December 30, 2014 Matt Landreman

Technical Documentation for version 3 of SFINCS

Introduction

In this document, we detail the equations implemented in version 3 of SFINCS: the Stellarator Fokker-Planck Iterative Neoclassical Conservative Solver. The normalizations and input and output quantities are also defined. We use SI units unless noted otherwise.

Differences between version 3 and previous versions of SFINCS include the following:

Single- and multi-species versions	Version 3
Adiabatic $\tilde{\Phi}$ assumed.	Full nonlinear effect of $\tilde{\Phi}$ can be included
Radial $\mathbf{E}\times\mathbf{B}$ drift is neglected.	Radial $\mathbf{E}\times\mathbf{B}$ drift can be included.
Magnetic drifts only appear in the inhomogeneous drive term.	Magnetic drifts acting on the perturbed f_s can also be included.
Boozer coordinates assumed.	Any flux coordinates can be used.

Kinetic equation

We begin with the drift-kinetic equation (19) of Hazeltine, Plasma Physics 15, 77 (1973):

$$\begin{aligned}
&\frac{\partial f_s}{\partial t}+\left(\upsilon_\| \mathbf{b}+\hat{\mathbf{u}}_s+\mathbf{v}_{Ds}\right)\cdot\left(\nabla f_s\right)_{\mu,W_s} \\
&+\left\{\frac{\upsilon_\|}{\Omega_s}\nabla\cdot\left(\frac{\partial\mathbf{b}}{\partial t}\times\mathbf{b}\right)-\frac{\mathbf{b}}{B}\cdot\frac{\partial\mathbf{A}}{\partial t}\mathbf{b}\cdot\nabla\times\mathbf{b}+\frac{\upsilon_\| B}{\Omega_s}\mathbf{b}\cdot\nabla\left(\frac{\upsilon_\|\mathbf{b}\cdot\nabla\times\mathbf{b}}{B}\right)\right\}\mu\frac{\partial f_s}{\partial\mu} \\
&-\left[\upsilon_\|\frac{\partial\upsilon_\|}{\partial t}+\frac{Z_s e}{m_s}\left(\upsilon_\|\mathbf{b}+\hat{\mathbf{u}}_s+\mathbf{v}_{Ds}\right)\cdot\frac{\partial\mathbf{A}}{\partial t}\right]m_s\frac{\partial f_s}{\partial W_s}=C_s\left\{f_s\right\}
\end{aligned} \tag{1}$$

where f_s is the full gyro-averaged distribution function, s denotes species, C_s is the collision operator, $\mu=\upsilon_\perp^2/\left(2B\right)$,

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

is the total energy, Z_s is the charge in units of the proton charge e, m_s is the mass, $\Omega_s=Z_s eB/m_s$ is the gyrofrequency (which is negative for electrons with $Z=-1$), $B=\left|\mathbf{B}\right|$, $\mathbf{b}=B^{-1}\mathbf{B}$, and $\mathbf{B}=\nabla\times\mathbf{A}$. Subscripts on partial derivatives indicate quantities held fixed in differentiation. The drifts in (1) are

$$\mathbf{v}_{Ds}=\frac{\mathbf{E}\times\mathbf{B}}{B^2}+\frac{1}{\Omega_s}\mathbf{b}\times\left(\mu\nabla B+\upsilon_\|^2\mathbf{b}\cdot\nabla\mathbf{b}+\upsilon_\|\frac{\partial\mathbf{b}}{\partial t}\right) \tag{3}$$

and

$$\hat{\mathbf{u}}_s=\frac{\upsilon_\perp^2}{2\Omega_s}\mathbf{b}\mathbf{b}\cdot\nabla\times\mathbf{b} \tag{4}$$

In (2), Φ is the electrostatic potential, which in general will vary on a flux surface.

For the slow neoclassical problem we wish to solve, we immediately drop all time derivative terms in (1) except for $\upsilon_\| \mathbf{b}\cdot\left(\partial \mathbf{A}/\partial t\right) m_s \left(\partial f_s/\partial W_s\right)$, which represents an effect of the inductive electric field (if one is present). There is often no inductive electric field in a stellarator, but we retain this term since the transport driven by the inductive electric field is used for computing monoenergetic transport coefficients, and thus for comparison with other codes such as DKES. In such codes, only the contribution from the leading-order Maxwellian

$$f_{Ms}\left(\psi\right) = n_s\left(\psi\right)\left[\frac{m_s}{2\pi T_s\left(\psi\right)}\right]^{3/2} \exp\left(-\frac{m_s \upsilon^2}{2T_s\left(\psi\right)}\right) \tag{5}$$

is retained in this inductive term, and we make the same approximation in sfincs. In (5), T_s denotes the leading order temperature, and n_s is the leading order density. Also, following appendix C of Landreman & Ernst, PPCF 54, 115006 (2012), we take the electromagnetic gauge to be chosen so that

$$-\mathbf{b}\cdot\frac{\partial \mathbf{A}}{\partial t} = \frac{\left\langle \mathbf{E}\cdot\mathbf{B}\right\rangle B}{\left\langle B^2\right\rangle} \tag{6}$$

where $\langle \ldots \rangle$ denotes a flux surface average. Thus, our kinetic equation (1) is reduced to

$$\left(\upsilon_\|\mathbf{b} + \hat{\mathbf{u}}_s + \mathbf{v}_{Ds}\right)\cdot\left(\nabla f_s\right)_{\mu,W_s} + \frac{\upsilon_\| B}{\Omega_s}\left\{\mathbf{b}\cdot\nabla\left(\frac{\upsilon_\|\mathbf{b}\cdot\nabla\times\mathbf{b}}{B}\right)\right\}\mu\frac{\partial f_s}{\partial\mu} - \frac{Z_s e}{T_s}\upsilon_\|\frac{\left\langle \mathbf{E}\cdot\mathbf{B}\right\rangle B}{\left\langle B^2\right\rangle} f_{Ms} = C_s\left\{f_s\right\}. \tag{7}$$

We next make the following changes:

- A source/sink term S_s is introduced, which is sometimes necessary to permit solvability, as discussed in the 2014 Phys. Plasmas paper on SFINCS.
- The $\partial f_s/\partial\mu$ term in (7) is neglected. Dropping this term is justified since $\mathbf{b}\cdot\nabla\times\mathbf{b} \sim \beta \ll 1$ and only the non-Maxwellian part of the distribution function $f_{s1} = f_s - f_{Ms}$ contributes to $\partial f_s/\partial\mu$, so overall this term has magnitude $\rho_* \varepsilon\beta f_{s1}$, which should be quite small.

With these changes, our kinetic equation becomes

$$K_s\left\{f_s\right\} = C_s\left\{f_s\right\} + S_s + \frac{Z_s e}{T_s}\upsilon_\|\frac{\left\langle \mathbf{E}\cdot\mathbf{B}\right\rangle B}{\left\langle B^2\right\rangle} f_{Ms} \tag{8}$$

where

$$K_s\left\{f_s\right\} = \left(\upsilon_\|\mathbf{b} + \mathbf{v}_E + \mathbf{v}_{m1s}\right)\cdot\left(\nabla f_s\right)_{\mu,W_s} \tag{9}$$

is the drift-kinetic operator,

$$\mathbf{v}_{m1s} = \frac{\mu}{\Omega_s}\mathbf{b}\times\nabla B + \frac{\upsilon_\|^2}{\Omega_s}\mathbf{b}\times\left(\mathbf{b}\cdot\nabla\mathbf{b}\right) + \frac{\upsilon_\perp^2}{2\Omega_s}\mathbf{b}\mathbf{b}\cdot\nabla\times\mathbf{b} \tag{10}$$

is the magnetic drift, and

$$\mathbf{v}_E = \frac{1}{B^2}\mathbf{B}\times\nabla\Phi\,. \tag{11}$$

The reason for the ‘1’ subscript in (10) will be clear in a moment.

Magnetic drifts

Sometimes in the literature, a magnetic drift is considered which is slightly different from (10):

$$\begin{aligned}\mathbf{v}_{m2s} &= \left(\upsilon_\parallel/\Omega\right)\nabla_{\mu,\upsilon}\times\left(\upsilon_\parallel\mathbf{b}\right) = \frac{\upsilon_\perp^2}{2\Omega_s B^2}\mathbf{B}\times\nabla B + \frac{\upsilon_\parallel^2}{\Omega_s}\nabla\times\mathbf{b} \\ &= \frac{\mu}{\Omega_s}\mathbf{b}\times\nabla B + \frac{\upsilon_\parallel^2}{\Omega_s}\mathbf{b}\times\left(\mathbf{b}\cdot\nabla\mathbf{b}\right) + \frac{\upsilon_\parallel^2}{\Omega_s}\mathbf{bb}\cdot\nabla\times\mathbf{b}.\end{aligned} \tag{12}$$

Notice that the two models for the magnetic drift ($\mathbf{v}_{m1s}$ and $\mathbf{v}_{m2s}$) differ only in whether $\upsilon_\perp^2/2$ or $\upsilon_\parallel^2$ appears in the parallel term $\propto \mathbf{bb}\cdot\nabla\times\mathbf{b}$. Since this parallel drift is smaller than the parallel streaming term $\upsilon_\parallel\mathbf{b}\cdot\nabla$ by a factor $\rho_*\beta \ll 1$, these 2 models for the magnetic drift should give nearly identical results. However, we provide both options in the code so they can be compared.

As shown in Appendix B of Landreman & Ernst, PPCF 54, 115006 (2012), the form $\mathbf{v}_{m2s}$ of the magnetic drifts is convenient for obtaining conservation laws.

Noting

$$\mathbf{b}\cdot\nabla\times\mathbf{b} = \frac{1}{B^2}\mathbf{B}\cdot\nabla\times\mathbf{B} \tag{13}$$

and

$$\begin{aligned}\mathbf{B}\times\left(\mathbf{b}\cdot\nabla\mathbf{b}\right) &= \mathbf{B}\times\left[\left(\nabla\times\mathbf{b}\right)\times\mathbf{b}\right] \\ &= B\left(\nabla\times\mathbf{b}\right) - \mathbf{bB}\cdot\nabla\times\mathbf{b} \\ &= \frac{1}{B}\mathbf{B}\times\nabla B + \nabla\times\mathbf{B} - \frac{1}{B^2}\mathbf{BB}\cdot\nabla\times\mathbf{B},\end{aligned} \tag{14}$$

then we can write the two forms of the magnetic drifts as

$$\mathbf{v}_{m1s} = \frac{m_s}{2Z_s eB^3}\left(\upsilon_\perp^2 + 2\upsilon_\parallel^2\right)\mathbf{B}\times\nabla B + \frac{m_s\upsilon_\parallel^2}{Z_s eB^2}\nabla\times\mathbf{B} + \frac{m_s}{2Z_s eB^4}\left(\upsilon_\perp^2 - 2\upsilon_\parallel^2\right)\mathbf{BB}\cdot\nabla\times\mathbf{B} \tag{15}$$

and

$$\mathbf{v}_{m2s} = \frac{m_s}{2Z_s eB^3}\left(\upsilon_\perp^2 + 2\upsilon_\parallel^2\right)\mathbf{B}\times\nabla B + \frac{m_s\upsilon_\parallel^2}{Z_s eB^2}\nabla\times\mathbf{B}. \tag{16}$$

We and therefore combine the two versions of the magnetic drifts into a single expression by writing

$$\mathbf{v}_{ms} = \frac{m_s}{2Z_s eB^3}\left(\upsilon_\perp^2 + 2\upsilon_\parallel^2\right)\mathbf{B}\times\nabla B + \frac{m_s\upsilon_\parallel^2}{Z_s eB^2}\nabla\times\mathbf{B} + \sigma_{mdo}\frac{m_s}{2Z_s eB^4}\left(\upsilon_\perp^2 - 2\upsilon_\parallel^2\right)\mathbf{BB}\cdot\nabla\times\mathbf{B} \tag{17}$$

where the 'magnetic drift option' σ_{mdo} is 1 for $\mathbf{v}_{m1s}$ and 0 for $\mathbf{v}_{m2s}$.

System of equations

For numerical solution, we will use coordinates $\left(\theta,\zeta,x_s,\xi\right)$ where $x_s = \upsilon/\upsilon_s$, $\upsilon_s = \sqrt{2T_s/m_s}$, and $\xi = \upsilon_\parallel/\upsilon$. We also choose a specific form for the source:

$$S_s = S_{1s}\left(\psi\right) f_{Ms} + S_{2s}\left(\psi\right) f_{Ms} x_s^2. \tag{18}$$

In this case, (8) can be written

$$K_s\{\theta\}\frac{\partial f_s}{\partial\theta}+K_s\{\zeta\}\frac{\partial f_s}{\partial\zeta}+K_s\{x_s\}\frac{\partial f_s}{\partial x_s}+K_s\{\xi\}\frac{\partial f_s}{\partial\xi}+K_s\{\psi\}\frac{\partial f_s}{\partial\psi}$$
$$-C_{\ell s}\{f_s\}-S_{1s}(\psi)\,f_{Ms}-S_{2s}(\psi)\,f_{Ms}x_s^2-\frac{Z_s e\upsilon_s}{T_s}x_s\xi\frac{\langle\mathbf{E}\cdot\mathbf{B}\rangle B}{\langle B^2\rangle}f_{Ms}=0. \tag{19}$$

In the numerical approach proposed here, we solve (19) together with the following equations:

$$\sum_s Z_s\int d^3\upsilon\, f_s+\lambda=0 \text{ (quasineutrality)} \tag{20}$$

$$\left\langle\int d^3\upsilon\, f_s\right\rangle=n_s(\psi) \tag{21}$$

$$\left\langle\frac{m_s}{3}\int d^3\upsilon\upsilon^2 f_s\right\rangle=n_s(\psi)T_s(\psi) \tag{22}$$

$$\langle\Phi_1\rangle=0 \tag{23}$$

where

$$\Phi_1=\Phi-\langle\Phi\rangle. \tag{24}$$

Notice the full f_s is used everywhere in the system of equations except in the radial derivative in (19). In this term we must substitute f_{Ms} for f_s, since otherwise the code would need to be 5D instead of 4D, and 5D is not feasible. For the same reason, everywhere in K_s that $\partial\Phi/\partial\psi$ appears, it will be approximated by $d\langle\Phi\rangle/d\psi$.

In (19), $C_{\ell s}$ is the collision operator linearized about a stationary Maxwellian; it could be either f_{Ms}, or a Maxwellian with the actual poloidally-varying density $\int d^3\upsilon f_s$ could be used. The more challenging latter approach might be important for high-Z impurities; we should think about how large we expect the impurity density asymmetry on a flux surface to be.

The profiles $S_{s1}(\psi)$ and $S_{s2}(\psi)$ represent additional particle and heat transport of species s required for a steady-state solution to exist.

The scalar quantity λ that appears in (20) is a sort of Lagrange multiplier which may be needed numerically to allow (23) to be satisfied. Flux-surface-averaging (20) and noting (21), then the code should always find $\lambda=0$ if the inputs n_s satisfy quasineutrality.

The unknowns in the system (19)-(23) are

$$\left\{f(\theta,\zeta,x,\xi,s),\ \Phi_1(\theta,\zeta),\ S_1(s),\ S_2(s),\ \lambda\right\} \tag{25}$$

Therefore, the number of degrees of freedom is

$$N_\theta N_\zeta N_x N_\xi N_s+N_\theta N_\zeta+2N_s+1 \tag{26}$$

where N_y is the number of degrees of freedom in the coordinate y upon discretization. As you can verify, the number of scalar equations in (19)-(23) is the same as the number of unknowns (26), so the system is “square”. If we had not included S_{s1}, S_{s2}, or λ, the system would not be square. For comparison, the number of degrees of freedom in SFINCS presently is $N_\theta N_\zeta N_x N_\xi N_s$, so (26) does not represent much of an increase.

Although (20)-(23) are linear in the unknowns, (19) is nonlinear in the unknowns. One type of nonlinearity occurs in collisionless terms $\propto \Phi_1 f$, such as the parallel acceleration term. If the collision operator is linearized about the actual density rather than $n_s(\psi)$, then the collision term would be nonlinear as well. The system of equations is solved by Newton's method, evaluating the Jacobian analytically. The first iteration would begin with the initial values $f_s = f_{Ms}$, $\Phi_1 = 0$, $S_{s1} = 0$, $S_{s2} = 0$, $\lambda = 0$. Since the nonlinear terms are quadratic in the unknowns, analytic differentiation of (19) is feasible.

Magnetic geometry

In the nonlinear version of SFINCS, we allow the magnetic geometry to be specified in any coordinates (ψ, θ, ζ) satisfying $\mathbf{B}\cdot\nabla\psi = 0$ where $2\pi\psi$ is the toroidal flux, as long as physical quantities are periodic in θ and ζ. Boozer coordinates can be used, as can VMEC coordinates. We will not assume the field lines are straight in the SFINCS coordinates, and in principle one could specify a magnetic field with $(\nabla\times\mathbf{B})\cdot\nabla\psi \neq 0$ (although any MHD equilibrium will have $(\nabla\times\mathbf{B})\cdot\nabla\psi = 0$). We will write the kinetic equation in terms of the following components of $\mathbf{B}$:

$$
\begin{aligned}
B^\theta(\psi,\theta,\zeta) &= \mathbf{B}\cdot\nabla\theta \\
B^\zeta(\psi,\theta,\zeta) &= \mathbf{B}\cdot\nabla\zeta \\
B_\psi(\psi,\theta,\zeta) &= \mathbf{B}\cdot\frac{\partial\mathbf{r}}{\partial\psi} = \frac{\mathbf{B}\cdot\nabla\theta\times\nabla\zeta}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta} \\
B_\theta(\psi,\theta,\zeta) &= \mathbf{B}\cdot\frac{\partial\mathbf{r}}{\partial\theta} = \frac{\mathbf{B}\cdot\nabla\zeta\times\nabla\psi}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta} \\
B_\zeta(\psi,\theta,\zeta) &= \mathbf{B}\cdot\frac{\partial\mathbf{r}}{\partial\zeta} = \frac{\mathbf{B}\cdot\nabla\psi\times\nabla\theta}{\nabla\psi\cdot\nabla\theta\times\nabla\zeta}
\end{aligned}
\tag{27}
$$

and the inverse Jacobian

$$D(\psi,\theta,\zeta) = \nabla\psi\cdot\nabla\theta\times\nabla\zeta\,. \tag{28}$$

In terms of the components (27), we have

$$\mathbf{B} = B_\psi\nabla\psi + B_\theta\nabla\theta + B_\zeta\nabla\zeta \tag{29}$$

and

$$\mathbf{B} = \frac{B^\theta}{D}\nabla\zeta\times\nabla\psi + \frac{B^\zeta}{D}\nabla\psi\times\nabla\theta. \tag{30}$$

Notice that for any quantity X, we have

$$\mathbf{B}\cdot\nabla X = B^\theta\frac{\partial X}{\partial\theta} + B^\zeta\frac{\partial X}{\partial\zeta} \tag{31}$$

and

$$\mathbf{B}\times\nabla\psi\cdot\nabla X = DB_\zeta\frac{\partial X}{\partial\theta} - DB_\theta\frac{\partial X}{\partial\zeta}\,. \tag{32}$$

To evaluate the components of the magnetic drifts, we will need to know the components of $\nabla\times\mathbf{B}$. These components may be evaluated using (29) and a couple of vector identities. The results are

$$\left(\nabla\times\mathbf{B}\right)\cdot\nabla\psi=\nabla\cdot\left(\mathbf{B}\times\nabla\psi\right)=\nabla\cdot\left(B_\theta\nabla\theta\times\nabla\psi+B_\zeta\nabla\zeta\times\nabla\psi\right)=D\left(\frac{\partial B_\zeta}{\partial\theta}-\frac{\partial B_\theta}{\partial\zeta}\right)\sigma_{fzrc}, \quad (33)$$

$$\left(\nabla\times\mathbf{B}\right)\cdot\nabla\theta=\nabla\cdot\left(\mathbf{B}\times\nabla\theta\right)=\nabla\cdot\left(B_\psi\nabla\psi\times\nabla\theta+B_\zeta\nabla\zeta\times\nabla\theta\right)=D\frac{\partial B_\psi}{\partial\zeta}-D\frac{\partial B_\zeta}{\partial\psi}, \quad (34)$$

$$\left(\nabla\times\mathbf{B}\right)\cdot\nabla\zeta=\nabla\cdot\left(\mathbf{B}\times\nabla\zeta\right)=\nabla\cdot\left(B_\psi\nabla\psi\times\nabla\zeta+B_\theta\nabla\theta\times\nabla\zeta\right)=D\frac{\partial B_\theta}{\partial\psi}-D\frac{\partial B_\psi}{\partial\theta}. \quad (35)$$

In (33), we have introduced the parameter σ_{fzrc} which is either 0 or 1. The user sets $\sigma_{fzrc}=0$ by setting forceZeroRadialCurrent = true in the input file. The rationale for introducing the parameter σ_{fzrc} is that some choices of coordinates (though not Boozer coordinates) permit there to be a nonzero radial current in the magnetic equilibrium, in which case a Maxwellian ends up giving a net radial current:

$$\left\langle\int d^3\upsilon\, f_M\mathbf{v}_m\cdot\nabla\psi\right\rangle\neq 0 \quad (36)$$

which seems like it could be pathological. We prove this fact following ???. Thus, the parameter σ_{fzrc} allows the user to determine whether the nonzero radial current in the magnetic geometry has any significant effect on the SFINCS output.

For evaluating the last term in the magnetic drifts (17), we define

$$A=\mathbf{B}\cdot\nabla\times\mathbf{B}. \quad (37)$$

Observe

$$\begin{aligned}A&=\mathbf{B}\cdot\nabla\times\mathbf{B}\\&=B_\psi\nabla\psi\cdot\nabla\times\mathbf{B}+B_\theta\nabla\theta\cdot\nabla\times\mathbf{B}+B_\zeta\nabla\zeta\cdot\nabla\times\mathbf{B}\\&=D\left(\left(\frac{\partial B_\zeta}{\partial\theta}-\frac{\partial B_\theta}{\partial\zeta}\right)B_\psi\sigma_{fzrc}+B_\theta\frac{\partial B_\psi}{\partial\zeta}-B_\theta\frac{\partial B_\zeta}{\partial\psi}+B_\zeta\frac{\partial B_\theta}{\partial\psi}-B_\zeta\frac{\partial B_\psi}{\partial\theta}\right).\end{aligned} \quad (38)$$

We will need to evaluate the components of the drifts. The components of the $\mathbf{E}\times\mathbf{B}$ drift are

$$\mathbf{v}_E\cdot\nabla\psi=\frac{DB_\theta}{B^2}\frac{\partial\Phi_1}{\partial\zeta}-\frac{DB_\zeta}{B^2}\frac{\partial\Phi_1}{\partial\theta}, \quad (39)$$

$$\mathbf{v}_E\cdot\nabla\theta=\frac{DB_\zeta}{B^2}\frac{\partial\left\langle\Phi\right\rangle}{\partial\psi}-\frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\zeta}, \quad (40)$$

$$\mathbf{v}_E\cdot\nabla\zeta=\frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\theta}-\frac{DB_\theta}{B^2}\frac{\partial\left\langle\Phi\right\rangle}{\partial\psi}, \quad (41)$$

where we have made the required approximation $\partial\Phi/\partial\psi\approx d\left\langle\Phi\right\rangle/d\psi$. For the DKES version of the $\mathbf{E}\times\mathbf{B}$ drift, we choose to only replace $1/B^2\to 1/\left\langle B^2\right\rangle$ in the $\partial\left\langle\Phi\right\rangle/\partial\psi$ terms, not the terms involving $\tilde{\Phi}$. We make this choice because DKES does not include $\tilde{\Phi}$. Thus,

$$\mathbf{v}_{E,DKES}\cdot\nabla\psi=-\frac{DB_\zeta}{B^2}\frac{\partial\Phi_1}{\partial\theta}+\frac{DB_\theta}{B^2}\frac{\partial\Phi_1}{\partial\zeta}\ \text{(unchanged)}, \quad (42)$$

$$\mathbf{v}_{E,DKES} \cdot \nabla\theta = \frac{DB_\zeta}{\left\langle B^2\right\rangle}\frac{\partial\left\langle\Phi\right\rangle}{\partial\psi} - \frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\zeta}, \tag{43}$$

$$\mathbf{v}_{E,DKES} \cdot \nabla\zeta = -\frac{DB_\theta}{\left\langle B^2\right\rangle}\frac{\partial\left\langle\Phi\right\rangle}{\partial\psi} + \frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\theta}. \tag{44}$$

To evaluate the magnetic drifts, we first re-write (17) as

$$\mathbf{v}_{ms} = \frac{\upsilon_s^2 x_s^2}{\Omega_s B^2}\left(\frac{1}{2}+\frac{\xi^2}{2}\right)\mathbf{B}\times\nabla B + \frac{\upsilon_s^2 x_s^2}{\Omega_s B}\xi^2\nabla\times\mathbf{B} + \sigma_{mdo}\frac{\upsilon_s^2 x_s^2}{2\Omega_s B^3}\left(1-3\xi^2\right)\mathbf{BB}\cdot\nabla\times\mathbf{B}. \tag{45}$$

Using (45) with (33)-(35), the components of the magnetic drifts are

$$\mathbf{v}_m \cdot \nabla\psi = \frac{T_s x_s^2 D}{Z_s e B^3}\left(1+\xi^2\right)\left(B_\theta\frac{\partial B}{\partial\zeta} - B_\zeta\frac{\partial B}{\partial\theta}\right) + \sigma_{fzrc}\frac{2T_s x_s^2 D}{Z_s e B^2}\xi^2\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right), \tag{46}$$

$$\begin{aligned}\mathbf{v}_{ms} \cdot \nabla\theta = {} & \frac{T_s x_s^2 D}{Z_s e B^3}\left(1+\xi^2\right)\left(B_\zeta\frac{\partial B}{\partial\psi} - B_\psi\frac{\partial B}{\partial\zeta}\right) + \frac{\upsilon_s^2 x_s^2 D}{\Omega_s B}\xi^2\left(\frac{\partial B_\psi}{\partial\zeta} - \frac{\partial B_\zeta}{\partial\psi}\right)\\ & +\sigma_{mdo}\frac{T_s x_s^2}{Z_s e B^4}\left(1-3\xi^2\right)AB^\theta,\end{aligned} \tag{47}$$

$$\begin{aligned}\mathbf{v}_{ms} \cdot \nabla\zeta = {} & \frac{T_s x_s^2 D}{Z_s e B^3}\left(1+\xi^2\right)\left(B_\psi\frac{\partial B}{\partial\theta} - B_\theta\frac{\partial B}{\partial\psi}\right) + \frac{2T_s x_s^2 D}{Z_s e B^2}\xi^2\left(\frac{\partial B_\theta}{\partial\psi} - \frac{\partial B_\psi}{\partial\theta}\right)\\ & +\sigma_{mdo}\frac{T_s x_s^2}{Z_s e B^4}\left(1-3\xi^2\right)AB^\zeta\end{aligned}. \tag{48}$$

We will need to evaluate flux surface averages. For any quantity X, the flux surface average is

$$\left\langle X\right\rangle = \frac{1}{V'}\int_0^{2\pi}d\theta\int_0^{2\pi}d\zeta\,\frac{X}{D} \tag{49}$$

where

$$V' = \int_0^{2\pi}d\theta\int_0^{2\pi}d\zeta\,\frac{1}{D}. \tag{50}$$

In the case that Boozer coordinates are used, then

$$\mathbf{B} = \nabla\psi\times\nabla\theta + \iota\nabla\zeta\times\nabla\psi, \tag{51}$$

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

$$\mathbf{B} = \beta\left(\psi,\theta,\zeta\right)\nabla\psi + I\left(\psi\right)\nabla\theta + G\left(\psi\right)\nabla\zeta. \tag{52}$$

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 (51) with (52) gives

$$D = \frac{B^2}{G+\iota I}. \tag{53}$$

The components of $\mathbf{B}$ become

$$
\begin{aligned}
B^{\theta} &= \iota \frac{B^2}{G+\iota I} \\
B^{\zeta} &= \frac{B^2}{G+\iota I} \\
B_{\psi} &= \beta \\
B_{\theta} &= I \\
B_{\zeta} &= G.
\end{aligned} \tag{54}
$$

Note that $(\nabla \times \mathbf{B})\cdot\nabla\psi = 0$ is assumed whenever Boozer coordinates are used, and indeed $B_{\theta} = I(\psi)$ and $B_{\zeta} = G(\psi)$ mean (33) vanishes. Thus, σ_{fzrc} is irrelevant for Boozer coordinates.

If we are given non-Boozer coordinates, it is possible to compute G and I without much effort. Consider a closed curve at fixed θ and ψ with $\zeta \in [0, 2\pi]$. Applying Ampere's Law,

$$
\oint \mathbf{B}\cdot d\mathbf{l} = \mu_0 i_p(\psi) \tag{55}
$$

where $i_p(\psi)$ is the poloidal current outside the flux surface. In the general coordinate system, we can write the length element along this curve as $d\mathbf{l} = (\nabla\psi \times \nabla\theta)/(\nabla\psi\cdot\nabla\theta\times\nabla\zeta)$. Then using (29), the left-hand side of (55) can be written

$$
\int_0^{2\pi} d\zeta\ B_{\zeta} = \mu_0 i_p(\psi). \tag{56}
$$

But this same analysis can be applied in Boozer coordinates, in which case the left-hand side is $2\pi G$. (The integration curves are somewhat different in the 2 coordinate systems, since different θ coordinates are held fixed, but the results of the integration must be the same according to Ampere's Law since the curves enclose the same current.) Thus,

$$
\int_0^{2\pi} d\zeta\ B_{\zeta} = 2\pi G \tag{57}
$$

where the left-hand side is evaluated in the non-Boozer system. The left-hand side must evidently be independent of θ, since the right-hand side is θ-independent. We choose to average (57) over θ since doing so may reduce numerical error slightly. Thus,

$$
G = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\ B_{\zeta}. \tag{58}
$$

We can repeat the analysis for a poloidally closed curve instead of a toroidally closed curve, giving

$$
I = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta\ B_{\theta}. \tag{59}
$$

Trajectory coefficients

Now let us evaluate the coefficients $K_s\{\ldots\}$ in (19) in terms of the coordinates used internally in SFINCS. First, we consider the spatial coefficients:

$$
\begin{aligned}
K_s\{\psi\} &= \mathbf{v}_E\cdot\nabla\psi + \mathbf{v}_{ms}\cdot\nabla\psi \\
&= -\frac{DB_{\zeta}}{B^2}\frac{\partial\Phi_1}{\partial\theta} + \frac{DB_{\theta}}{B^2}\frac{\partial\Phi_1}{\partial\zeta} + \frac{T_s x_s^2 D}{Z_s e B^3}\left(1+\xi^2\right)\left(B_{\theta}\frac{\partial B}{\partial\zeta} - B_{\zeta}\frac{\partial B}{\partial\theta}\right) + \sigma_{fzrc} 2\frac{T_s x_s^2 D}{Z_s e B^2}\xi^2\left(\frac{\partial B_{\zeta}}{\partial\theta} - \frac{\partial B_{\theta}}{\partial\zeta}\right),
\end{aligned} \tag{60}
$$

$$K_s\{\theta\} = \upsilon_\parallel \mathbf{b}\cdot\nabla\theta + \mathbf{v}_E\cdot\nabla\theta + \mathbf{v}_{ms}\cdot\nabla\theta$$
$$= \frac{\upsilon_s x_s \xi B^\theta}{B} + \frac{DB_\zeta}{B^2}\frac{\partial\langle\Phi\rangle}{\partial\psi} - \frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\zeta} \tag{61}$$
$$+\sigma_{islmdt}\frac{T_s x_s^2 D}{Z_s e B^3}\left[\left(1+\xi^2\right)\left(B_\zeta\frac{\partial B}{\partial\psi} - B_\psi\frac{\partial B}{\partial\zeta}\right) + 2\xi^2 B\left(\frac{\partial B_\psi}{\partial\zeta} - \frac{\partial B_\zeta}{\partial\psi}\right) + \sigma_{mdo}\left(1-3\xi^2\right)\frac{A}{DB}B^\theta\right],$$

and

$$K_s\{\zeta\} = \upsilon_\parallel \mathbf{b}\cdot\nabla\zeta + \mathbf{v}_E\cdot\nabla\zeta + \mathbf{v}_{ms}\cdot\nabla\zeta$$
$$= \frac{\upsilon_s x_s \xi B^\zeta}{B} - \frac{DB_\theta}{B^2}\frac{\partial\langle\Phi\rangle}{\partial\psi} + \frac{DB_\psi}{B^2}\frac{\partial\Phi_1}{\partial\theta} \tag{62}$$
$$+\sigma_{islmdt}\frac{T_s x_s^2 D}{Z_s e B^3}\left[\left(1+\xi^2\right)\left(B_\psi\frac{\partial B}{\partial\theta} - B_\theta\frac{\partial B}{\partial\psi}\right) + 2\xi^2 B\left(\frac{\partial B_\theta}{\partial\psi} - \frac{\partial B_\psi}{\partial\theta}\right) + \sigma_{mdo}\left(1-3\xi^2\right)\frac{A}{DB}B^\zeta\right],$$

where we have introduced $\sigma_{islmdt} = 0$ or 1. In the bottom lines of (60)-(62), the black terms are the terms included in the older versions of SFINCS. The blue terms in (61)-(62) are associated with the poloidal or toroidal magnetic drifts, and are turned on and off by the parameter magneticDriftOption, corresponding to $\sigma_{islmdt} = 1$ or 0. The magenta terms in (60) are *linear* terms that are unique to the nonlinear version of SFINCS, because they involve Φ_1 but will multiply only the known quantity $\partial f_{Ms}/\partial\psi$. The green terms in (61)-(62) are nonlinear, since they involve Φ_1 and will multiply derivatives of the full f_s. (Note that $\mathbf{v}_E\cdot\nabla\theta$ and $\mathbf{v}_E\cdot\nabla\zeta$ each contain one linear and one nonlinear term.)

Next, let us evaluate $K_s\{x_s\}$. To do so, we first write

$$0 = K_s\{W_s\} = x_s^2 K_s\{T_s\} + 2T_s x_s K_s\{x_s\} + Z_s e K_s\{\Phi\}, \tag{63}$$

so

$$K_s\{x_s\} = -\frac{x_s}{2}K_s\{\psi\}\frac{1}{T_s}\frac{dT_s}{d\psi} - \frac{Z_s e}{2T_s x_s}K_s\{\Phi\}. \tag{64}$$

Plugging in (60)-(62), several cancellations occur, leaving

$$K_s\{x_s\} = \sigma_{itgt}\left[\frac{DB_\zeta x_s}{2B^2}\frac{\partial\Phi_1}{\partial\theta} - \frac{DB_\theta x_s}{2B^2}\frac{\partial\Phi_1}{\partial\zeta} - \frac{T_s x_s^3 D}{2Z_s e B^3}\left(1+\xi^2\right)\left(B_\theta\frac{\partial B}{\partial\zeta} - B_\zeta\frac{\partial B}{\partial\theta}\right) - \sigma_{fzrc}\frac{T_s x_s^3 D}{Z_s e B^2}\xi^2\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\right]\frac{1}{T_s}\frac{dT_s}{d\psi}$$
$$-\sigma_{ixdt}\frac{x_s D}{2B^3}\left[\left(1+\xi^2\right)\left(B_\theta\frac{\partial B}{\partial\zeta} - B_\zeta\frac{\partial B}{\partial\theta}\right) + \sigma_{fzrc}2\xi^2 B\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\right]\frac{\partial\langle\Phi\rangle}{\partial\psi} \tag{65}$$
$$+\left[-\frac{Z_s e\upsilon_s\xi B^\theta}{2T_s B} - \sigma_{isnmdt}\frac{x_s D}{2B^3}\left\{\left(1+\xi^2\right)\left(B_\zeta\frac{\partial B}{\partial\psi} - B_\psi\frac{\partial B}{\partial\zeta}\right) + 2\xi^2 B\left(\frac{\partial B_\psi}{\partial\zeta} - \frac{\partial B_\zeta}{\partial\psi}\right)\right\} + \sigma_{mdo}\left(1-3\xi^2\right)\frac{A}{DB}B^\theta\right]\frac{\partial\Phi_1}{\partial\theta}$$
$$+\left[-\frac{Z_s e\upsilon_s\xi B^\zeta}{2T_s B} - \sigma_{isnmdt}\frac{x_s D}{2B^3}\left\{\left(1+\xi^2\right)\left(B_\psi\frac{\partial B}{\partial\theta} - B_\theta\frac{\partial B}{\partial\psi}\right) + 2\xi^2 B\left(\frac{\partial B_\theta}{\partial\psi} - \frac{\partial B_\psi}{\partial\theta}\right)\right\} + \sigma_{mdo}\left(1-3\xi^2\right)\frac{A}{DB}B^\zeta\right]\frac{\partial\Phi_1}{\partial\zeta},$$

where we have introduced σ_{itgt}, σ_{ixdt}, and σ_{isnmdt}, which are either 0 or 1. In (65), the cyan and red terms are present in the linear version of SFINCS, although these terms are slightly simpler in the linear version because $(\nabla\times\mathbf{B})\cdot\nabla\psi = 0$ is assumed in that version. In the linear version of SFINCS, the cyan and red terms both act on the Maxwellian contribution $\partial f_{Ms}/\partial x_s$. In the linear version of SFINCS, the cyan term does not act on the perturbation $\partial(f_s - f_{Ms})/\partial x_s$, while in the nonlinear version, we do allow this cyan term to act on the full f_s if includeTemperatureGradientTerms = true, corresponding to $\sigma_{itgt}=1$. The red terms in (65) always act on the Maxwellian term $\partial f_{Ms}/\partial x_s$. The red terms may or may not also act on the perturbation $\partial\left(f_s - f_{Ms}\right)/\partial x_s$; this action is turned on and off by the parameter includeXDotTerm, corresponding to $\sigma_{ixdt}=1$ or 0, as in the linear version of SFINCS. The blue terms in (65) are small, as they involve both the poloidal/toroidal magnetic drifts and Φ_1. These blue terms are turned on and off by the parameter includeSmallNonlinearMagneticDriftTerms, corresponding to $\sigma_{isnmdt}=1$ or 0. Both the blue and green terms are nonlinear, since they involve Φ_1 and will multiply $\partial f_s/\partial x_s$.

Note that the last 2 green terms in (65) are $\propto Z_s$, so these terms may be important for heavy impurities.

Next, let us evaluate $K_s\{\xi\}$. To do so, we first write

$$\begin{aligned}0 &= K_s\{\mu\} = \frac{1}{m_s}K_s\left\{\frac{T_s x_s^2\left(1-\xi^2\right)}{B}\right\} \\ &= -\frac{1}{B^2 m_s}T_s x_s^2\left(1-\xi^2\right)K_s\{B\} + \frac{1}{Bm_s}x_s^2\left(1-\xi^2\right)K_s\{\psi\}\frac{dT_s}{d\psi} + \frac{2x_s T_s}{Bm_s}\left(1-\xi^2\right)K_s\{x_s\} - 2\xi\frac{x_s^2 T_s}{Bm_s}K_s\{\xi\}\end{aligned} \tag{66}$$

and so

$$K_s\{\xi\} = -\frac{1}{2\xi B}\left(1-\xi^2\right)K_s\{B\} + \frac{1}{2\xi}\left(1-\xi^2\right)K_s\{\psi\}\frac{1}{T_s}\frac{dT_s}{d\psi} + \frac{1}{\xi x_s}\left(1-\xi^2\right)K_s\{x_s\}. \tag{67}$$

Into (67) we substitute (60)-(62) and (65). Several cancellations occur. After some algebra, the results simplify to

$$\begin{aligned}K_s\{\xi\} &= -\left(1-\xi^2\right)\frac{\upsilon_s x_s}{2B^2}\left(B^\theta\frac{\partial B}{\partial\theta} + B^\zeta\frac{\partial B}{\partial\zeta}\right) \\ &+\sigma_{ieftixd}\left[B_\zeta\frac{\partial B}{\partial\theta} - B_\theta\frac{\partial B}{\partial\zeta} - \sigma_{fzrc}2B\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\right]\frac{D}{2B^3}\xi\left(1-\xi^2\right)\frac{\partial\langle\Phi\rangle}{\partial\psi} \\ &+\left[\begin{array}{l}-\frac{Z_s e\upsilon_s B^\theta}{2T_s x_s B}\left(1-\xi^2\right) - \sigma_{isnmdt}\frac{D}{2B^3}\left(1-\xi^2\right)\xi\left(B_\zeta\frac{\partial B}{\partial\psi} - B_\psi\frac{\partial B}{\partial\zeta} + 2B\frac{\partial B_\psi}{\partial\zeta} - 2B\frac{\partial B_\zeta}{\partial\psi}\right) \\ +\sigma_{mdo}\frac{\left(1-\xi^2\right)\left(1-3\xi^2\right)}{\xi}\frac{A}{x_s DB}B^\theta\end{array}\right]\frac{\partial\Phi_1}{\partial\theta} \\ &+\left[\begin{array}{l}-\frac{Z_s e\upsilon_s B^\zeta}{2T_s x_s B}\left(1-\xi^2\right) - \sigma_{isnmdt}\frac{D}{2B^3}\left(1-\xi^2\right)\xi\left(B_\psi\frac{\partial B}{\partial\theta} - B_\theta\frac{\partial B}{\partial\psi} + 2B\frac{\partial B_\theta}{\partial\psi} - 2B\frac{\partial B_\psi}{\partial\theta}\right) \\ +\sigma_{mdo}\frac{\left(1-\xi^2\right)\left(1-3\xi^2\right)}{\xi}\frac{A}{x_s DB}B^\zeta\end{array}\right]\frac{\partial\Phi_1}{\partial\zeta} \\ &-\sigma_{islmdt}\frac{T_s x_s^2 D}{Z_s eB^3}\left(1-\xi^2\right)\xi\left[\sigma_{fzrc}\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\frac{\partial B}{\partial\psi} + \left(\frac{\partial B_\psi}{\partial\zeta} - \frac{\partial B_\zeta}{\partial\psi}\right)\frac{\partial B}{\partial\theta} + \left(\frac{\partial B_\theta}{\partial\psi} - \frac{\partial B_\psi}{\partial\theta}\right)\frac{\partial B}{\partial\zeta}\right] \\ &-\sigma_{mdo}\frac{1}{\xi}\left(1-\xi^2\right)\left(1-3\xi^2\right)\frac{T_s x_s^2 D}{2Z_s eB^4}\frac{A}{DB}\left(B^\zeta\frac{\partial B}{\partial\zeta} + B^\theta\frac{\partial B}{\partial\theta}\right).\end{aligned} \tag{68}$$

The red terms are the terms proportional to σ_{ndo}, and notice these terms are all proportional to $1/\xi$. Due to this singularity, these terms have a dense representation in the Legendre polynomial index, and for this reason we drop them. (Perhaps these terms might become regular if the $\partial f / \partial\mu$ term in (7) is retained?) For all the black terms in (68), there are no factors of ξ remaining in the denominators. These remaining terms are

$$
\begin{aligned}
K_s\{\xi\} = & -\left(1-\xi^2\right)\frac{\upsilon_s x_s}{2B^2}\left(B^\theta \frac{\partial B}{\partial\theta} + B^\zeta \frac{\partial B}{\partial\zeta}\right) \\
& +\sigma_{ieftixd}\left[B_\zeta \frac{\partial B}{\partial\theta} - B_\theta \frac{\partial B}{\partial\zeta} - \sigma_{fzrc} 2B\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\right]\frac{D}{2B^3}\xi\left(1-\xi^2\right)\frac{\partial\langle\Phi\rangle}{\partial\psi} \\
& +\left[-\frac{Z_s e\upsilon_s B^\theta}{2T_s x_s B}\left(1-\xi^2\right) - \sigma_{isnmdt}\frac{D}{2B^3}\left(1-\xi^2\right)\xi\left(B_\zeta \frac{\partial B}{\partial\psi} - B_\psi \frac{\partial B}{\partial\zeta} + 2B\frac{\partial B_\psi}{\partial\zeta} - 2B\frac{\partial B_\zeta}{\partial\psi}\right)\right]\frac{\partial\Phi_1}{\partial\theta} \\
& +\left[-\frac{Z_s e\upsilon_s B^\zeta}{2T_s x_s B}\left(1-\xi^2\right) - \sigma_{isnmdt}\frac{D}{2B^3}\left(1-\xi^2\right)\xi\left(B_\psi \frac{\partial B}{\partial\theta} - B_\theta \frac{\partial B}{\partial\psi} + 2B\frac{\partial B_\theta}{\partial\psi} - 2B\frac{\partial B_\psi}{\partial\theta}\right)\right]\frac{\partial\Phi_1}{\partial\zeta} \\
& -\sigma_{islmdt}\frac{T_s x_s^2 D}{Z_s e B^3}\left(1-\xi^2\right)\xi\left[\sigma_{fzrc}\left(\frac{\partial B_\zeta}{\partial\theta} - \frac{\partial B_\theta}{\partial\zeta}\right)\frac{\partial B}{\partial\psi} + \left(\frac{\partial B_\psi}{\partial\zeta} - \frac{\partial B_\zeta}{\partial\psi}\right)\frac{\partial B}{\partial\theta} + \left(\frac{\partial B_\theta}{\partial\psi} - \frac{\partial B_\psi}{\partial\theta}\right)\frac{\partial B}{\partial\zeta}\right].
\end{aligned}
\tag{69}
$$

The σ factors have been inserted here to reflect the actual implementation in the code for turning various terms on and off, and are not "derived" from previous equations. The first line of (69), in black, is the familiar mirror force term, also present in the older versions of SFINCS. The next line, in red, is also present in previous versions of SFINCS, and may be turned on or off with the includeElectricFieldTermInXDot parameter, corresponding to $\sigma_{ieftixd} = 1$ or 0. The next two lines, in green, are nonlinear, as they involve Φ_1 and will multiply $\partial f_s / \partial\xi$. The last line of (69), in blue, is linear but is not present in the older versions of SFINCS, as it arises from the magnetic drifts.

Normalizations

Let's suppose we are given T_s, $dT_s / d\psi_N$, n_s, $dn_s / d\psi_N$, $d\langle\Phi\rangle / d\psi_N$, $B(\theta,\zeta)$, 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. $10^{20}/\mathrm{m}^3$), $\bar{\Phi}$ (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

$$\hat{m}_s = m_s / \bar{m}, \tag{70}$$

$$\hat{T}_s = T_s / \bar{T}, \tag{71}$$

$$\hat{n}_s = n_s / \bar{n}, \tag{72}$$

$$d\hat{T}_s / d\psi_N = \left(dT_s / d\psi_N\right) / \bar{T}, \tag{73}$$

$$d\hat{n}_s / d\psi_N = \left(dn_s / d\psi_N\right) / \bar{n}, \tag{74}$$

$$d\langle\hat{\Phi}\rangle / d\psi_N = \left(d\langle\Phi\rangle / d\psi_N\right) / \bar{\Phi}, \tag{75}$$

$$\hat{\Phi}_1 = \Phi_1 / \bar{\Phi}, \tag{76}$$

$$\hat{B} = B / \bar{B}, \tag{77}$$

$$\hat{B}^\theta = \frac{\bar{R}}{\bar{B}} B^\theta, \tag{78}$$

$$\hat{B}^\zeta = \frac{\bar{R}}{\bar{B}} B^\zeta, \tag{79}$$

$$\hat{B}_\psi = \bar{R} B_\psi, \tag{80}$$

$$\hat{B}_\theta = \frac{1}{\bar{R}\bar{B}} B_\theta, \tag{81}$$

$$\hat{B}_\zeta = \frac{1}{\bar{R}\bar{B}} B_\zeta, \tag{82}$$

$$\hat{D} = \frac{\bar{R}}{\bar{B}} D, \tag{83}$$

$$\hat{\psi} = \psi / \left(\bar{R}^2 \bar{B}\right) \tag{84}$$

$$\hat{\psi}_a = \psi_a / \left(\bar{B}\bar{R}^2\right), \tag{85}$$

$$\hat{A} = \frac{\bar{R}}{\bar{B}^2} \mathbf{B} \cdot \nabla \times \mathbf{B} = \frac{\bar{R} A}{\bar{B}^2} \text{ (called } \texttt{BDotCurlB} \text{ in the code)} \tag{86}$$

and

$$\hat{E} = \left\langle E_\| B \right\rangle \frac{\bar{R}}{\bar{\Phi}\bar{B}}. \tag{87}$$

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

$$\frac{dX}{d\psi} = \frac{1}{\hat{\psi}_a \bar{R}^2 \bar{B}} \frac{dX}{d\psi_N} \tag{88}$$

for any flux function X. If Boozer coordinates are used, then we also have

$$\hat{G} = \frac{1}{\bar{R}\bar{B}} G, \tag{89}$$

$$\hat{I} = \frac{1}{\bar{R}\bar{B}} I. \tag{90}$$

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

$$\bar{\upsilon} = \sqrt{2\bar{T} / \bar{m}}, \tag{91}$$

$$\Delta = \frac{\bar{m}\bar{\upsilon}}{e\bar{B}\bar{R}} \tag{92}$$

(which resembles $\rho_* = \rho / R$; note that $\Delta = \bar{m}\bar{\upsilon}c / \left(e\bar{B}\bar{R}\right)$ has a factor of c in Gaussian units),

$$\alpha = \frac{e\bar{\Phi}}{\bar{T}}, \tag{93}$$

and a normalized collisionality

$$\nu_n = \bar{\nu}\bar{R} / \bar{\upsilon} \tag{94}$$

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

$$\bar{\nu} = \frac{1}{\left(4\pi\varepsilon_0\right)^2} \frac{4\sqrt{2\pi}\bar{n}e^4 \ln\Lambda}{3\bar{m}^{1/2}\bar{T}^{3/2}} \text{ (SI units)}, \tag{95}$$

$$\bar{\nu} = \frac{4\sqrt{2\pi}\bar{n}e^4 \ln\Lambda}{3\bar{m}^{1/2}\bar{T}^{3/2}} \text{ (Gaussian units)} \tag{96}$$

We assume $\ln\Lambda$ has the same value for all species. Notice that

$$\frac{\upsilon_s}{\bar{\upsilon}} = \sqrt{\frac{\hat{T}_s}{\hat{m}_s}} \tag{97}$$

with no 2 inside the square root.

As in the multi-species version of SFINCS, **we define a normalized distribution function $\hat{f}_s$ as follows:**

$$f_s = \frac{\bar{n}}{\bar{\upsilon}^3} \hat{f}_s. \tag{98}$$

Notice this normalization is the same for each species.

The kinetic equation (19) for each species is made dimensionless by multiplying through by

$$\frac{\bar{\upsilon}^3}{\bar{n}} \frac{\bar{R}}{\bar{\upsilon}}. \tag{99}$$

This normalization is slightly different from the linear version of SFINCS. The associated normalized trajectory coefficients may then be written as

$$\hat{K}_s\{\ldots\} = \frac{\bar{R}}{\bar{\upsilon}} K_s\{\ldots\} \tag{100}$$

so the kinetic equation is

$$\begin{aligned} &\hat{K}_s\{\theta\}\frac{\partial \hat{f}_s}{\partial\theta} + \hat{K}_s\{\zeta\}\frac{\partial \hat{f}_s}{\partial\zeta} + \hat{K}_s\{x\}\frac{\partial \hat{f}_s}{\partial x} + \hat{K}_s\{\xi\}\frac{\partial \hat{f}_s}{\partial\xi} + \hat{K}_s\{\hat{\psi}\}\frac{\partial \hat{f}_{Ms}}{\partial\hat{\psi}} \\ &-\hat{C}_{\ell s}\left\{\hat{f}_s\right\} - \hat{S}_{s1}\hat{f}_{Ms} - \hat{S}_{s2}\hat{f}_{Ms}x^2 - \frac{\hat{E}\alpha Z_s \hat{B}}{\sqrt{\hat{m}_s\hat{T}_s}\left\langle \hat{B}^2\right\rangle} x_s \xi \hat{f}_{Ms} = 0 \end{aligned} \tag{101}$$

where

$$\hat{C}_s\left\{\hat{f}_s\right\} = \frac{1}{\bar{\nu}} C_s\left\{\hat{f}_s\right\} \tag{102}$$

is the normalized collision operator and

$$\hat{S}_{sj} = \frac{\bar{R}}{\bar{\upsilon}} S_{sj} \tag{103}$$

denote the normalized sources. Applying our normalizations to (60)-(62), (65), and (69), the normalized trajectory coefficients are

$$
\begin{aligned}
\hat{K}_s\{\hat{\psi}\} = & -\alpha\Delta\frac{\hat{D}\hat{B}_\zeta}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\theta}+\alpha\Delta\frac{\hat{D}\hat{B}_\theta}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\zeta} \\
& +\frac{\Delta\hat{T}_s x_s^2\hat{D}}{2Z_s\hat{B}^3}\left(1+\xi^2\right)\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)+\sigma_{fzrc}\Delta\frac{\hat{T}_s x_s^2\hat{D}}{Z_s\hat{B}^2}\xi^2\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right),
\end{aligned}
\tag{104}
$$

$$
\begin{aligned}
\hat{K}_s\{\theta\} = & \sqrt{\frac{\hat{T}_s}{\hat{m}_s}}\frac{x_s\xi\hat{B}^\theta}{\hat{B}}+\alpha\Delta\frac{\hat{D}\hat{B}_\zeta}{2\hat{B}^2}\frac{\partial\left\langle\hat{\Phi}\right\rangle}{\partial\hat{\psi}}-\alpha\Delta\frac{\hat{D}\hat{B}_\psi}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\zeta} \\
& +\sigma_{islmdt}\frac{\Delta\hat{T}_s x_s^2\hat{D}}{2Z_s\hat{B}^3}\left[\left(1+\xi^2\right)\left(\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\hat{\psi}}-\hat{B}_\psi\frac{\partial\hat{B}}{\partial\zeta}\right)+2\xi^2\hat{B}\left(\frac{\partial\hat{B}_\psi}{\partial\zeta}-\frac{\partial\hat{B}_\zeta}{\partial\hat{\psi}}\right)+\sigma_{mdo}\left(1-3\xi^2\right)\frac{\hat{A}}{\hat{D}\hat{B}}\hat{B}^\theta\right],
\end{aligned}
\tag{105}
$$

$$
\begin{aligned}
\hat{K}_s\{\zeta\} = & \sqrt{\frac{\hat{T}_s}{\hat{m}_s}}\frac{x_s\xi\hat{B}^\zeta}{\hat{B}}-\alpha\Delta\frac{\hat{D}\hat{B}_\theta}{2\hat{B}^2}\frac{\partial\left\langle\hat{\Phi}\right\rangle}{\partial\hat{\psi}}+\alpha\Delta\frac{\hat{D}\hat{B}_\psi}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\theta} \\
& +\sigma_{islmdt}\frac{\Delta\hat{T}_s x_s^2\hat{D}}{2Z_s\hat{B}^3}\left[\left(1+\xi^2\right)\left(\hat{B}_\psi\frac{\partial\hat{B}}{\partial\theta}-\hat{B}_\theta\frac{\partial\hat{B}}{\partial\hat{\psi}}\right)+2\xi^2\hat{B}\left(\frac{\partial\hat{B}_\theta}{\partial\hat{\psi}}-\frac{\partial\hat{B}_\psi}{\partial\theta}\right)+\sigma_{mdo}\left(1-3\xi^2\right)\frac{\hat{A}}{\hat{D}\hat{B}}\hat{B}^\zeta\right],
\end{aligned}
\tag{106}
$$

$$
\begin{aligned}
\hat{K}_s\{x_s\} = & \sigma_{itgt}\left[\alpha\Delta\frac{\hat{D}\hat{B}_\zeta x_s}{4\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\theta}-\alpha\Delta\frac{\hat{D}\hat{B}_\theta x_s}{4\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\zeta}-\Delta\frac{\hat{T}_s x_s^3\hat{D}}{4Z_s\hat{B}^3}\left(1+\xi^2\right)\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)-\sigma_{fzrc}\Delta\frac{\hat{T}_s x_s^3\hat{D}}{2Z_s\hat{B}^2}\xi^2\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\right]\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\hat{\psi}} \\
& -\sigma_{ixdt}\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left[\left(1+\xi^2\right)\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)+\sigma_{fzrc}2\xi^2\hat{B}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\right]\frac{\partial\left\langle\hat{\Phi}\right\rangle}{\partial\hat{\psi}} \\
& +\left[-\alpha\frac{Z_s\xi\hat{B}^\theta}{2\sqrt{\hat{T}_s\hat{m}_s}\hat{B}}-\sigma_{isnmdt}\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left\{\left(1+\xi^2\right)\left(\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\hat{\psi}}-\hat{B}_\psi\frac{\partial\hat{B}}{\partial\zeta}\right)+2\xi^2\hat{B}\left(\frac{\partial\hat{B}_\psi}{\partial\zeta}-\frac{\partial\hat{B}_\zeta}{\partial\hat{\psi}}\right)+\sigma_{mdo}\left(1-3\xi^2\right)\frac{\hat{A}}{\hat{D}\hat{B}}\hat{B}^\theta\right\}\right]\frac{\partial\hat{\Phi}_1}{\partial\theta} \\
& +\left[-\alpha\frac{Z_s\xi\hat{B}^\zeta}{2\sqrt{\hat{T}_s\hat{m}_s}\hat{B}}-\sigma_{isnmdt}\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left\{\left(1+\xi^2\right)\left(\hat{B}_\psi\frac{\partial\hat{B}}{\partial\theta}-\hat{B}_\theta\frac{\partial\hat{B}}{\partial\hat{\psi}}\right)+2\xi^2\hat{B}\left(\frac{\partial\hat{B}_\theta}{\partial\hat{\psi}}-\frac{\partial\hat{B}_\psi}{\partial\theta}\right)+\sigma_{mdo}\left(1-3\xi^2\right)\frac{\hat{A}}{\hat{D}\hat{B}}\hat{B}^\zeta\right\}\right]\frac{\partial\hat{\Phi}_1}{\partial\zeta},
\end{aligned}
\tag{107}
$$

and

$$
\begin{aligned}
\hat{K}_s\{\xi\} = &-\sqrt{\frac{\hat{T}_s}{\hat{m}_s}}\left(1-\xi^2\right)\frac{x_s}{2\hat{B}^2}\left(\hat{B}^\theta \frac{\partial \hat{B}}{\partial \theta} + \hat{B}^\zeta \frac{\partial \hat{B}}{\partial \zeta}\right) \\
&+\sigma_{ieftixd}\left[\hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} - \hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \sigma_{fzrc} 2\hat{B}\left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta}\right)\right]\frac{\alpha \Delta \hat{D}}{4\hat{B}^3}\xi\left(1-\xi^2\right)\frac{\partial \langle \hat{\Phi} \rangle}{\partial \hat{\psi}} \\
&-\frac{\alpha Z_s \hat{B}^\theta}{2\sqrt{\hat{m}_s \hat{T}_s}\, x_s \hat{B}}\left(1-\xi^2\right)\frac{\partial \hat{\Phi}_1}{\partial \theta} \\
&-\alpha \Delta \sigma_{isnmdt}\frac{\hat{D}}{4\hat{B}^3}\left(1-\xi^2\right)\xi\left(\hat{B}_\zeta \frac{\partial \hat{B}}{\partial \hat{\psi}} - \hat{B}_\psi \frac{\partial \hat{B}}{\partial \zeta} + 2\hat{B}\frac{\partial \hat{B}_\psi}{\partial \zeta} - 2\hat{B}\frac{\partial \hat{B}_\zeta}{\partial \hat{\psi}}\right)\frac{\partial \hat{\Phi}_1}{\partial \theta} \\
&-\frac{\alpha Z_s \hat{B}^\zeta}{2\sqrt{\hat{m}_s \hat{T}_s}\, x_s \hat{B}}\left(1-\xi^2\right)\frac{\partial \hat{\Phi}_1}{\partial \zeta} \\
&-\alpha \Delta \sigma_{isnmdt}\frac{\hat{D}}{4\hat{B}^3}\left(1-\xi^2\right)\xi\left(\hat{B}_\psi \frac{\partial \hat{B}}{\partial \theta} - \hat{B}_\theta \frac{\partial \hat{B}}{\partial \hat{\psi}} + 2\hat{B}\frac{\partial \hat{B}_\theta}{\partial \hat{\psi}} - 2\hat{B}\frac{\partial \hat{B}_\psi}{\partial \theta}\right)\frac{\partial \hat{\Phi}_1}{\partial \zeta} \\
&-\sigma_{islmdt}\frac{\Delta \hat{D}\hat{T}_s x_s^2}{2Z_s \hat{B}^3}\left(1-\xi^2\right)\xi\left[\sigma_{fzrc}\left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta}\right)\frac{\partial \hat{B}}{\partial \hat{\psi}} + \left(\frac{\partial \hat{B}_\psi}{\partial \zeta} - \frac{\partial \hat{B}_\zeta}{\partial \hat{\psi}}\right)\frac{\partial \hat{B}}{\partial \theta} + \left(\frac{\partial \hat{B}_\theta}{\partial \hat{\psi}} - \frac{\partial \hat{B}_\psi}{\partial \theta}\right)\frac{\partial \hat{B}}{\partial \zeta}\right].
\end{aligned}
\tag{108}
$$

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 $P_\ell(\xi)$:

$$\hat{f}_s = \sum_\ell f_{s,\ell} P_\ell(\xi). \tag{109}$$

We discretize the kinetic equation (101) by applying

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\, P_L(\xi)(\quad\cdot\quad). \tag{110}$$

To evaluate the various integrals that result, we use the orthogonality relation

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\, P_L(\xi) P_\ell(\xi) = \delta_{L,\ell}, \tag{111}$$

as well as the following identities:

$$\frac{2L+1}{2}\int_{-1}^{1} d\xi\, \xi P_L(\xi) P_\ell(\xi) = \frac{L+1}{2L+3}\delta_{L+1,\ell} + \frac{L}{2L-1}\delta_{L-1,\ell}, \tag{112}$$

$$
\begin{aligned}
\frac{2L+1}{2}\int_{-1}^{1} d\xi\, \left(1+\xi^2\right) P_L(\xi) P_\ell(\xi) = &\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)}\delta_{L,\ell} \\
&+\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell} + \frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell},
\end{aligned}
\tag{113}
$$

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\ \xi^2 P_L(\xi)P_\ell(\xi)=\frac{2L^2+2L-1}{(2L+3)(2L-1)}\delta_{L,\ell}+\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell}+\frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell}, \tag{114}$$

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\ \left(1-\xi^2\right)P_L(\xi)\frac{dP_\ell}{d\xi}=\frac{(L+1)(L+2)}{2L+3}\delta_{L+1,\ell}-\frac{(L-1)L}{2L-1}\delta_{L-1,\ell}, \tag{115}$$

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\ \left(1-\xi^2\right)\xi P_L(\xi)\frac{dP_\ell}{d\xi}=\frac{(L+1)L}{(2L-1)(2L+3)}\delta_{L,\ell}+\frac{(L+3)(L+2)(L+1)}{(2L+5)(2L+3)}\delta_{L+2,\ell}-\frac{L(L-1)(L-2)}{(2L-3)(2L-1)}\delta_{L-2,\ell}, \tag{116}$$

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\ P_L(\xi)\xi=\delta_{L,1}, \tag{117}$$

and

$$\frac{2L+1}{2}\int_{-1}^{1}d\xi\ P_L(\xi)\left(1+\xi^2\right)=\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}. \tag{118}$$

As a result, (101) may be written

$$\dot{\hat{\psi}}_{s,L}\frac{\partial\hat{f}_{Ms}}{\partial\hat{\psi}}+\sum_\ell\left(M_{s,L,\ell}\hat{f}_{s,\ell}\right)+\mathcal{E}_s=0 \tag{119}$$

where

$$\mathcal{E}=-\frac{\hat{E}\alpha Z_s\hat{B}}{\left\langle\hat{B}^2\right\rangle}x_s\frac{\hat{n}_s\hat{m}_s}{\pi^{3/2}\hat{T}_s^2}\exp\left(-x_s^2\right)\delta_{L,1} \tag{120}$$

$$M_{s,L,\ell}=\dot{\theta}_{s,L,\ell}\frac{\partial}{\partial\theta}+\dot{\zeta}_{s,L,\ell}\frac{\partial}{\partial\zeta}+M_{s,L,\ell}^{(\xi)}+\dot{x}_{s,L,\ell}\frac{\partial}{\partial x_s}-\nu_n\hat{C}_{s,L}\delta_{L,\ell}, \tag{121}$$

$$\dot{\hat{\psi}}_{s,L}=-\alpha\Delta\frac{\hat{D}\hat{B}_\zeta}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\theta}\delta_{L,0}+\alpha\Delta\frac{\hat{D}\hat{B}_\theta}{2\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\zeta}\delta_{L,0}+\frac{\Delta\hat{T}_s x_s^2\hat{D}}{2Z_s\hat{B}^3}\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)+\sigma_{fzrc}\Delta\frac{\hat{T}_s x_s^2\hat{D}}{Z_s\hat{B}^2}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right), \tag{122}$$

(Since $\dot{\psi}_{N,s,L}$ only acts on the Maxwellian, we only need to consider $\ell=0$ in the identities (113)-(114)),

$$\dot{\theta}_{s,L,\ell} = \sqrt{\frac{\hat{T}_s}{\hat{m}_s}} \frac{x_s \hat{B}^\theta}{\hat{B}} \left(\frac{L+1}{2L+3} \delta_{L+1,\ell} + \frac{L}{2L-1} \delta_{L-1,\ell} \right) + \alpha\Delta \frac{\hat{D}\hat{B}_\zeta}{2\hat{B}^2} \frac{\partial \langle \hat{\Phi} \rangle}{\partial \hat{\psi}} \delta_{L,\ell} - \alpha\Delta \frac{\hat{D}\hat{B}_\psi}{2\hat{B}^2} \frac{\partial \hat{\Phi}_1}{\partial \zeta} \delta_{L,\ell}$$
$$+\sigma_{islmdt} \frac{\Delta \hat{T}_s x_s^2 \hat{D}}{2 Z_s \hat{B}^3} \left[\begin{array}{l} \left(\hat{B}_\zeta \frac{\partial \hat{B}}{\partial \hat{\psi}} - \hat{B}_\psi \frac{\partial \hat{B}}{\partial \zeta} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \delta_{L,\ell} + \frac{L-1}{2L-3} \frac{L}{2L-1} \delta_{L-2,\ell} + \frac{L+2}{2L+5} \frac{L+1}{2L+3} \delta_{L+2,\ell} \right) \\ +2\hat{B} \left(\frac{\partial \hat{B}_\psi}{\partial \zeta} - \frac{\partial \hat{B}_\zeta}{\partial \hat{\psi}} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \delta_{L,\ell} + \frac{L-1}{2L-3} \frac{L}{2L-1} \delta_{L-2,\ell} + \frac{L+2}{2L+5} \frac{L+1}{2L+3} \delta_{L+2,\ell} \right) \end{array} \right], \tag{123}$$

$$\dot{\zeta}_{s,L,\ell} = \sqrt{\frac{\hat{T}_s}{\hat{m}_s}} \frac{x_s \hat{B}^\zeta}{\hat{B}} \left(\frac{L+1}{2L+3} \delta_{L+1,\ell} + \frac{L}{2L-1} \delta_{L-1,\ell} \right) - \alpha\Delta \frac{\hat{D}\hat{B}_\theta}{2\hat{B}^2} \frac{\partial \langle \hat{\Phi} \rangle}{\partial \hat{\psi}} \delta_{L,\ell} + \alpha\Delta \frac{\hat{D}\hat{B}_\psi}{2\hat{B}^2} \frac{\partial \hat{\Phi}_1}{\partial \theta} \delta_{L,\ell}$$
$$+\sigma_{islmdt} \frac{\Delta \hat{T}_s x_s^2 \hat{D}}{2 Z_s \hat{B}^3} \left[\begin{array}{l} \left(\hat{B}_\psi \frac{\partial \hat{B}}{\partial \theta} - \hat{B}_\theta \frac{\partial \hat{B}}{\partial \hat{\psi}} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \delta_{L,\ell} + \frac{L-1}{2L-3} \frac{L}{2L-1} \delta_{L-2,\ell} + \frac{L+2}{2L+5} \frac{L+1}{2L+3} \delta_{L+2,\ell} \right) \\ +2\hat{B} \left(\frac{\partial \hat{B}_\theta}{\partial \hat{\psi}} - \frac{\partial \hat{B}_\psi}{\partial \theta} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \delta_{L,\ell} + \frac{L-1}{2L-3} \frac{L}{2L-1} \delta_{L-2,\ell} + \frac{L+2}{2L+5} \frac{L+1}{2L+3} \delta_{L+2,\ell} \right) \end{array} \right], \tag{124}$$

$$\begin{aligned}
\dot{x}_{s,L,\ell} = {}& \sigma_{itgt} \left[\alpha\Delta \frac{\hat{D}\hat{B}_\zeta x_s}{4\hat{B}^2} \frac{\partial \hat{\Phi}_1}{\partial \theta} \delta_{L,\ell} - \alpha\Delta \frac{\hat{D}\hat{B}_\theta x_s}{4\hat{B}^2} \frac{\partial \hat{\Phi}_1}{\partial \zeta} \delta_{L,\ell} \right] \frac{1}{\hat{T}_s} \frac{d\hat{T}_s}{d\hat{\psi}} \\
& -\sigma_{itgt} \Delta \frac{\hat{T}_s x_s^3 \hat{D}}{4 Z_s \hat{B}^3} \left[\begin{array}{l} \left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \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} \right) \\ +\sigma_{fzrc} 2\hat{B} \left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \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} \right) \end{array} \right] \frac{1}{\hat{T}_s} \frac{d\hat{T}_s}{d\hat{\psi}} \\
& -\sigma_{ixdt} \alpha\Delta \frac{x_s \hat{D}}{4\hat{B}^3} \left[\begin{array}{l} \left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \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} \right) \\ +\sigma_{fzrc} 2\hat{B} \left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \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} \right) \end{array} \right] \frac{\partial \langle \hat{\Phi} \rangle}{\partial \hat{\psi}} \\
& -\alpha \frac{Z_s \hat{B}^\theta}{2\sqrt{\hat{T}_s \hat{m}_s} \hat{B}} \left(\frac{L+1}{2L+3} \delta_{L+1,\ell} + \frac{L}{2L-1} \delta_{L-1,\ell} \right) \frac{\partial \hat{\Phi}_1}{\partial \theta} \\
& -\sigma_{isnmdt} \alpha\Delta \frac{x_s \hat{D}}{4\hat{B}^3} \left\{ \begin{array}{l} \left(\hat{B}_\zeta \frac{\partial \hat{B}}{\partial \hat{\psi}} - \hat{B}_\psi \frac{\partial \hat{B}}{\partial \zeta} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \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} \right) \\ +2\hat{B} \left(\frac{\partial \hat{B}_\psi}{\partial \zeta} - \frac{\partial \hat{B}_\zeta}{\partial \hat{\psi}} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \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} \right) \end{array} \right\} \frac{\partial \hat{\Phi}_1}{\partial \theta} \\
& -\alpha \frac{Z_s \hat{B}^\zeta}{2\sqrt{\hat{T}_s \hat{m}_s} \hat{B}} \left(\frac{L+1}{2L+3} \delta_{L+1,\ell} + \frac{L}{2L-1} \delta_{L-1,\ell} \right) \frac{\partial \hat{\Phi}_1}{\partial \zeta} \\
& -\sigma_{isnmdt} \alpha\Delta \frac{x_s \hat{D}}{4\hat{B}^3} \left\{ \begin{array}{l} \left(\hat{B}_\psi \frac{\partial \hat{B}}{\partial \theta} - \hat{B}_\theta \frac{\partial \hat{B}}{\partial \hat{\psi}} \right) \left(\frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)} \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} \right) \\ +2\hat{B} \left(\frac{\partial \hat{B}_\theta}{\partial \hat{\psi}} - \frac{\partial \hat{B}_\psi}{\partial \theta} \right) \left(\frac{2L^2+2L-1}{(2L+3)(2L-1)} \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} \right) \end{array} \right\} \frac{\partial \hat{\Phi}_1}{\partial \zeta},
\end{aligned} \tag{125}$$

and

$$
\begin{aligned}
M_{s,L,\ell}^{(\xi)} =& -\sqrt{\frac{\hat{T}_s}{\hat{m}_s}}\frac{x_s}{2\hat{B}^2}\left(\hat{B}^\theta\frac{\partial\hat{B}}{\partial\theta}+\hat{B}^\zeta\frac{\partial\hat{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] \\
&+\sigma_{ieftixd}\left[\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}-\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\sigma_{fzrc}2\hat{B}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\right]\frac{\alpha\Delta\hat{D}}{4\hat{B}^3}\frac{\partial\langle\hat{\Phi}\rangle}{\partial\hat{\psi}}\left[\frac{(L+1)L}{(2L-1)(2L+3)}\delta_{L,\ell}+\frac{(L+3)(L+2)(L+1)}{(2L+5)(2L+3)}\delta_{L+2,\ell}-\frac{L(L-1)(L-2)}{(2L-3)(2L-1)}\delta_{L-2,\ell}\right] \\
&-\frac{\alpha Z_s\hat{B}^\theta}{2\sqrt{\hat{m}_s\hat{T}_s}x_s\hat{B}}\left[\frac{(L+1)(L+2)}{2L+3}\delta_{L+1,\ell}-\frac{(L-1)L}{2L-1}\delta_{L-1,\ell}\right]\frac{\partial\hat{\Phi}_1}{\partial\theta} \\
&-\alpha\Delta\sigma_{isnmdt}\frac{\hat{D}}{4\hat{B}^3}\left(\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\hat{\psi}}-\hat{B}_\psi\frac{\partial\hat{B}}{\partial\zeta}+2\hat{B}\frac{\partial\hat{B}_\psi}{\partial\zeta}-2\hat{B}\frac{\partial\hat{B}_\zeta}{\partial\hat{\psi}}\right)\left[\frac{(L+1)L}{(2L-1)(2L+3)}\delta_{L,\ell}+\frac{(L+3)(L+2)(L+1)}{(2L+5)(2L+3)}\delta_{L+2,\ell}-\frac{L(L-1)(L-2)}{(2L-3)(2L-1)}\delta_{L-2,\ell}\right]\frac{\partial\hat{\Phi}_1}{\partial\theta} \\
&-\frac{\alpha Z_s\hat{B}^\zeta}{2\sqrt{\hat{m}_s\hat{T}_s}x_s\hat{B}}\left[\frac{(L+1)(L+2)}{2L+3}\delta_{L+1,\ell}-\frac{(L-1)L}{2L-1}\delta_{L-1,\ell}\right]\frac{\partial\hat{\Phi}_1}{\partial\zeta} \\
&-\alpha\Delta\sigma_{isnmdt}\frac{\hat{D}}{4\hat{B}^3}\left(\hat{B}_\psi\frac{\partial\hat{B}}{\partial\theta}-\hat{B}_\theta\frac{\partial\hat{B}}{\partial\hat{\psi}}+2\hat{B}\frac{\partial\hat{B}_\theta}{\partial\hat{\psi}}-2\hat{B}\frac{\partial\hat{B}_\psi}{\partial\theta}\right)\left[\frac{(L+1)L}{(2L-1)(2L+3)}\delta_{L,\ell}+\frac{(L+3)(L+2)(L+1)}{(2L+5)(2L+3)}\delta_{L+2,\ell}-\frac{L(L-1)(L-2)}{(2L-3)(2L-1)}\delta_{L-2,\ell}\right]\frac{\partial\hat{\Phi}_1}{\partial\zeta} \\
&-\sigma_{islmdt}\frac{\Delta\hat{D}\hat{T}_s x_s^2}{2Z_s\hat{B}^3}\left[\sigma_{fzrc}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\frac{\partial\hat{B}}{\partial\hat{\psi}}+\left(\frac{\partial\hat{B}_\psi}{\partial\zeta}-\frac{\partial\hat{B}_\zeta}{\partial\hat{\psi}}\right)\frac{\partial\hat{B}}{\partial\theta}+\left(\frac{\partial\hat{B}_\theta}{\partial\hat{\psi}}-\frac{\partial\hat{B}_\psi}{\partial\theta}\right)\frac{\partial\hat{B}}{\partial\zeta}\right]\left[\frac{(L+1)L}{(2L-1)(2L+3)}\delta_{L,\ell}+\frac{(L+3)(L+2)(L+1)}{(2L+5)(2L+3)}\delta_{L+2,\ell}-\frac{L(L-1)(L-2)}{(2L-3)(2L-1)}\delta_{L-2,\ell}\right].
\end{aligned}
\tag{126}
$$

When the $\dot{x}_s$ term operates on the Maxwellian, we only care about the $\ell = 0$ terms:

$$
\begin{aligned}
\dot{x}_{s,L,\ell} =& \sigma_{itgt}\left[\alpha\Delta\frac{\hat{D}\hat{B}_\zeta x_s}{4\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\theta}\delta_{L,0}-\alpha\Delta\frac{\hat{D}\hat{B}_\theta x_s}{4\hat{B}^2}\frac{\partial\hat{\Phi}_1}{\partial\zeta}\delta_{L,0}\right]\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\hat{\psi}} \\
&-\sigma_{itgt}\Delta\frac{\hat{T}_s x_s^3\hat{D}}{4Z_s\hat{B}^3}\left[\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)+\sigma_{fzrc}2\hat{B}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)\right]\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\hat{\psi}} \\
&-\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left[\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta}-\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)+\sigma_{fzrc}2\hat{B}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta}-\frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)\right]\frac{\partial\langle\hat{\Phi}\rangle}{\partial\hat{\psi}} \\
&-\alpha\frac{Z_s\hat{B}^\theta}{2\sqrt{\hat{T}_s\hat{m}_s}\hat{B}}\delta_{L,1}\frac{\partial\hat{\Phi}_1}{\partial\theta}-\alpha\frac{Z_s\hat{B}^\zeta}{2\sqrt{\hat{T}_s\hat{m}_s}\hat{B}}\delta_{L,1}\frac{\partial\hat{\Phi}_1}{\partial\zeta} \\
&-\sigma_{isnmdt}\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left\{\begin{matrix}\left(\hat{B}_\zeta\frac{\partial\hat{B}}{\partial\hat{\psi}}-\hat{B}_\psi\frac{\partial\hat{B}}{\partial\zeta}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right) \\ +2\hat{B}\left(\frac{\partial\hat{B}_\psi}{\partial\zeta}-\frac{\partial\hat{B}_\zeta}{\partial\hat{\psi}}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)\end{matrix}\right\}\frac{\partial\hat{\Phi}_1}{\partial\theta} \\
&-\sigma_{isnmdt}\alpha\Delta\frac{x_s\hat{D}}{4\hat{B}^3}\left\{\begin{matrix}\left(\hat{B}_\psi\frac{\partial\hat{B}}{\partial\theta}-\hat{B}_\theta\frac{\partial\hat{B}}{\partial\hat{\psi}}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right) \\ +2\hat{B}\left(\frac{\partial\hat{B}_\theta}{\partial\hat{\psi}}-\frac{\partial\hat{B}_\psi}{\partial\theta}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right)\end{matrix}\right\}\frac{\partial\hat{\Phi}_1}{\partial\zeta},
\end{aligned}
\tag{127}
$$

$$
f_{Ms} = \frac{n_s}{\pi^{3/2}\upsilon_s^3}\exp\left(-x_s^2\right), \tag{128}
$$

$$
\hat{f}_{Ms} = \left(\frac{\hat{m}_s}{\hat{T}_s}\right)^{3/2}\frac{\hat{n}_s}{\pi^{3/2}}\exp\left(-x_s^2\right), \tag{129}
$$

$$
\frac{\partial\hat{f}_{Ms}}{\partial x_s} = -2x_s\left(\frac{\hat{m}_s}{\hat{T}_s}\right)^{3/2}\frac{\hat{n}_s}{\pi^{3/2}}\exp\left(-x_s^2\right), \tag{130}
$$

$$\dot{x}_{s,L,\ell} = \frac{\alpha\Delta}{4\hat{\psi}_a \hat{B}^3}\frac{d\hat{\Phi}}{d\psi_N} x_s \left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]\left[\begin{array}{l} \frac{2\left[3L^2+3L-2\right]}{(2L+3)(2L-1)}\delta_{L,\ell} \\ +\frac{L-1}{2L-3}\frac{L}{2L-1}\delta_{L-2,\ell} + \frac{L+2}{2L+5}\frac{L+1}{2L+3}\delta_{L+2,\ell} \end{array}\right], \quad (131)$$

$$Y = -\frac{d\hat{\Phi}}{d\psi_N}\frac{\Delta\alpha}{\hat{\psi}_a \hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right], \quad (132)$$

and

$$\begin{aligned} \dot{\psi}_{s,L} &= -\alpha\Delta\frac{\hat{J}\hat{B}_\zeta}{2\hat{B}^2}\frac{\partial \hat{\Phi}_1}{\partial \theta}\delta_{L,0} + \alpha\Delta\frac{\hat{J}\hat{B}_\theta}{2\hat{B}^2}\frac{\partial \hat{\Phi}_1}{\partial \zeta}\delta_{L,0} \\ &+\frac{\Delta \hat{T}_s x_s^2 \hat{J}}{2Z_s \hat{B}^3}\left(\hat{B}_\theta\frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta\frac{\partial \hat{B}}{\partial \theta}\right)\left(\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right) + \sigma_{fzrc}\Delta\frac{\hat{T}_s x_s^2 \hat{J}}{Z_s \hat{B}^2}\left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta}\right)\left(\frac{1}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right), \end{aligned} \quad (133)$$

$$\begin{aligned} R_{s,L} &= \frac{\Delta \hat{n}_s \hat{T}_s}{2\pi^{3/2}\hat{\psi}_a Z_s \hat{B}^3}\left(\frac{\hat{m}_s}{\hat{T}_s}\right)^{3/2} x_s^2\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right] e^{-x_s^2}\left[\frac{1}{\hat{n}_s}\frac{d\hat{n}_s}{d\psi_N} + \frac{\alpha Z_s}{\hat{T}_s}\frac{d\hat{\Phi}}{d\psi_N} + \left(x_s^2-\frac{3}{2}\right)\frac{1}{\hat{T}_s}\frac{d\hat{T}_s}{d\psi_N}\right]\left[\frac{4}{3}\delta_{L,0}+\frac{2}{3}\delta_{L,2}\right] \\ &+\alpha\frac{\hat{G}+\iota\hat{I}}{\hat{B}}\frac{Z_s}{\hat{T}_s^2}x_s \xi \hat{E}\frac{1}{\left\langle \hat{B}^2\right\rangle}\frac{\hat{n}_s \hat{m}_s}{\pi^{3/2}} e^{-x_s^2}\delta_{L,1} \end{aligned} \quad (134)$$

Collision operator

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

$$C_a = \sum_b C_{ab}\,. \quad (135)$$

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

$$C_{ab} = C_{ab}^L + C_{ab}^E + C_{ab}^F, \quad (136)$$

where the Lorentz part of the collision term is

$$C_{ab}^L = \frac{\nu_{Dab}}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial f_{a1}}{\partial \xi} \quad (137)$$

with

$$\nu_{Dab} = \frac{\Gamma_{ab} n_b}{\upsilon^3}\left[\mathrm{erf}\,(x_b) - \Psi(x_b)\right], \quad (138)$$

$$\Gamma_{ab} = \frac{4\pi Z_a^2 Z_b^2 e^4 \ln\Lambda}{m_a^2}, \quad (139)$$

$$\Psi(x_b) = \frac{\mathrm{erf}\,(x_b) - x_b \mathrm{erf}'(x_b)}{2x_b^2}. \quad (140)$$

The energy scattering contribution is

$$C_{ab}^E = \nu_{\|ab}\left[\frac{\upsilon^2}{2}\frac{\partial^2 f_{a1}}{\partial \upsilon^2} - x_b^2\left(1-\frac{m_a}{m_b}\right)\upsilon\frac{\partial f_{a1}}{\partial \upsilon}\right] + \nu_{Dab}\upsilon\frac{\partial f_{a1}}{\partial \upsilon} + 4\pi\Gamma_{ab}\frac{m_a}{m_b} f_{Mb} f_{a1} \quad (141)$$

where

$$\nu_{\|ab} = 2\frac{\Gamma_{ab} n_b}{\upsilon^3}\Psi\left(x_b\right). \tag{142}$$

The field term is

$$C_{ab}^F = \Gamma_{ab} f_{Ma}\left[\frac{2\upsilon^2}{\upsilon_a^4}\frac{\partial^2 G_{b1}}{\partial \upsilon^2} - \frac{2\upsilon}{\upsilon_a^2}\left(1-\frac{m_a}{m_b}\right)\frac{\partial H_{b1}}{\partial \upsilon} - \frac{2}{\upsilon_a^2}H_{b1} + 4\pi\frac{m_a}{m_b} f_{b1}\right] \tag{143}$$

where the potentials are defined by

$$\nabla_\upsilon^2 H_{b1} = -4\pi f_{b1} \tag{144}$$

and

$$\nabla_\upsilon^2 G_{b1} = 2H_{b1}. \tag{145}$$

We write the field term as

$$C_{ab}^F = C_{ab}^H + C_{ab}^G + C_{ab}^D \tag{146}$$

where

$$C_{ab}^G = \Gamma_{ab} f_{Ma}\frac{2\upsilon^2}{\upsilon_a^4}\frac{\partial^2 G_{b1}}{\partial \upsilon^2} \tag{147}$$

$$C_{ab}^H = \Gamma_{ab} f_{Ma}\left[-\frac{2\upsilon}{\upsilon_a^2}\left(1-\frac{m_a}{m_b}\right)\frac{\partial H_{b1}}{\partial \upsilon} - \frac{2}{\upsilon_a^2}H_{b1}\right] \tag{148}$$

$$C_{ab}^D = \Gamma_{ab} f_{Ma} 4\pi\frac{m_a}{m_b} f_{b1} = \frac{\Gamma_{ab} n_a}{\upsilon_a^3}\exp\left(-x_a^2\right)\frac{4}{\pi^{1/2}}\frac{m_a}{m_b} f_{b1} \tag{149}$$

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

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial H_{b1}}{\partial x_b} - \ell\left(\ell+1\right) H_{b1} = -4\pi\upsilon^2 f_{b1} \tag{150}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial G_{b1}}{\partial x_b} - \ell\left(\ell+1\right) G_{b1} = 2\upsilon^2 H_{b1}. \tag{151}$$

Let us define

$$\hat{H}_{b1} = H_{b1} / \upsilon_b^2 \tag{152}$$

$$\hat{G}_{b1} = G_{b1} / \upsilon_b^4 \tag{153}$$

so the defining equations for the potentials become

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{H}_{b1}}{\partial x_b} - \ell\left(\ell+1\right) \hat{H}_{b1} = -4\pi x_b^2 f_{b1} \tag{154}$$

$$\frac{\partial}{\partial x_b} x_b^2 \frac{\partial \hat{G}_{b1}}{\partial x_b} - \ell\left(\ell+1\right) \hat{G}_{b1} = 2x_b^2 \hat{H}_{b1}. \tag{155}$$

Next, recall that in the kinetic equation (121), we need to evaluate

$$\hat{C}_{ab} = \frac{1}{\bar{\nu}} C_{ab} \tag{156}$$

where $\bar{\nu}$ is defined in (96). It is convenient to note

$$\frac{\Gamma_{ab}}{\bar{\nu}} = \frac{3\sqrt{\pi}}{4}\frac{1}{\bar{n}}\frac{Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\upsilon_a^3 \tag{157}$$

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

$$\hat{C}_{ab}^L = \frac{\hat{\nu}_{Dab}}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial f_{a1}}{\partial\xi} \tag{158}$$

where

$$\hat{\nu}_{Dab} = \frac{3\sqrt{\pi}}{4}\frac{\hat{n}_b Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\frac{1}{x_a^3}\left[\operatorname{erf}\left(x_b\right) - \Psi\left(x_b\right)\right] \tag{159}$$

The energy scattering component is

$$\hat{C}_{ab}^E\left\{f_{a1}\right\} = \frac{3\sqrt{\pi}}{4}\frac{\hat{n}_b Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left[\begin{array}{l} \dfrac{1}{x_a}\Psi\left(x_b\right)\dfrac{\partial^2 f_{a1}}{\partial x_a^2} \\ +\left\{-2\dfrac{\hat{T}_a}{\hat{T}_b}\dfrac{\hat{m}_b}{\hat{m}_a}\Psi\left(x_b\right)\left(1-\dfrac{\hat{m}_a}{\hat{m}_b}\right) + \dfrac{1}{x_a^2}\left[\operatorname{erf}\left(x_b\right) - \Psi\left(x_b\right)\right]\right\}\dfrac{\partial f_{a1}}{\partial x_a} \\ +\dfrac{4}{\sqrt{\pi}}\left(\dfrac{\hat{T}_a}{\hat{T}_b}\right)^{3/2}\left(\dfrac{\hat{m}_b}{\hat{m}_a}\right)^{1/2} e^{-x_b^2} f_{a1} \end{array}\right] \tag{160}$$

The diagonal term is

$$\hat{C}_{ab}^D = 3\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\frac{\hat{m}_a}{\hat{m}_b}\exp\left(-x_a^2\right) f_{b1} \tag{161}$$

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

$$\begin{aligned} \hat{C}_{ab}^G &= \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right)^2 e^{-x_a^2} x_b^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_b^2} \\ &= \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right) e^{-x_a^2} x_a^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_b^2}. \end{aligned} \tag{162}$$

Although in principle we would also be free to write

$$\hat{C}_{ab}^G = \frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\left(\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b}\right)^2 e^{-x_a^2} x_a^2 \frac{\partial^2 \hat{G}_{b1}}{\partial x_a^2} \tag{163}$$

(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

$$\hat{C}_{ab}^H = -\frac{3}{2\pi}\frac{\hat{n}_a Z_a^2 Z_b^2}{\hat{T}_a^{3/2}\hat{m}_a^{1/2}}\frac{\hat{T}_b}{\hat{T}_a}\frac{\hat{m}_a}{\hat{m}_b} e^{-x_a^2}\left[\left(1-\frac{\hat{m}_a}{\hat{m}_b}\right) x_b \frac{\partial \hat{H}_{b1}}{\partial x_b} + \hat{H}_{b1}\right] \tag{164}$$

Radial coordinates

There are many flux surface labels which may be used as radial coordinates. Examples include the toroidal flux (divided by 2π) normalized to the reference values:

$$\hat{\psi} = \psi / \left(\bar{R}\bar{B} \right), \tag{165}$$

the toroidal flux normalized to the flux at the last closed magnetic surface:

$$\psi_N = \psi / \psi_a = \hat{\psi} / \hat{\psi}_a , \tag{166}$$

a normalized effective minor radius:

$$r_N = \sqrt{\psi_N} \tag{167}$$

(where ρ is called `normradius` in the code), and an effective minor radius:

$$\hat{r} = \frac{a}{\bar{R}} \sqrt{\psi_N} = \hat{a}\sqrt{\psi_N} \tag{168}$$

where a is any effective minor radius of the last closed flux surface and

$$\hat{a} = a / \bar{R}. \tag{169}$$

Put another way, there are $2 \times 2 = 4$ main options: the flux or the square root of the flux, normalized either by the "Bar" quantities or normalized by values at the last closed flux surface. The input gradients (i.e. gradients of density, temperature, and electrostatic potential) may be specified as derivatives with respect to any of these 4 radial coordinates; you choose between these options using the parameter gradientInputScheme. Whichever choice you make, sfincs converts all gradients to $d / d\hat{\psi}$ derivatives internally for the main computations. For any quantity X, this conversion is done using

$$\frac{dX}{d\hat{\psi}} = \frac{1}{\hat{\psi}_a} \frac{dX}{d\psi_N}, \tag{170}$$

$$\frac{dX}{d\hat{\psi}} = \frac{1}{2\hat{\psi}_a \sqrt{\psi_N}} \frac{dX}{dr_N}, \tag{171}$$

$$\frac{dX}{d\hat{\psi}} = \frac{\hat{a}}{2\hat{\psi}_a \sqrt{\psi_N}} \frac{dX}{d\hat{r}}. \tag{172}$$

A similar conversion is done for output fluxes. For example, the code first computes the radial particle flux with respect to the coordinate $\hat{\psi}$, i.e. $\left\langle \Gamma \cdot \nabla \hat{\psi} \right\rangle$. Fluxes with respect to other radial coordinates are then computed using

$$\left\langle \Gamma \cdot \nabla \psi_N \right\rangle = \frac{1}{\hat{\psi}_a} \left\langle \Gamma \cdot \nabla \hat{\psi} \right\rangle, \tag{173}$$

$$\left\langle \Gamma \cdot \nabla r_N \right\rangle = \frac{1}{2\hat{\psi}_a \sqrt{\psi_N}} \left\langle \Gamma \cdot \nabla \hat{\psi} \right\rangle, \tag{174}$$

$$\left\langle \Gamma \cdot \nabla \hat{r} \right\rangle = \frac{\hat{a}}{2\hat{\psi}_a \sqrt{\psi_N}} \left\langle \Gamma \cdot \nabla \hat{\psi} \right\rangle. \tag{175}$$

Output quantities

In the definitions below, recall that n_s and T_s are flux functions - the average density and temperature on the flux surface, not the *total* density and temperature.

Flux surface averages:

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

$$\left\langle X \right\rangle = \frac{1}{\hat{V}'}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{X}{\hat{D}} \tag{176}$$

where

$$\texttt{VPrimeHat} = \hat{V}' = \frac{\bar{B}}{\bar{R}} V' = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{D}}. \tag{177}$$

One output quantity we give for convenience is

$$\texttt{FSABHat2} = \left\langle \hat{B}^2 \right\rangle = \frac{1}{\bar{B}^2} \left\langle B^2 \right\rangle. \tag{178}$$

Density

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

$$\texttt{densityPerturbation} = \frac{1}{\bar{n}} \int d^3 \upsilon f_{s1} = 4\pi \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{3/2} \int_0^\infty dx_s x_s^2 \hat{f}_{s,L=0}. \tag{179}$$

We also return the total density

$$\texttt{totalDensity} = \frac{1}{\bar{n}} \int d^3 \upsilon f_s = \hat{n}_s + \left(\texttt{densityPerturbation} \right). \tag{180}$$

Another quantity saved is

$$\begin{aligned} \texttt{FSADensityPerturbation} &= \left\langle \frac{1}{\bar{n}} \int d^3 \upsilon f_{s1} \right\rangle \\ &= \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{\texttt{densityPerturbation}}{\hat{D}} \end{aligned} \tag{181}$$

which should be nearly zero, within roundoff error or so.

Pressure perturbation

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

$$\begin{aligned} \texttt{pressurePerturbation} &= \frac{1}{\bar{n}\bar{T}} \frac{m_s}{3} \int d^3 \upsilon \, \upsilon^2 f_{s1} \\ &= \frac{8\pi \hat{m}_s}{3} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \int_0^\infty dx_s x_s^4 \hat{f}_{s,L=0}. \end{aligned} \tag{182}$$

The total pressure is also saved:

$$\texttt{totalPressure} = \frac{1}{\bar{n}\bar{T}} \frac{m_s}{3} \int d^3 \upsilon \, \upsilon^2 f_s = \hat{n}_s \hat{T}_s + \left(\texttt{pressurePerturbation} \right) \tag{183}$$

Upon flux surface averaging, we obtain

$$\texttt{FSAPressurePerturbation} = \left\langle \frac{1}{\bar{n}\bar{T}} \frac{m_s}{3} \int d^3 v v^2 f_{s1} \right\rangle = \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \, \frac{\texttt{pressurePerturbation}}{\hat{B}^2}. \tag{184}$$

Perhaps I should also save pressures with the velocity shifted by the mean flow?

I could also save temperatures.

Flow

Several quantities related to the parallel fluid flow are available in the output file:

$$\texttt{flow} = \frac{1}{\bar{n}\bar{v}} \int d^3v \, v_{\|} f_s = \frac{4\pi}{3} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^2 \int_0^\infty dx_s x_s^3 \hat{f}_{s,L=1}, \tag{185}$$

$$\texttt{velocityUsingFSADensity} = \frac{1}{\bar{v}} \frac{1}{n_s} \int d^3v \, v_{\|} f_s = \frac{\texttt{flow}}{\hat{n}_s}, \tag{186}$$

$$\texttt{velocityUsingTotalDensity} = \frac{1}{\bar{v}} \frac{\int d^3v \, v_{\|} f_s}{\int d^3v \, f_s} = \frac{\texttt{flow}}{\texttt{totalDensity}}, \tag{187}$$

and

$$\texttt{MachUsingFSAThermalSpeed} = \frac{1}{n_s v_s} \int d^3v \, v_{\|} f_s = \sqrt{\frac{\hat{m}_s}{\hat{T}_s}} \frac{\texttt{flow}}{\hat{n}_s}. \tag{188}$$

I might want to eventually also include the Mach number computed from the local thermal speed.

Both numerical and analytic calculations often employ a weighted average flow, such as $\langle V_{\|} B \rangle$. In SFINCS, we save several variants of this average parallel velocity:

$$\texttt{FSABFlow} = \frac{1}{\bar{v}\bar{B}\bar{n}} \left\langle B \int d^3v \, v_{\|} f_s \right\rangle = \frac{1}{\hat{V}'} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \, \frac{\hat{B}}{\hat{D}} (\texttt{flow}), \tag{189}$$

$$\texttt{FSABVelocityUsingFSADensity} = \frac{1}{\bar{v}\bar{B}} \frac{1}{n_s} \left\langle B \int d^3v \, v_{\|} f_s \right\rangle = \frac{1}{\hat{n}_s} (\texttt{FSABFlow}), \tag{190}$$

$$\texttt{FSABVelocityUsingFSADensityOverB0} = \frac{1}{\bar{v}} \frac{1}{B_0 n_s} \left\langle B \int d^3v \, v_{\|} f_s \right\rangle = \frac{\bar{B}}{B_0} \frac{1}{\hat{n}_s} (\texttt{FSABFlow}), \tag{191}$$

$$\texttt{FSABVelocityUsingFSADensityOverRootFSAB2} = \frac{1}{\bar{v}} \frac{1}{n_s} \frac{\left\langle B \int d^3v \, v_{\|} f_s \right\rangle}{\left\langle B^2 \right\rangle^{1/2}} = \frac{1}{\hat{n}_s} \frac{(\texttt{FSABFlow})}{(\texttt{FSABHat2})^{1/2}}. \tag{192}$$

Parallel current

Closely related to the parallel flow is the parallel current

$$\texttt{jHat} = \frac{\mathbf{j} \cdot \mathbf{b}}{e\bar{n}\bar{v}} = \frac{1}{e\bar{n}\bar{v}} \sum_s Z_s e \int d^3v v_{\|} f_s = \sum_s Z_s (\texttt{flow}). \tag{193}$$

The weighted average parallel current $\langle \mathbf{j} \cdot \mathbf{B} \rangle$ is often considered, and it is available in the code as

$$\texttt{FSABjHat} = \frac{1}{e\bar{n}\bar{\upsilon}\bar{B}}\left\langle B\sum_s Z_s e\int d^3\upsilon\, f_s \upsilon_\| \right\rangle = \sum_s Z_s \left(\texttt{FSABFlow}_s\right). \tag{194}$$

In order to give an average parallel current without the overall scaling by B, we also provide two other related outputs:

$$\texttt{FSABjHatOverB0} = \frac{1}{e\bar{n}\bar{\upsilon}}\frac{1}{B_0}\left\langle B\sum_s Z_s e\int d^3\upsilon\, f_s \upsilon_\| \right\rangle = \frac{\bar{B}}{B_0}\sum_s Z_s \left(\texttt{FSABFlow}_s\right) \tag{195}$$

and

$$\begin{aligned}\texttt{FSABjHatOverRootFSAB2} &= \frac{1}{e\bar{n}\bar{\upsilon}}\frac{\left\langle B\sum_s Z_s e\int d^3\upsilon\, f_s \upsilon_\| \right\rangle}{\left\langle B^2\right\rangle^{1/2}} \\ &= \frac{1}{\left(\texttt{FSABHat2}\right)^{1/2}}\sum_s Z_s \left(\texttt{FSABFlow}_s\right).\end{aligned} \tag{196}$$

General comments on radial fluxes

The radial fluxes have the form

$$\left\langle \mathbf{X}\cdot\nabla Y\right\rangle \tag{197}$$

where Y is a flux surface label. In SFINCS we give fluxes for 4 possible flux surface labels: $\hat{\psi}$, ψ_N, $\hat{r}$, and r_N, indicated by the suffix `_psiHat`, `_psiN`, `_rHat`, or `_rN` to the variable names in the code and in the .h5 output file. Below, we illustrate calculations for the specific case $Y = \hat{\psi}$. (While we give the flux-surface-averaged fluxes with respect to multiple radial coordinates, for the "beforeSurfaceIntegral" versions of the fluxes we only give results for the psiHat radial coordinate.)

For the flux of each quantity (particles, momentum, and energy), and for each radial coordinate, one can compute the flux associated with the leading-order Maxwellian or with the full distribution function. One can also compute the flux associated with the radial magnetic drift, with the radial $\mathbf{E}\times\mathbf{B}$ drift, and with the total $\mathbf{v}_{ds} = \mathbf{v}_{ms} + \mathbf{v}_E$. In SFINCS the following fluxes are recorded, using the particle flux as an example:

Variable name	**Definition, up to normalization**
`particleFlux_vm0_psiHat`	$\left\langle \int d^3\upsilon\, f_{Ms}\mathbf{v}_{ms}\cdot\nabla\hat{\psi}\right\rangle$ i.e. just the Maxwellian. This quantity should be 0 to high precision unless there is a radial current in the magnetic equilibrium.
`particleFlux_vm_psiHat`	$\left\langle \int d^3\upsilon\, f_s\mathbf{v}_{ms}\cdot\nabla\hat{\psi}\right\rangle$ i.e., the full distribution function
`particleFlux_vE0_psiHat`	$\left\langle \int d^3\upsilon\, f_{Ms}\mathbf{v}_{E}\cdot\nabla\hat{\psi}\right\rangle$ i.e. just the Maxwellian. This flux is typically nonzero, unlike `particleFlux_vm0_psiHat`.

particleFlux_vE_psiHat	$\left\langle \int d^3\upsilon f_s \mathbf{v}_E \cdot \nabla\hat{\psi} \right\rangle$ i.e., the full distribution function
particleFlux_vd1_psiHat	particleFlux_vm_psiHat +particleFlux_vE0_psiHat
particleFlux_vd_psiHat	$\left\langle \int d^3\upsilon f_s \mathbf{v}_{ds} \cdot \nabla\hat{\psi} \right\rangle$ i.e., the full distribution function. In a sense this is the most complete radial flux available in sfincs.

When `includePhi1` is false, only the first 2 fluxes in the table are computed.

The rationale for defining `particleFlux_vd1_psiHat` is that (at least for $E_r = 0$) this quantity (computed only when `includePhi1=.true.`) gives the particle flux that would be expected if `includePhi1=.false.`, such as the flux computed in the older versions of sfincs. This relationship is proved in separate notes ?????

For a similar reason, we also define one other version of the heat flux:

For calculating the fluxes below, it is useful to note that from (104) we know

$$\frac{\bar{R}}{\bar{\upsilon}}\mathbf{v}_m \cdot \nabla\hat{\psi} = \frac{\Delta \hat{T}_s x_s^2 \hat{D}}{2Z_s \hat{B}^3}\left[\left(1+\xi^2\right)\left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta}\right) + \sigma_{fzrc} 2\xi^2 \hat{B}\left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta}\right)\right] \tag{198}$$

and

$$\frac{\bar{R}}{\bar{\upsilon}}\mathbf{v}_E \cdot \nabla\hat{\psi} = \alpha\Delta \frac{\hat{D}}{2\hat{B}^2}\left[\hat{B}_\theta \frac{\partial \hat{\Phi}_1}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{\Phi}_1}{\partial \theta}\right]. \tag{199}$$

We will also repeatedly use

$$\int d^3\upsilon X = \bar{\upsilon}^3 \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} 2\pi \int_{-1}^{1} d\xi \int_0^\infty dx_s x_s^2 X \ . \tag{200}$$

Particle fluxes

The contribution to the particle flux from the magnetic drift which we save in SFINCS is defined to be

$$\texttt{particleFlux\_vm\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{\upsilon}}\left\langle \int d^3\upsilon f_s \mathbf{v}_m \cdot \nabla\hat{\psi} \right\rangle. \tag{201}$$

Using (98), (176), (198), and (200), we write (201) as

$$\texttt{particleFlux\_vm\_psiHat} = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \left(\texttt{particleFluxBeforeSurfaceIntegral\_vm}\right) \tag{202}$$

where

$$\texttt{particleFluxBeforeSurfaceIntegral\_vm}$$
$$= \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \frac{1}{\hat{B}^3} \int_{-1}^{1} d\xi \int_0^\infty dx_s x_s^4 \hat{f}_s \left[\left(1+\xi^2\right)\left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta}\right) + \sigma_{fzrc} 2\xi^2 \hat{B}\left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta}\right)\right]. \tag{203}$$

Using (109) and the identities

$$\int_{-1}^{1} d\xi\, P_L(\xi)\left(1+\xi^2\right) = \frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{204}$$

and

$$\int_{-1}^{1} d\xi\, P_L(\xi)\,\xi^2 = \frac{2}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{205}$$

we obtain

$$\begin{aligned}&\texttt{particleFluxBeforeSurfaceIntegral\_vm}\\ &= \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \frac{\pi\Delta\hat{T}_s}{Z_s\hat{V}'}\frac{1}{\hat{B}^3}\left[\left(\hat{B}_\theta\frac{\partial\hat{B}}{\partial\zeta} - \hat{B}_\zeta\frac{\partial\hat{B}}{\partial\theta}\right)\left(\frac{8}{3}\delta_{L,0}+\frac{4}{15}\delta_{L,2}\right) + \sigma_{fzrc}2\hat{B}\left(\frac{\partial\hat{B}_\zeta}{\partial\theta} - \frac{\partial\hat{B}_\theta}{\partial\zeta}\right)\left(\frac{2}{3}\delta_{L,0}+\frac{4}{15}\delta_{L,2}\right)\right]\int_0^\infty dx_s x_s^4\,\hat{f}_{s,L}.\end{aligned} \tag{206}$$

Repeating the last few steps for the radial $\mathbf{E}\times\mathbf{B}$ drift instead of the magnetic drift,

$$\texttt{particleFlux\_vE\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{\upsilon}}\left\langle \int d^3\upsilon\, f_s \mathbf{v}_E\cdot\nabla\hat{\psi}\right\rangle, \tag{207}$$

we find

$$\texttt{particleFlux\_vE\_psiHat} = \int_0^{2\pi}d\theta\int_0^{2\pi}d\zeta\left(\texttt{particleFluxBeforeSurfaceIntegral\_vE}\right) \tag{208}$$

where

$$\begin{aligned}&\texttt{particleFluxBeforeSurfaceIntegral\_vE}\\ &= \frac{2\pi\alpha\Delta}{\hat{V}'}\left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2}\frac{1}{\hat{B}^2}\left[\hat{B}_\theta\frac{\partial\hat{\Phi}_1}{\partial\zeta} - \hat{B}_\zeta\frac{\partial\hat{\Phi}_1}{\partial\theta}\right]\int_0^\infty dx_s x_s^2\,\hat{f}_{s,L=0}.\end{aligned} \tag{209}$$

The quantities `particleFlux_vm_psiHat` and `particleFluxBeforeSurfaceIntegral_vm` in the nonlinear version of SFINCS are equivalent (i.e. normalized in the same way) to the quantities `particleFlux` and `particleFluxBeforeSufaceIntegral` in the linear multispecies version.

Momentum flux

Particle and heat fluxes are usually more important than momentum fluxes, but just in case it ever turns out to be useful, we do compute and save a momentum flux in SFINCS. Since the parallel flow moments are often computed with an extra factor of B in the flux surface average, we do the same here for the momentum fluxes. (This factor of B was not included in previous linear versions of SFINCS!) The momentum flux due to magnetic drifts that we save is

$$\texttt{momentumFlux\_vm\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{\upsilon}^2\bar{B}\bar{m}}\left\langle\int d^3\upsilon\, f_s B m_s \upsilon_\| \mathbf{v}_m\cdot\nabla\hat{\psi}\right\rangle, \tag{210}$$

i.e., compared to the particle flux there is an extra factor of

$$\frac{B\upsilon_\| m_s}{\bar{\upsilon}\bar{B}\bar{m}} = \hat{B}\xi x_s\sqrt{\hat{T}_s\hat{m}_s}\,. \tag{211}$$

Thus, in place of (202)-(203) we have

$$\texttt{momentumFlux\_vm\_psiHat} = \int_0^{2\pi}d\theta\int_0^{2\pi}d\zeta\left(\texttt{momentumFluxBeforeSurfaceIntegral\_vm}\right) \tag{212}$$

where

momentumFluxBeforeSurfaceIntegral_vm

$$= \frac{\hat{T}_s^3}{\hat{m}_s} \frac{\pi\Delta}{Z_s \hat{V}'} \frac{1}{\hat{B}^2} \int_{-1}^{1} d\xi \int_0^\infty dx_s x_s^5 \hat{f}_s \left[\left(\xi + \xi^3\right) \left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} \right) + \sigma_{fzrc} 2\xi^3 \hat{B} \left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta} \right) \right]. \tag{213}$$

(Differences from the particle flux are highlighted in red.) To evaluate the ξ integrals we can use

$$\int_{-1}^{1} d\xi \, P_L(\xi) \xi \left(1+\xi^2\right) = \frac{16}{15}\delta_{L,1} + \frac{4}{35}\delta_{L,3} \tag{214}$$

and

$$\int_{-1}^{1} d\xi \, P_L(\xi) \xi^3 = \frac{2}{5}\delta_{L,1} + \frac{4}{35}\delta_{L,3}, \tag{215}$$

so (213) becomes

momentumFluxBeforeSurfaceIntegral_vm

$$= \frac{\hat{T}_s^3}{\hat{m}_s} \frac{\pi\Delta}{Z_s \hat{V}'} \frac{1}{\hat{B}^2} \int_0^\infty dx_s x_s^5 \hat{f}_s \left[\left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} \right) \left(\frac{16}{15}\delta_{L,1} + \frac{4}{35}\delta_{L,3} \right) + \sigma_{fzrc} 2\hat{B} \left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta} \right) \left(\frac{2}{5}\delta_{L,1} + \frac{4}{35}\delta_{L,3} \right) \right]. \tag{216}$$

Similarly, the contribution to the momentum flux from the radial $\mathbf{E}\times\mathbf{B}$ drift is

$$\texttt{momentumFlux\_vE\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{\upsilon}^2 \bar{B}\bar{m}} \left\langle \int d^3\upsilon \, f_s B m_s \upsilon_\| \mathbf{v}_E \cdot \nabla \hat{\psi} \right\rangle. \tag{217}$$

Furthermore,

$$\texttt{momentumFlux\_vE\_psiHat} = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \left(\texttt{momentumFluxBeforeSurfaceIntegral\_vE} \right) \tag{218}$$

where

momentumFluxBeforeSurfaceIntegral_vE

$$= \frac{2\pi\alpha\Delta}{\hat{V}'} \frac{\hat{T}_s^2}{\hat{m}_s} \frac{1}{\hat{B}^1} \left[\hat{B}_\theta \frac{\partial \hat{\Phi}_1}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{\Phi}_1}{\partial \theta} \right] \int_0^\infty dx_s x_s^3 \hat{f}_{s,L} \left(\delta_{L,1} \frac{2}{3} \right). \tag{219}$$

Heat flux

The contribution to the heat flux from the magnetic drift which we save in SFINCS is defined to be

$$\texttt{heatFlux\_vm\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{m}\bar{\upsilon}^3} \left\langle \int d^3\upsilon \, f_s \frac{m_s \upsilon^2}{2} \mathbf{v}_m \cdot \nabla \hat{\psi} \right\rangle. \tag{220}$$

In other words, there is an extra factor of

$$\frac{1}{\bar{m}\bar{\upsilon}^2} \frac{m_s \upsilon^2}{2} = \frac{\hat{T}_s x_s^2}{2} \tag{221}$$

compared to the particle flux. Thus, instead of (202) and (206) we have

$$\texttt{heatFlux\_vm\_psiHat} = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \left(\texttt{heatFluxBeforeSurfaceIntegral\_vm} \right) \tag{222}$$

and

heatFluxBeforeSurfaceIntegral_vm

$$= \frac{\hat{T}_s}{2} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{3/2} \frac{\pi\Delta\hat{T}_s}{Z_s \hat{V}'} \frac{1}{\hat{B}^3} \left[\left(\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta} \right) \left(\frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \right) + \sigma_{fzrc} 2\hat{B} \left(\frac{\partial \hat{B}_\zeta}{\partial \theta} - \frac{\partial \hat{B}_\theta}{\partial \zeta} \right) \left(\frac{2}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \right) \right] \int_0^\infty dx_s x_s^6 \hat{f}_{s,L}. \tag{223}$$

where differences from the particle flux are given in red. Similarly, the contribution to the radial heat flux from the radial $\mathbf{E}\times\mathbf{B}$ drift is

$$\texttt{heatFlux\_vE\_psiHat} = \frac{\bar{R}}{\bar{n}\bar{m}\bar{\upsilon}^3}\left\langle \int d^3\upsilon\, f_s \frac{m_s \upsilon^2}{2} \mathbf{v}_E \cdot \nabla \hat{\psi} \right\rangle, \tag{224}$$

given by

$$\texttt{heatFlux\_vE\_psiHat} = \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \left(\texttt{heatFluxBeforeSurfaceIntegral\_vE}\right) \tag{225}$$

where

$$\begin{aligned}&\texttt{heatFluxBeforeSurfaceIntegral\_vE}\\ &= \frac{\hat{T}_s}{2}\frac{2\pi\alpha\Delta}{\hat{V}'}\left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2}\frac{1}{\hat{B}^2}\left[\hat{B}_\theta \frac{\partial \hat{\Phi}_1}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{\Phi}_1}{\partial \theta}\right]\int_0^\infty dx_s x_s^4 \hat{f}_{s,L=0}.\end{aligned} \tag{226}$$

The quantities `heatFlux_vm_psiHat` and `heatFluxBeforeSurfaceIntegral_vm` in the nonlinear version of SFINCS are equivalent (i.e. normalized in the same way) to the quantities `heatFlux` and `heatFluxBeforeSufaceIntegral` in the linear multispecies version.

The following expression is useful for evaluating the radial fluxes:

$$\mathbf{v}_{ms} \cdot \nabla \psi = -\bar{\upsilon}\bar{R}\bar{B}\frac{\Delta \hat{T}_s}{2Z_s \hat{B}} x_s^2 \left(1+\xi^2\right)\frac{1}{\hat{G}+\iota \hat{I}}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]. \tag{227}$$

We may write the radial particle flux as

$$\begin{aligned}\left\langle \int d^3\upsilon\, f_{s1} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle &= -\bar{n}\bar{\upsilon}\bar{R}\bar{B}\frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'}\left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2}\frac{1}{\hat{G}+\iota \hat{I}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]\\ &\times \int_{-1}^{1} d\xi \int_0^\infty dx_s \hat{f}_s x_s^4 \left(1+\xi^2\right).\end{aligned} \tag{228}$$

Using

$$\int_{-1}^{1} d\xi\, P_L(\xi)\left(1+\xi^2\right) = \frac{8}{3}\delta_{L,0} + \frac{4}{15}\delta_{L,2} \tag{229}$$

then

$$\left\langle \int d^3\upsilon\, f_{s1} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = \bar{n}\bar{\upsilon}\bar{R}\bar{B}\left(\texttt{particleFlux}\right) \tag{230}$$

where

$$\begin{aligned}\texttt{particleFlux} &= -\frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'}\left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2}\frac{1}{\hat{G}+\iota \hat{I}}\int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3}\left[\hat{G}\frac{\partial \hat{B}}{\partial \theta} - \hat{I}\frac{\partial \hat{B}}{\partial \zeta}\right]\\ &\times \int_0^\infty dx_s x_s^4 \left[\frac{8}{3}\hat{f}_{s,L=0} + \frac{4}{15}\hat{f}_{s,L=2}\right].\end{aligned} \tag{231}$$

Momentum flux

We may write a radial momentum flux as

$$\left\langle \int d^3 \upsilon\, f_{s1} m_s \upsilon_\| \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = -\bar{n}\bar{m}\bar{\upsilon}^2 \bar{R}\bar{B} \frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^2 \frac{\hat{m}_s}{\hat{G}+\iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_{-1}^{1} d\xi \int_0^\infty dx_s\, \hat{f}_s x_s^5 \xi \left(1+\xi^2 \right). \tag{232}$$

Using

$$\int_{-1}^{1} d\xi\, P_L(\xi) \xi \left(1+\xi^2\right) = \frac{16}{15} \delta_{L,1} + \frac{4}{35} \delta_{L,3} \tag{233}$$

then

$$\left\langle \int d^3 \upsilon\, f_{s1} \upsilon_\| \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = \bar{n}\bar{m}\bar{\upsilon}^2 \bar{R}\bar{B} \left(\texttt{momentumFlux} \right) \tag{234}$$

where

$$\texttt{momentumFlux} = -\frac{\pi \Delta \hat{T}_s}{Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^2 \frac{\hat{m}_s}{\hat{G}+\iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_0^\infty dx_s x_s^5 \left[\frac{16}{15} \hat{f}_{s,L=1} + \frac{4}{35} \hat{f}_{s,L=3} \right]. \tag{235}$$

Heat flux

We may write the radial energy flux as

$$\left\langle \int d^3 \upsilon\, f_{s1} \frac{m_s \upsilon^2}{2} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = -\bar{n}\bar{m}\bar{\upsilon}^3 \bar{R}\bar{B} \frac{\pi \Delta \hat{T}_s \hat{m}_s}{2 Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \frac{1}{\hat{G}+\iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_{-1}^{1} d\xi \int_0^\infty dx_s\, \hat{f}_s x_s^6 \left(1+\xi^2 \right). \tag{236}$$

Using (229), then

$$\left\langle \int d^3 \upsilon\, f_{s1} \frac{m_s \upsilon^2}{2} \mathbf{v}_{ms} \cdot \nabla \psi \right\rangle = \bar{n}\bar{m}\bar{\upsilon}^3 \bar{R}\bar{B} \left(\texttt{heatFlux} \right) \tag{237}$$

where

$$\texttt{heatFlux} = -\frac{\pi \Delta \hat{T}_s \hat{m}_s}{2 Z_s \hat{V}'} \left(\frac{\hat{T}_s}{\hat{m}_s} \right)^{5/2} \frac{1}{\hat{G}+\iota \hat{I}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\zeta \frac{1}{\hat{B}^3} \left[\hat{G} \frac{\partial \hat{B}}{\partial \theta} - \hat{I} \frac{\partial \hat{B}}{\partial \zeta} \right] \times \int_0^\infty dx_s\, \hat{f}_s x_s^6 \left[\frac{8}{3} \hat{f}_{s,L=0} + \frac{4}{15} \hat{f}_{s,L=2} \right]. \tag{238}$$

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

$$e\Phi_1 \sum_a \frac{Z_a^2 n_a}{T_a} = \sum_a Z_a \int d^3 \upsilon\, f_{a1}. \tag{239}$$

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

$$\hat{\Phi}_1 = \frac{\sum_a Z_a \frac{1}{n}\int d^3\upsilon f_{a1}}{\alpha \sum_a \frac{Z_a^2 \hat{n}_a}{\hat{T}_a}} = \frac{\sum_a Z_a\left(\texttt{densityPerturbation}\right)}{\alpha \sum_a \frac{Z_a^2 \hat{n}_a}{\hat{T}_a}}. \tag{240}$$

$$\Gamma\cdot\nabla\psi_N = \Gamma\cdot\nabla\hat{\psi}\frac{d\psi_N}{d\hat{\psi}} \tag{241}$$

$$\frac{dX}{d\hat{\psi}} = \frac{d\psi_N}{d\hat{\psi}}\frac{dX}{d\psi_N} \tag{242}$$

Transport matrix

$$\begin{pmatrix} \frac{Ze\left(G+\iota I\right)}{ncTG}\left\langle \int d^3\upsilon f \mathbf{v}_d\cdot\nabla\psi \right\rangle \\ \frac{Ze\left(G+\iota I\right)}{ncTG}\left\langle \int d^3\upsilon f \frac{m\upsilon^2}{2T}\mathbf{v}_d\cdot\nabla\psi \right\rangle \\ \frac{1}{\upsilon_{th}B_0}\left\langle BV_\| \right\rangle \end{pmatrix} = \begin{pmatrix} L_{1,1} & L_{1,2} & L_{1,3} \\ L_{2,1} & L_{2,2} & L_{2,3} \\ L_{3,1} & L_{3,2} & L_{3,3} \end{pmatrix} \begin{pmatrix} \frac{GTc}{ZeB_0\upsilon_{th}}\left[\frac{1}{n}\frac{dn}{d\psi} + \frac{Ze}{T}\frac{d\Phi}{d\psi} - \frac{3}{2}\frac{1}{T}\frac{dT}{d\psi}\right] \\ \frac{GTc}{ZeB_0\upsilon_{th}}\frac{1}{T}\frac{dT}{d\psi} \\ \frac{Ze}{T}\left(G+\iota I\right)\frac{\left\langle E_\| B\right\rangle}{\left\langle B^2\right\rangle} \end{pmatrix}. \tag{243}$$

$$\begin{aligned} L_{11} &= \frac{\frac{Ze\left(G+\iota I\right)}{nTG}\left\langle \int d^3\upsilon f \mathbf{v}_m\cdot\nabla\psi \right\rangle}{\frac{GT}{ZeB_0\upsilon_i}\frac{1}{n}\frac{dn}{d\psi}} \\ &= \frac{4}{\Delta^2}\sqrt{\frac{\hat{T}}{\hat{m}}}\frac{Z^2\left(\hat{G}+\iota\hat{I}\right)}{\hat{T}^2\hat{G}^2\frac{d\hat{n}}{d\hat{\psi}}}\frac{B_0}{\bar{B}}\left(\texttt{particleFlux\_vm\_psiHat}\right) \end{aligned} \tag{244}\backslash$$

$$\begin{aligned} L_{12} &= \frac{\frac{Ze\left(G+\iota I\right)}{ncTG}\left\langle \int d^3\upsilon f \mathbf{v}_d\cdot\nabla\psi \right\rangle}{\frac{GTc}{ZeB_0\upsilon_{th}}\frac{1}{T}\frac{dT}{d\psi}} \\ &= \frac{4}{\Delta^2}\sqrt{\frac{\hat{T}}{\hat{m}}}\frac{Z^2\left(\hat{G}+\iota\hat{I}\right)}{\hat{n}\hat{G}^2\hat{T}\frac{d\hat{T}}{d\hat{\psi}}}\frac{B_0}{\bar{B}}\left(\texttt{particleFlux\_vm\_psiHat}\right) \end{aligned} \tag{245}$$

$$L_{13} = \frac{1}{\hat{E}}\frac{1}{\alpha\Delta}\frac{2\left\langle \hat{B}^2\right\rangle}{\hat{n}\hat{G}}\left(\texttt{particleFlux\_vm\_psiHat}\right) \tag{246}$$

$$L_{21} = \frac{8}{\Delta^2}\sqrt{\frac{\hat{T}}{\hat{m}}}\frac{Z^2\left(\hat{G}+\iota\hat{I}\right)}{\hat{T}^3\hat{G}^2\frac{d\hat{n}}{d\hat{\psi}}}\frac{B_0}{\overline{B}}\left(\texttt{heatFlux\_vm\_psiHat}\right) \tag{247}$$

$$L_{22} = \frac{8}{\Delta^2}\sqrt{\frac{\hat{T}}{\hat{m}}}\frac{Z^2\left(\hat{G}+\iota\hat{I}\right)}{\hat{n}\hat{T}^2\hat{G}^2\frac{d\hat{T}}{d\hat{\psi}}}\frac{B_0}{\overline{B}}\left(\texttt{heatFlux\_vm\_psiHat}\right) \tag{248}$$

$$L_{23} = \frac{4}{\alpha\Delta}\frac{\left\langle \hat{B}^2\right\rangle}{\hat{E}}\frac{1}{\hat{n}\hat{G}\hat{T}}\left(\texttt{heatFlux\_vm\_psiHat}\right) \tag{249}$$

$$L_{31} = \frac{2Z}{\Delta\hat{T}\hat{G}\frac{d\hat{n}}{d\hat{\psi}}}\left(\texttt{FSABFlow}\right) \tag{250}$$

$$L_{32} = \frac{2Z}{\Delta\hat{n}\hat{G}\frac{d\hat{T}}{d\hat{\psi}}}\left(\texttt{FSABFlow}\right) \tag{251}$$

$$L_{33} = \frac{\frac{1}{\upsilon_{th}B_0}\left\langle BV_\parallel\right\rangle}{\frac{Ze}{T}\left(G+\iota I\right)\frac{\left\langle E_\parallel B\right\rangle}{\left\langle B^2\right\rangle}} = \frac{1}{\hat{E}}\sqrt{\frac{\hat{m}}{\hat{T}}}\frac{\hat{T}\left\langle \hat{B}^2\right\rangle}{\alpha Z\left(\hat{G}+\iota\hat{I}\right)\hat{n}}\frac{\overline{B}}{B_0}\left(\texttt{FSABFlow}\right) \tag{252}$$