right] \tag{120}$$

and (26) shows that one reasonable choice is the following:

$$A_1 = \frac{GTc}{ZeB_0\upsilon_{th}}\left[\frac{1}{n}\frac{dn}{d\psi} + \frac{Ze}{T}\frac{d\Phi}{d\psi} - \frac{3}{2}\frac{1}{T}\frac{dT}{d\psi}\right] \tag{121}$$

$$A_2 = \frac{GTc}{ZeB_0\upsilon_{th}}\frac{1}{T}\frac{dT}{d\psi} \tag{122}$$

$$A_3 = \frac{Ze}{T}\left(G+\iota I\right)\frac{\left\langle E_\| B\right\rangle}{\left\langle B^2\right\rangle} \tag{123}$$

where B_0 is the $(0,\ 0)$ harmonic of the Boozer spectrum. You can verify that all the A_j are indeed dimensionless. Applying (116), (121)-(123), and (120) in (1), we find the equations satisfied by the $\hat{f}_j$ are

$$x\xi\frac{\partial\hat{f}_1}{\partial\zeta} - \frac{B_0}{B}\nu'\hat{C}\left\{\hat{f}_1\right\} = \frac{B_0}{B^2}e^{-x^2}x^2\left(1+\xi^2\right)\left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta}\right], \tag{124}$$

$$x\xi\frac{\partial\hat{f}_2}{\partial\zeta} - \frac{B_0}{B}\nu'\hat{C}\left\{\hat{f}_2\right\} = \frac{B_0}{B^2}e^{-x^2}x^4\left(1+\xi^2\right)\left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta}\right], \tag{125}$$

and

$$x\xi\frac{\partial\hat{f}_3}{\partial\zeta} - \frac{B_0}{B}\nu'\hat{C}\left\{\hat{f}_3\right\} = x\xi e^{-x^2}. \tag{126}$$

with a new dimensionless collisionality

$$\nu' = \frac{\nu_{ii}\left(G+\iota I\right)}{\upsilon_{th}B_0} = \frac{1}{\hat{T}^{1/2}}\frac{\bar{B}}{B_0}\left(\hat{G}+\iota\hat{I}\right)\nu_n \tag{127}$$

and $\hat{C} = \nu_{ii}^{-1}C$ as before. (Equations (124)-(125) differ in the power of x on the right-hand side.) The $\partial/\partial\zeta$ derivatives in (124)-(126) are performed at fixed μ and field line, and the electric field terms have been omitted for simplicity. Notice $\hat{C}$ is independent of all parameters (density, temperature, etc.) It is then evident from (124)-(126) that the $\hat{f}_j$ depend on the input parameters only through the combinations B/B_0, ι, I/G, and ν'. There is no additional dependence on the density, temperature, G, B, or I individually.

Fluxes

The three output quantities of greatest interest are the particle flux

$$\left\langle \int d^3\upsilon f \mathbf{v}_d \cdot \nabla\psi \right\rangle = -\frac{ncTG}{\pi^{3/2} Ze(G+\iota I)} \left\langle \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x^2 \left(1+\xi^2\right) \frac{1}{B} \left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta} \right] \right\rangle, \tag{128}$$

the heat flux

$$\left\langle \int d^3\upsilon f x^2 \mathbf{v}_d \cdot \nabla\psi \right\rangle = -\frac{ncTG}{\pi^{3/2} Ze(G+\iota I)} \left\langle \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x^4 \left(1+\xi^2\right) \frac{1}{B} \left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta} \right] \right\rangle, \tag{129}$$

and the flux-surface-averaged parallel flow

$$\left\langle B \int d^3\upsilon \upsilon_\parallel f \right\rangle = \frac{\upsilon_{th} n B_0}{\pi^{3/2}} \left\langle \frac{B}{B_0} \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x\xi \right\rangle. \tag{130}$$

The right-hand sides of (128)-(130) resemble the right-hand sides of (124)-(126). This correspondence suggests that we define three fluxes as follows:

$$\begin{aligned} I_1 &= \frac{Ze(G+\iota I)}{ncTG} \left\langle \int d^3\upsilon f \mathbf{v}_d \cdot \nabla\psi \right\rangle \\ &= -\frac{1}{\pi^{3/2}} \left\langle \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x^2 \left(1+\xi^2\right) \frac{1}{B} \left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta} \right] \right\rangle, \end{aligned} \tag{131}$$

$$\begin{aligned} I_2 &= \frac{Ze(G+\iota I)}{ncTG} \left\langle \int d^3\upsilon f x^2 \mathbf{v}_d \cdot \nabla\psi \right\rangle \\ &= -\frac{1}{\pi^{3/2}} \left\langle \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x^4 \left(1+\xi^2\right) \frac{1}{B} \left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta} \right] \right\rangle, \end{aligned} \tag{132}$$

and

$$I_3 = \frac{1}{\upsilon_{th} n B_0} \left\langle B \int d^3\upsilon \upsilon_\parallel f \right\rangle = \frac{1}{\pi^{3/2}} \left\langle \frac{B}{B_0} \int d^3x \left(A_1 \hat{f}_1 + A_2 \hat{f}_2 + A_3 \hat{f}_3 \right) x\xi \right\rangle. \tag{133}$$

These definitions are chosen so right-hand sides of (131)-(133) have the same ratio as (124)-(126), except for the sign of I_3. It turns out this sign change is necessary in order for the matrix to be symmetric. The definitions of the I_3 are not unique in that only the choices (131)-(133) will turn out to yield a symmetric transport matrix (given our choices of A_j), as we will show below.

If we now define a transport matrix $L_{i,j}$ by the relation

$$I_i = \sum_j L_{i,j} A_j\ , \tag{134}$$

the $L_{i,j}$ matrix elements will be dimensionless, unlike those in Ref. [6]. Notice the $L_{i,j}$ elements are integrals of the $\hat{f}_j$, with the integrands depending on the input parameters only through B/B_0 and I/G. Therefore, exactly like the $\hat{f}_j$, the A_j depend on the input parameters only through the combinations B/B_0, ι, I/G, and ν'. There is no additional dependence on the density, temperature, G, B, or I individually.

In summary, the transport matrix equation is

$$\begin{pmatrix} \frac{Ze(G+\iota I)}{ncTG}\left\langle \int d^3\upsilon f \mathbf{v}_d \cdot \nabla\psi \right\rangle \\ \frac{Ze(G+\iota I)}{ncTG}\left\langle \int d^3\upsilon f \frac{m\upsilon^2}{2T}\mathbf{v}_d \cdot \nabla\psi \right\rangle \\ \frac{1}{\upsilon_{th}B_0}\left\langle BV_\parallel \right\rangle \end{pmatrix} = \begin{pmatrix} L_{1,1} & L_{1,2} & L_{1,3} \\ L_{2,1} & L_{2,2} & L_{2,3} \\ L_{3,1} & L_{3,2} & L_{3,3} \end{pmatrix} \begin{pmatrix} \frac{GTc}{ZeB_0\upsilon_{th}}\left[\frac{1}{n}\frac{dn}{d\psi} + \frac{Ze}{T}\frac{d\Phi}{d\psi} - \frac{3}{2}\frac{1}{T}\frac{dT}{d\psi}\right] \\ \frac{GTc}{ZeB_0\upsilon_{th}}\frac{1}{T}\frac{dT}{d\psi} \\ \frac{Ze}{T}(G+\iota I)\frac{\left\langle E_\parallel B\right\rangle}{\left\langle B^2 \right\rangle} \end{pmatrix}. \quad (135)$$

Matrix elements in SFINCS units

The matrix elements of $L_{i,j}$ are computed in SFINCS by solving the kinetic equation for three separate right-hand sides: each one with only one of the A_j nonzero. The first solve uses $d\hat{n}/d\psi_N = 1$, $d\hat{T}/d\psi_N = 0$, $\hat{E} = 0$, and $d\hat{\Phi}/d\psi_N = 0$ on the right-hand side, though $d\hat{\Phi}/d\psi_N$ is allowed to be nonzero on the left-hand side terms. The second solve uses $d\hat{n}/d\psi_N = (3/2)\hat{n}/\hat{T}$, $d\hat{T}/d\psi_N = 1$, and $d\hat{\Phi}/d\psi_N = 0$ to make $A_1 = 0$ but A_2 nonzero. Again, $d\hat{\Phi}/d\psi_N$ is allowed to be nonzero on the left-hand side terms, and $\hat{E} = 0$. For the third solve, $d\hat{n}/d\psi_N = 0$, $d\hat{T}/d\psi_N = 0$ and $d\hat{\Phi}/d\psi_N = 0$ on the right-hand side, $d\hat{\Phi}/d\psi_N$ is nonzero on the left-hand side, and this time $\hat{E} = 1$. Straightforward but tedious manipulation of (34)-(47), (100), (101), and (109) then gives expressions for the matrix elements:

$$L_{1,1} = \frac{I_1}{A_1} = (\texttt{particleFlux})\frac{\bar{R}}{V\bar{B}}\frac{4(\hat{G}+\iota\hat{I})}{\hat{G}}\frac{\hat{n}}{\hat{G}\hat{T}^{3/2}}\frac{B_0}{\bar{B}}\left(\frac{d\hat{n}}{d\psi_N}\right)^{-1} \quad (136)$$

$$L_{1,2} = \frac{I_1}{A_2} = (\texttt{particleFlux})\frac{\bar{R}}{V\bar{B}}\frac{4(\hat{G}+\iota\hat{I})}{\hat{G}}\frac{1}{\hat{T}^{1/2}\hat{G}}\frac{B_0}{\bar{B}}\left(\frac{d\hat{T}}{d\psi_N}\right)^{-1} \quad (137)$$

$$L_{1,3} = \frac{I_1}{A_3} = (\texttt{particleFlux})\frac{\bar{R}}{V\bar{B}}\frac{\Delta^2}{\hat{\psi}_a\hat{G}\omega}\left\langle \hat{B}^2\right\rangle \hat{E}^{-1} \quad (138)$$

$$L_{2,1} = \frac{I_2}{A_1} = (\texttt{heatFlux})\frac{\bar{R}}{V\bar{B}}\frac{8(\hat{G}+\iota\hat{I})}{\hat{G}}\frac{\hat{n}}{\hat{G}\hat{T}^{5/2}}\frac{B_0}{\bar{B}}\left(\frac{d\hat{n}}{d\psi_N}\right)^{-1} \quad (139)$$

$$L_{2,2} = \frac{I_2}{A_2} = (\texttt{heatFlux})\frac{\bar{R}}{V\bar{B}}\frac{8(\hat{G}+\iota\hat{I})}{\hat{G}}\frac{1}{\hat{T}^{3/2}\hat{G}}\frac{B_0}{\bar{B}}\left(\frac{d\hat{T}}{d\psi_N}\right)^{-1} \quad (140)$$

$$L_{2,3} = \frac{I_2}{A_3} = (\texttt{heatFlux})\frac{\bar{R}}{V\bar{B}}\frac{2\Delta^2}{\hat{G}\hat{\psi}_a\hat{T}\omega}\left\langle \hat{B}^2\right\rangle \hat{E}^{-1} \quad (141)$$

$$L_{3,1} = \frac{I_3}{A_1} = (\texttt{FSAFlow})\frac{2\hat{n}}{\hat{G}\hat{T}}\left(\frac{d\hat{n}}{d\psi_N}\right)^{-1} \tag{142}$$

$$L_{3,2} = \frac{I_3}{A_2} = (\texttt{FSAFlow})\frac{2}{\hat{G}}\left(\frac{d\hat{T}}{d\psi_N}\right)^{-1} \tag{143}$$

$$L_{3,3} = \frac{I_3}{A_3} = (\texttt{FSAFlow})\frac{1}{\left(\hat{G}+\iota\hat{I}\right)}\frac{\Delta^2\hat{T}^{1/2}}{2\hat{\psi}_a\omega}\frac{\bar{B}}{B_0}\left\langle\hat{B}^2\right\rangle\hat{E}^{-1} \tag{144}$$

Each of these expressions is to be evaluated using the particleFlux, heatFlux, or FSAFlow from the appropriate right-hand side, the right-most quantity in each case is the value 1 used in the associated right-hand side.

Sign of diagonal elements

Several properties of the $L_{i,j}$ matrix can be proved. We begin with $L_{1,1}$, substituting (124) into the right-hand side of (131), giving

$$\begin{aligned} L_{11} = \frac{I_1}{A_1} &= -\frac{1}{\pi^{3/2}}\frac{(G+\iota I)}{\upsilon_{th}B_0}\left\langle\int d^3x\frac{1}{e^{-x^2}}\left[\hat{f}_1\upsilon_\parallel\nabla_\parallel\hat{f}_1 - \hat{f}_1 C\left\{\hat{f}_1\right\}\right]\right\rangle \\ &= \frac{1}{\pi^{3/2}}\frac{(G+\iota I)}{\upsilon_{th}B_0}\underbrace{\left\langle\int d^3x\frac{1}{e^{-x^2}}\hat{f}_1 C\left\{\hat{f}_1\right\}\right\rangle}_{Y}. \end{aligned} \tag{145}$$

To obtain the last line, we have noted that $\left\langle\int d^3\upsilon\upsilon_\parallel\nabla_\parallel U\right\rangle = 0$ for any U. The quantity Y represents (negative) entropy generation, and it can be proved that $Y \le 0$ for the linearized Fokker-Planck operator. Therefore,

$$\operatorname{sgn}\left(L_{1,1}\right) = -\operatorname{sgn}\left(\frac{G+\iota I}{B_0}\right). \tag{146}$$

The analysis and result for $L_{2,2}$ is similar:

$$\operatorname{sgn}\left(L_{2,2}\right) = -\operatorname{sgn}\left(\frac{G+\iota I}{B_0}\right). \tag{147}$$

To determine the sign of $L_{3,3}$, we substitute (126) into the right-hand side of (133), giving

$$\begin{aligned} L_{3,3} = \frac{I_3}{A_3} &= \frac{1}{\pi^{3/2}}\frac{G+\iota I}{\upsilon_{th}B_0}\left\langle\int d^3x\frac{1}{e^{-x^2}}\left[\hat{f}_3\upsilon_\parallel\nabla_\parallel\hat{f}_3 - \hat{f}_3 C\left\{\hat{f}_3\right\}\right]\right\rangle \\ &= -\frac{1}{\pi^{3/2}}\frac{G+\iota I}{\upsilon_{th}B_0}\underbrace{\left\langle\int d^3x\frac{1}{e^{-x^2}}\hat{f}_3 C\left\{\hat{f}_3\right\}\right\rangle}_{\le 0} \end{aligned} \tag{148}$$

so

$$\operatorname{sgn}\left(L_{3,3}\right) = \operatorname{sgn}\left(\frac{G+\iota I}{B_0}\right). \tag{149}$$

It should be noted that while $Y \leq 0$ for the linearized Fokker-Planck operator, Y could possibly be positive for model collision operators.

Onsager symmetry

We can also prove that the matrix $L_{i,j}$ is symmetric, which is the ultimate reason for defining the fluxes I_j as we have done. To complete the proof, we must separate each $\hat{f}_j$ into the parts that are symmetric and antisymmetric with respect to $\upsilon_\|$: $\hat{f}_1 = \hat{f}_{1+} + \hat{f}_{1-}$ where

$$\hat{f}_{1+} = \frac{1}{2}\left[\hat{f}_1\left(\upsilon_\|\right) + \hat{f}_1\left(-\upsilon_\|\right)\right] \tag{150}$$

$$\hat{f}_{1-} = \frac{1}{2}\left[\hat{f}_1\left(\upsilon_\|\right) - \hat{f}_1\left(-\upsilon_\|\right)\right] \tag{151}$$

with analogous definitions for $\hat{f}_2$ and $\hat{f}_3$. The kinetic equations (124)-(126) may then be separated into symmetric and antisymmetric parts:

$$\upsilon_\|\nabla_\|\hat{f}_{1-} - C\left\{\hat{f}_{1+}\right\} = \upsilon_{th}\frac{1}{G+\iota I}\frac{B_0}{B}e^{-x^2}x^2\left(1+\xi^2\right)\left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta}\right] \tag{152}$$

$$\upsilon_\|\nabla_\|\hat{f}_{1+} - C\left\{\hat{f}_{1-}\right\} = 0 \tag{153}$$

$$\upsilon_\|\nabla_\|\hat{f}_{2-} - C\left\{\hat{f}_{2+}\right\} = \upsilon_{th}\frac{1}{G+\iota I}\frac{B_0}{B}e^{-x^2}x^4\left(1+\xi^2\right)\left[\frac{\partial B}{\partial\theta} - \frac{I}{G}\frac{\partial B}{\partial\zeta}\right] \tag{154}$$

$$\upsilon_\|\nabla_\|\hat{f}_{2+} - C\left\{\hat{f}_{2-}\right\} = 0 \tag{155}$$

$$\upsilon_\|\nabla_\|\hat{f}_{3+} - C\left\{\hat{f}_{3-}\right\} = \frac{\upsilon_{th}}{B}\frac{B^2}{G+\iota I}x\xi e^{-x^2} \tag{156}$$

$$\upsilon_\|\nabla_\|\hat{f}_{3-} - C\left\{\hat{f}_{3+}\right\} = 0 \tag{157}$$

To prove $L_{i,j} = L_{j,i}$, we then substitute (152), (154), or (156) into the right-hand side of (131)-(133) as appropriate. The results are then manipulated using the integration-by-parts rule

$$\left\langle\int d^3\upsilon\, y_1\upsilon_\|\nabla_\| y_2\right\rangle = -\left\langle\int d^3\upsilon\, y_2\upsilon_\|\nabla_\| y_1\right\rangle, \tag{158}$$

and the self-adjointness property of C:

$$\int d^3\upsilon\frac{y_1}{e^{-x^2}}C\left\{y_2\right\} = \int d^3\upsilon\frac{y_2}{e^{-x^2}}C\left\{y_1\right\}, \tag{159}$$

(both true for any physical y_1 and y_2) as well as (153), (155), and (157).

Tokamak limits

For benchmarking purposes, it is useful to note the values of the transport matrix elements in the case of axisymmetry $\left(B/B_0 = 1+\varepsilon\cos\theta\right)$ in the limit $\nu' \gg 1$ (since high collisionality requires lower resolution than low collisionality.) In axisymmetry, certain matrix elements can be fact be determined exactly for any value of ν'; these elements are denoted with (*) below. These results are derived in separate notes.

Pure pitch-angle scattering:

$$L = \begin{pmatrix} -2.13135\varepsilon^2\nu'/\iota^2 & -2.828427\varepsilon^2\nu'/\iota^2 & 0 \\ -2.828427\varepsilon^2\nu'/\iota^2 & -6.363961\varepsilon^2\nu'/\iota^2 & 0 \\ 0 & 0 & 2.0244/\nu' \end{pmatrix} \qquad (160)$$

Momentum-conserving model:

$$L = \begin{pmatrix} 0\ (*) & 0\ (*) & -1/\iota\ (*) \\ 0\ (*) & -2.6104889\varepsilon^2\nu'/\iota^2 & ? \\ -1/\iota\ (*) & ? & ? \end{pmatrix} \qquad (161)$$

Full linearized Fokker-Planck operator:

$$L = \begin{pmatrix} 0\ (*) & 0\ (*) & -1/\iota\ (*) \\ 0\ (*) & -4.5\varepsilon^2\nu'/\iota^2 & -4.57/\iota \\ -1/\iota\ (*) & -4.57/\iota & ? \end{pmatrix} \qquad (162)$$

References

[1] Landreman and Catto, “Conservation of energy and magnetic moment in neoclassical calculations for optimized stellarators”, submitted to Plasma Phys Controlled Fusion (2013).

[2] Li and Ernst, Phys. Rev. Lett. 106, 195002 (2011).

[3] Rosenbluth, McDonald, and Judd, Phys. Rev. 107, 1 (1957).

[4] Landreman and Ernst, J. Comp. Phys., http://dx.doi.org/10.1016/j.jcp.2013.02.041 (2013).

[5] Landreman and Catto, Plasma Phys Controlled Fusion 53, 015004 (2011).

[6] Beidler et al, Nuclear Fusion 51, 076001 (2011).