Implementation of Φ_1 in SFINCS

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EUTERPE old equations vs new equations

We want to modify the implementation of the old EUTERPE equations [1] in SFINCS to the new equations [2].

The old equations for the particle trajectories and the drift-kinetic equation are

$$\dot{\boldsymbol{R}} = v_\| \boldsymbol{b} - \frac{\nabla\Phi_0 \times \boldsymbol{b}}{B} \tag{1}$$

$$\dot{v}_\| = -\frac{q}{m}\boldsymbol{b}\cdot\nabla\Phi_1 - \mu\boldsymbol{b}\cdot\nabla B - \frac{v_\|}{B^2}\left(\boldsymbol{b}\times\nabla B\right)\cdot\nabla\Phi_0 \tag{2}$$

$$\dot{\mu} = 0 \tag{3}$$

and

$$\frac{\partial f_1}{\partial t} + \dot{\boldsymbol{R}}\cdot\nabla f_1 + \dot{v}_\| \frac{\partial f_1}{\partial v_\|} - C =$$
$$= -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right](\boldsymbol{v}_d + \boldsymbol{v}_{E1})\cdot\nabla\psi - \frac{q}{m}\frac{f_M}{v_{\rm th}^2}\left(v_\|\boldsymbol{b} + \boldsymbol{v}_d\right)\cdot\left(\nabla\Phi_0 + \nabla\Phi_1\right). \tag{4}$$

The new equations are

$$\dot{\boldsymbol{R}} = v_\| \boldsymbol{b} - \frac{\nabla\Phi_0 \times \boldsymbol{b}}{B} \tag{5}$$

$$\dot{v}_\| = -\frac{q}{m}\boldsymbol{b}\cdot\nabla\Phi_1 - \mu\boldsymbol{b}\cdot\nabla B - \frac{v_\|}{B^2}\left(\boldsymbol{b}\times\nabla B\right)\cdot\nabla\Phi_0 \tag{6}$$

$$\dot{\mu} = 0 \tag{7}$$

and

$$\frac{\partial f_1}{\partial t} + \dot{\boldsymbol{R}}\cdot\nabla f_1 + \dot{v}_\| \frac{\partial f_1}{\partial v_\|} - C =$$
$$= -f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right](\boldsymbol{v}_d + \boldsymbol{v}_{E1})\cdot\nabla\psi. \tag{8}$$

Here we have the definitions

$$\Phi(\psi,\theta,\varphi) \equiv \Phi_0(\psi) + \Phi_1(\theta,\varphi), \tag{9}$$

$$\boldsymbol{v}_d = \frac{m}{q}\frac{\mu B + v_\parallel^2}{B^2}\boldsymbol{b}\times\nabla B, \tag{10}$$

$$\boldsymbol{v}_{E1} = -\frac{\nabla\Phi_1\times\boldsymbol{b}}{B}, \tag{11}$$

$$f_0 = f_M \exp(-q\Phi_1/T) = \frac{n_0(\psi)}{(2\pi)^{3/2} v_{\mathrm{th}}^3}\exp\left[-\frac{\left(v_\parallel^2 + v_\perp^2\right)}{2v_{\mathrm{th}}^2}\right]\exp(-q\Phi_1/T), \tag{12}$$

$q = Ze$ and $v_{\mathrm{th}}^2 = T/m$.

The only differences appear in the RHS:s of Eqs. 4 and 8:
Firstly, f_M has been replaced by f_0 containing the $\exp(-q\Phi_1/T)$ factor.
Secondly, some of the terms have been modified. We rewrite the RHS of 8:

$$\begin{aligned}
\mathrm{RHS}_{\mathrm{NEW}} = &-f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right](\boldsymbol{v}_d + \boldsymbol{v}_{E1})\cdot\nabla\psi = \\
= &-f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right](\boldsymbol{v}_d + \boldsymbol{v}_{E1})\cdot\nabla\psi + \\
&- f_0\frac{q}{T}\Phi_1\frac{1}{T}\frac{\partial T}{\partial\psi}(\boldsymbol{v}_d + \boldsymbol{v}_{E1})\cdot\nabla\psi = \\
= &-f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_d\cdot\nabla\psi + \\
&- f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_{E1}\cdot\nabla\psi - f_0\frac{q}{T}\frac{\partial\Phi_0}{\partial\psi}\boldsymbol{v}_{E1}\cdot\nabla\psi + \\
&- f_0\frac{q}{T}\Phi_1\frac{\nabla T}{T}\cdot(\boldsymbol{v}_d + \boldsymbol{v}_{E1}) = \\
= &-f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_d\cdot\nabla\psi + \\
&{\color{blue}-f_0\left[\frac{1}{n}\frac{\partial n}{\partial\psi} + \left(\frac{mv^2}{2T} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_{E1}\cdot\nabla\psi +} \\
&{\color{red}-f_0\frac{q}{T}\left[\nabla\Phi_0\cdot\boldsymbol{v}_{E1} + \Phi_1\frac{\nabla T}{T}\cdot\boldsymbol{v}_d + \Phi_1\frac{\nabla T}{T}\cdot\boldsymbol{v}_{E1}\right]}.
\end{aligned} \tag{13}$$

Similarly, the RHS of 4 is rewritten as:

$$\begin{aligned}\mathrm{RHS}_{\mathrm{OLD}} &= -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi}+\left(\frac{mv^2}{2T}-\frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right](\boldsymbol{v}_d+\boldsymbol{v}_{E1})\cdot\nabla\psi-\frac{q}{m}\frac{f_M}{v_{\mathrm{th}}^2}\left(v_\parallel\boldsymbol{b}+\boldsymbol{v}_d\right)\cdot(\nabla\Phi_0+\nabla\Phi_1)= \\ &= -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi}+\frac{q}{T}\frac{\partial\Phi_0}{\partial\psi}+\left(\frac{mv^2}{2T}-\frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_d\cdot\nabla\psi+ \\ &\quad -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi}+\left(\frac{mv^2}{2T}-\frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_{E1}\cdot\nabla\psi+ \\ &\quad -f_M\frac{q}{T}\left[v_\parallel\boldsymbol{b}\cdot\nabla\Phi_1+\boldsymbol{v}_d\cdot\nabla\Phi_1\right]. \end{aligned}\tag{14}$$

Comparing $\mathrm{RHS}_{\mathrm{NEW}}$ to $\mathrm{RHS}_{\mathrm{OLD}}$ we see that, apart from $f_M\to f_0$, only the terms in red have changed.

What has to be changed in SFINCS

The only part of the drift-kinetic equation block we need to modify is the RHS, where we need to update the red terms and substitute $f_M\to f_0$. SFINCS had earlier neglected the $\boldsymbol{v}_d\cdot\nabla\Phi_1$-term which is small in the standard ρ_*-expansion. The RHS that was implemented is (see Matt's ISHW poster, also note that $\boldsymbol{v}_E\cdot\nabla\psi=\boldsymbol{v}_{E1}\cdot\nabla\psi$)

$$\begin{aligned}\mathrm{RHS}_{\mathrm{SFINCS,OLD}} &= -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi}+\frac{q}{T}\frac{\partial\Phi_0}{\partial\psi}+\left(\frac{mv^2}{2T}-\frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_d\cdot\nabla\psi+ \\ &\quad -f_M\left[\frac{1}{n}\frac{\partial n}{\partial\psi}+\left(\frac{mv^2}{2T}-\frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial\psi}\right]\boldsymbol{v}_E\cdot\nabla\psi-f_M\frac{q}{T}v_\parallel\boldsymbol{b}\cdot\nabla\Phi_1.\end{aligned}\tag{15}$$

We thus replace

$$v_\parallel\boldsymbol{b}\cdot\nabla\Phi_1\tag{16}$$

with

$$\nabla\Phi_0\cdot\boldsymbol{v}_E+\Phi_1\frac{\nabla T}{T}\cdot\boldsymbol{v}_d+\Phi_1\frac{\nabla T}{T}\cdot\boldsymbol{v}_E,\tag{17}$$

and make the substitution

$$f_M\to f_0=f_M\exp\left(-q\Phi_1/T\right).\tag{18}$$

All terms which contain Φ_1 are now nonlinear. It does not make sense to have both switches **includePhi1** and **nonlinear** still available in SFINCS, and consequently we will remove the **nonlinear** switch.

We will also introduce to possibility to run SFINCS with an adiabatic species.

Implementation in SFINCS

Of the equations implemented in SFINCS [4], the only two we need to modify are the kinetic equation

$$R\left(f_1,\Phi_1\right) = K\left\{\theta\right\}\frac{\partial f}{\partial \theta} + K\left\{\zeta\right\}\frac{\partial f}{\partial \zeta} + K\left\{x\right\}\frac{\partial f}{\partial x} + K\left\{\xi\right\}\frac{\partial f}{\partial \xi} + K\left\{\psi\right\}\frac{\partial f_M}{\partial \psi} + \\ - C\left\{f\right\} - S_1 f_M - S_2 f_M x^2 - \frac{Zev}{T}x\xi\frac{\langle \boldsymbol{E}\cdot\boldsymbol{B}\rangle B}{\langle B^2\rangle}f_M = 0 \quad (19)$$

and the quasineutrality equation

$$\sum_s Z_s \int d^3v\, f_s + \lambda = 0. \quad (20)$$

Here $x = v/v_s = v/\sqrt{2T/m}$ and $\xi = v_\parallel/v$.

In the implementation we need to rewrite all our equations into SFINCS units, using the following identities:
$m = \hat{m}\bar{m}$, $n = \hat{n}\bar{n}$, $T = \hat{T}\bar{T}$, $\Phi = \hat{\Phi}\bar{\Phi}$, $B = \hat{B}\bar{B}$, $B_\zeta = \bar{R}\bar{B}\hat{B}_\zeta$, $B_\theta = \bar{R}\bar{B}\hat{B}_\theta$, $D = \bar{B}\hat{D}/\bar{R}$, $\bar{v} = \sqrt{2\bar{T}/\bar{m}}$, $\alpha = e\bar{\Phi}/\bar{T}$, $\Delta = \bar{m}\bar{v}/\left(e\bar{B}\bar{R}\right)$, $\dfrac{dX}{d\psi} = \dfrac{1}{\hat{\psi}_a\bar{R}^2\bar{B}}\dfrac{dX}{d\psi_N}$ and $\alpha\cdot\Delta = \dfrac{e\bar{\Phi}}{\bar{T}}\cdot\dfrac{\bar{m}\bar{v}}{e\bar{B}\bar{R}} = \dfrac{2^{1/2}\bar{m}^{1/2}\bar{\Phi}}{\bar{B}\bar{R}\bar{T}^{1/2}}$. Furthermore, we note that the kinetic equation is made dimensionless by multiplying with the factor

$$\frac{\bar{v}^3}{\bar{n}}\frac{\bar{R}}{\bar{v}} = \frac{2\bar{T}\bar{R}}{\bar{m}\bar{n}}. \quad (21)$$

Newton's method

In each iteration step we want to calculate the residual and Jacobian of $R\left(\boldsymbol{X}\right) = 0$ with $\boldsymbol{X} = \left(f_1,\Phi_1\right)$. The residual is R itself, and the Jacobian is $R' = \dfrac{\delta R\left(\boldsymbol{X}\right)}{\delta \boldsymbol{X}}$. The state-vector is updated as

$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n - \frac{R\left(\boldsymbol{X}_n\right)}{R'\left(\boldsymbol{X}_n\right)}. \quad (22)$$

Drift-kinetic equation

For the residual $R(f_1, \Phi_1)$ the only term in the kinetic equation we need to modify is the one in yellow in Eq. 19. We replace $f_M \to f_0 = f_M \exp(-q\Phi_1/T)$, and use that $K\{\psi\} = \boldsymbol{v}_E \cdot \nabla\psi + \boldsymbol{v}_d \cdot \nabla\psi = \boldsymbol{v}_{E1} \cdot \nabla\psi + \boldsymbol{v}_d \cdot \nabla\psi$ to write

$$\begin{aligned}
K\{\psi\}\frac{\partial f_M}{\partial \psi} &= \exp(-q\Phi_1/T)\frac{\partial f_M}{\partial \psi}\left(\boldsymbol{v}_{E1} \cdot \nabla\psi + \boldsymbol{v}_d \cdot \nabla\psi\right) = \\
&= \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right]\left(-\frac{\nabla\Phi_1 \times \boldsymbol{b}}{B} \cdot \nabla\psi + \boldsymbol{v}_d \cdot \nabla\psi\right) = \\
&= \left\| -\frac{\nabla\Phi_1 \times \boldsymbol{b}}{B} \cdot \nabla\psi = -\frac{\boldsymbol{B} \times \nabla\psi}{B^2} \cdot \nabla\Phi_1 = \frac{1}{B^2} D\left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right] \right\| = \\
&= \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \cdot \\
&\qquad \left(\frac{1}{B^2} D\left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right] + \boldsymbol{v}_d \cdot \nabla\psi\right)
\end{aligned} \tag{23}$$

(Here $D = \nabla\psi \cdot \nabla\theta \times \nabla\zeta$.) Written like this we explicitly see the places where Φ_1 appears in $K\{\psi\}\frac{\partial f_M}{\partial \psi}$. From Eq. 23 we obtain the corresponing terms in the Jacobian matrix

$$\begin{aligned}
\frac{\delta}{\delta\Phi_1}\left(K\{\psi\}\frac{\partial f_M}{\partial \psi}\right) &= -\frac{q}{T}\exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \cdot \\
&\qquad \left(\frac{1}{B^2} D\left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right] + \boldsymbol{v}_d \cdot \nabla\psi\right) + \\
&+ \exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\frac{1}{T}\frac{\partial T}{\partial \psi}\left(\frac{1}{B^2} D\left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right] + \boldsymbol{v}_d \cdot \nabla\psi\right) + \\
&+ \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \cdot \\
&\qquad \left(\frac{1}{B^2} D\left[B_\theta \frac{\partial}{\partial \zeta} - B_\zeta \frac{\partial}{\partial \theta}\right]\right)
\end{aligned} \tag{24}$$

Residual

Many of the terms involving $\boldsymbol{v}_d \cdot \nabla\psi$ are almost implemented in SFINCS already except that they now contain the $\exp\left(-\frac{q\Phi_1}{T}\right)$-factor. We therefore rewrite Eq. 23 as

$$K\{\psi\}\frac{\partial f_M}{\partial \psi} = R_m + R_E \tag{25}$$

where

$$R_m = \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right]\boldsymbol{v}_d \cdot \nabla\psi \tag{26}$$

and

$$R_E = \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(\frac{mv^2}{2T} - \frac{3}{2} + \frac{q}{T}\Phi_1\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \frac{1}{B^2} D \left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right]. \tag{27}$$

$\boldsymbol{R_m}$

R_m will be implemented in evaluateResidual.F90. We write the term as

$$R_m = \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi} + \left(x^2 - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \boldsymbol{v}_d \cdot \nabla \psi + \\ + \exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1 \frac{1}{T}\frac{\partial T}{\partial \psi} \boldsymbol{v}_d \cdot \nabla \psi. \tag{28}$$

Note that the first term in Eq. 28 can only be implemented in evaluateResidual.F90, since it is not of the form $L[\Phi_1]$ where $L[]$ is a linear operator.
The first term in Eq. 28 is already implemented in evaluateResidual.F90 except for the factor

$$\exp\left(-\frac{q\Phi_1}{T}\right) = \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right)$$

which has to be added.
The second term in Eq. 28 we rewrite in SFINCS units (also considering the factor Eq. 21) as

$$\left(\exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1 \frac{1}{T}\frac{\partial T}{\partial \psi} \boldsymbol{v}_d \cdot \nabla \psi\right)_{\text{SFINCS}} = \\ = \frac{\alpha\Delta}{3\pi^{3/2}} \frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{5/2}\hat{B}^3\hat{\psi}_a} \hat{\Phi}_1 \frac{\partial \hat{T}}{\partial \psi_N} x^2 \left(P_2(\xi) + 2\right) \exp\left(-x^2\right) \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right) \left[\hat{B}_\theta \frac{\partial \hat{B}}{\partial \zeta} - \hat{B}_\zeta \frac{\partial \hat{B}}{\partial \theta}\right]. \tag{29}$$

$\boldsymbol{R_E}$

R_E we will instead implement in populateMatrix.F90. We write the term as

$$R_E = \exp\left(-\frac{q\Phi_1}{T}\right) f_M \left[\frac{1}{n}\frac{\partial n}{\partial \psi} + \left(x^2 - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial \psi}\right] \frac{1}{B^2} D \left[B_\theta \frac{\partial}{\partial \zeta} - B_\zeta \frac{\partial}{\partial \theta}\right] \Phi_1 + \\ + \exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\frac{\partial \Phi_0}{\partial \psi}\frac{1}{B^2} D \left[B_\theta \frac{\partial}{\partial \zeta} - B_\zeta \frac{\partial}{\partial \theta}\right] \Phi_1 + \\ + \exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1 \frac{1}{T}\frac{\partial T}{\partial \psi}\frac{1}{B^2} D \left[B_\theta \frac{\partial}{\partial \zeta} - B_\zeta \frac{\partial}{\partial \theta}\right] \Phi_1. \tag{30}$$

Note that in the code when evaluating the residual, the matrix added in populateMatrix.F90 is multiplied by the state-vector in evaluateResidual.F90 and therefore the right-most Φ_1 should not be added inside populateMatrix.F90.

The first term in Eq. 30 is already implemented in populateMatrix.F90 except for the factor

$$\exp\left(-\frac{q\Phi_1}{T}\right) = \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right)$$

which has to be added.
The second term in Eq. 30 we rewrite in SFINCS units (also considering the factor Eq. 21) as

$$\begin{aligned}\left(\exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\frac{\partial\Phi_0}{\partial\psi}\frac{1}{B^2} D\left[B_\theta\frac{\partial\Phi_1}{\partial\zeta} - B_\zeta\frac{\partial\Phi_1}{\partial\theta}\right]\right)_{\text{SFINCS}} &= \\ = \frac{Z\alpha^2\Delta}{2\pi^{3/2}}\frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{5/2}\hat{B}^2\hat{\psi}_a}\frac{\partial\hat{\Phi}_0}{\partial\psi_N}\exp\left(-x^2\right)\exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right)\left[\hat{B}_\theta\frac{\partial}{\partial\zeta} - \hat{B}_\zeta\frac{\partial}{\partial\theta}\right]\hat{\Phi}_1.\end{aligned} \tag{31}$$

The third term in Eq. 30 we rewrite in SFINCS units (also considering the factor Eq. 21) as

$$\begin{aligned}\left(\exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1\frac{1}{T}\frac{\partial T}{\partial\psi}\frac{1}{B^2} D\left[B_\theta\frac{\partial\Phi_1}{\partial\zeta} - B_\zeta\frac{\partial\Phi_1}{\partial\theta}\right]\right)_{\text{SFINCS}} &= \\ = \frac{Z\alpha^2\Delta}{2\pi^{3/2}}\frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{7/2}\hat{B}^2\hat{\psi}_a}\frac{\partial\hat{T}}{\partial\psi_N}\hat{\Phi}_1\exp\left(-x^2\right)\exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right)\left[\hat{B}_\theta\frac{\partial}{\partial\zeta} - \hat{B}_\zeta\frac{\partial}{\partial\theta}\right]\hat{\Phi}_1.\end{aligned} \tag{32}$$

Files to change:

Jacobian

The Jacobian terms will be implemented in populateMatrix.F90. In the code we use SFINCS units, and the Jacobian is calculated from taking the derivative of the residual in SFINCS units with respect to the state-vector in SFINCS units (also considering the factor Eq. 21). This implies that what we are calculating here is

$$\frac{\delta}{\delta\hat{\Phi}_1}\left(\hat{R}_m + \hat{R}_E\right),$$

where $\hat{R}_m$ and $\hat{R}_E$ are how the components of the residual are written in SFINCS.
We see that the last term in the Jacobian in Eq. 24 corresponds to R_E in Eq. 27 (since the rightmost Φ_1 in the residual is not implemented in populateMatrix.F90), so this term is already implemented by the residual.

The other two terms should only be added when 'whichMatrix==0' or 'whichMatrix==1'.
The first term in the Jacobian is the residual multiplied by $-q/T$. However, since the exponential is $\exp\left(-\frac{q\Phi_1}{T}\right) = \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right)$, in SFINCS the term will be implemented as

$$-\frac{Z\alpha}{\hat{T}}\left(\hat{R}_m + \hat{R}_E\right). \tag{33}$$

The second term in the Jacobian can be written as

$$\exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\frac{1}{T}\frac{\partial T}{\partial \psi}\left(\frac{1}{B^2}D\left[B_\theta \frac{\partial \Phi_1}{\partial \zeta} - B_\zeta \frac{\partial \Phi_1}{\partial \theta}\right] + \boldsymbol{v}_d \cdot \nabla\psi\right) =$$
$$= \frac{1}{\Phi_1}\left(\exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1 \frac{1}{T}\frac{\partial T}{\partial \psi}\frac{1}{B^2}D\left[B_\theta \frac{\partial}{\partial \zeta} - B_\zeta \frac{\partial}{\partial \theta}\right]\Phi_1 + \exp\left(-\frac{q\Phi_1}{T}\right) f_M \frac{q}{T}\Phi_1 \frac{1}{T}\frac{\partial T}{\partial \psi}\boldsymbol{v}_d \cdot \nabla\psi\right), \tag{34}$$

where the two terms inside the brackets have already been implemented in R_E and R_m respectively. Consequently, to obtain this term we sum these two terms written in code units, and multiply by $1/\hat{\Phi}_1$.
Although the first term and the second term of the Jacobian consist of terms available in other terms, we need to rewrite them since we cannot access code in evaluateResidual.F90 from populateMatrix.F90, and also the residual terms in populateMatrix.F90 contain a factor Φ_1 less which instead is in the state-vector.

Files to change:

Additional implementation related to the kinetic equation

Besides implementing the above terms, we need to remove the former term in SFINCS corresponding to $\frac{Ze}{T} f_M v_\parallel \nabla_\parallel \Phi_1$.

We will remove the **nonlinear** switch from the code, since all terms related to Φ_1 are now nonlinear.

Files to change:

Quasi-neutrality equation

In EUTERPE Φ_1 is calculated from quasi-neutrality by expanding the exponential, assuming adiabatic electrons and neglecting the impurities. However, this is not a generic quasi-neutrality equation and in SFINCS we can easily implement the full equation. To be able to compare to results from EUTERPE we will allow for both possibilities in the code, and implement an adiabatic species. The option **quasineutralityOption = 1** corresponds to the full quasi-neutrality equation and is the default, whereas **quasineutralityOption = 2** corresponds to the EUTERPE equations.

Adiabatic species

We will allow for the possibility to run SFINCS with an adiabatic species. The following input parameters will be introduced (with their default value in brackets) in the **speciesParameters** namelist:

```
logical :: withAdiabatic  (.false.)
PetscScalar :: adiabaticZ  (-1)
PetscScalar :: adiabaticMHat  (5.446170214E-4)
PetscScalar :: adiabaticNHat  (1.0)
PetscScalar :: adiabaticTHat  (1.0)
```

Files to change:

```
globalVariables.F90
populateMatrix.F90
readInput.F90
sfincs.F90
validateInput.F90
writeHDF5Output.F90
```

Full quasi-neutrality equation, quasineutralityOption = 1

Firstly, we need to make sure that the input densities fulfill quasi-neutrality (also considering the adiabatic species if it is used):

$$\sum_s Z_s \hat{n}_s = 0. \tag{35}$$

The densities can be written

$$n_s = n_{s0}(\psi) \exp\left(-q_s \Phi_1 / T_s\right) + n_{s1}, \tag{36}$$

and the quasi-neutrality equation is

$$\sum_s Z_s n_s = 0. \tag{37}$$

For an adiabatic species a

$$n_{a1} = 0.$$

The velocity integration in SFINCS is done in $(x, \xi) = \left(v/v_s, v_\parallel/v\right)$, and

$$\int d^3v = 2\pi v_s^3 \int_0^\infty dx\, x^2 \int_{-1}^1 d\xi \tag{38}$$

where $v_s = \sqrt{2T_s/m_S}$. Since

$$n_{s1} = \int d^3v\, f_{s1}, \tag{39}$$

we can rewrite quasi-neutrality in form of its contribution to the residual as

$$R_{QN}\left(f_{s1}, \Phi_1\right) = \sum_s Z_s n_{s0} \exp\left(-\frac{Z_s e \Phi_1}{T_s}\right) + 2\pi \sum_{s\backslash a} v_s^3 Z_s \int_0^\infty dx\, x^2 \int_{-1}^1 d\xi\, f_{s1} = 0 \tag{40}$$

(note that the adiabatic species is excluded in the second summation).

In SFINCS we add a Lagrange multiplier λ, divide Eq. 40 by $\bar{n}$, and use $n = \hat{n}\bar{n}$, $\bar{v} = \sqrt{2\bar{T}/\bar{m}}$, $v_s/\bar{v} = \sqrt{\hat{T}_s/\hat{m}_s}$, $f_s = \bar{n}\hat{f}_s/\bar{v}^3$, $\exp\left(-\frac{q_s\Phi_1}{T_s}\right) = \exp\left(-\frac{Z_s\alpha\hat{\Phi}_1}{\hat{T}_s}\right)$, to write

$$\hat{R}_{QN}\left(\hat{f}_{s1}, \hat{\Phi}_1, \lambda\right) = \sum_s Z_s \hat{n}_{s0} \exp\left(-\frac{Z_s\alpha\hat{\Phi}_1}{\hat{T}_s}\right) + \\ + 2\pi \sum_{s\backslash a} Z_s \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \int_0^\infty dx\, x^2 \int_{-1}^1 d\xi\, \hat{f}_{s1} + \lambda = 0. \tag{41}$$

The first term in Eq. 41 must be implemented in evaluateResidual.F90 because it does not include a linear operation on $\hat{\Phi}_1$. The other terms will be implemented in populateMatrix.F90.

When implementing the Jacobian terms, we note that

$$\frac{\delta \hat{R}_{QN}}{\delta \hat{f}_{s1}} = 2\pi Z_s \left(\frac{\hat{T}_s}{\hat{m}_s}\right)^{3/2} \int_0^\infty dx\, x^2 \int_{-1}^1 d\xi, \tag{42}$$

$$\frac{\delta \hat{R}_{QN}}{\delta \lambda} = 1, \tag{43}$$

which means that these two terms are the same as the corresponding terms in the residual and are thus implemented in populateMatrix.F90. Moreover,

$$\frac{\delta \hat{R}_{QN}}{\delta \hat{\Phi}_1} = \sum_s -\frac{Z_s^2\alpha}{\hat{T}_s} \hat{n}_{s0} \exp\left(-\frac{Z_s\alpha\hat{\Phi}_1}{\hat{T}_s}\right) \tag{44}$$

will also be implemented in populateMatrix.F90 when 'whichMatrix==0' or 'whichMatrix==1'.

Files to change:

EUTERPE quasi-neutrality equation, quasineutralityOption = 2

EUTERPE equations:

$$n_s = n_{s0}\left(\psi\right)\,\exp\left(-q_s\Phi_1/T_s\right) + n_{s1}, \tag{45}$$

$$\sum_s Z_s n_s = 0, \tag{46}$$

$$\Rightarrow \quad 0 \simeq \sum_s Z_s\left[n_{s0}\left(1 - q_s\Phi_1/T_s\right) + n_{s1}\right] \quad \Leftrightarrow$$

$$\sum_s Z_s\left[n_{s0} + n_{s1}\right] = \sum_s \frac{Z_s^2 e}{T_s}\Phi_1 n_{s0}.$$

Since $n_{s0}\left(\psi\right)$ is obtained by integrating the Maxwellian f_{Ms} over velocity space we must have

$$\sum_s Z_s n_{s0} = 0,$$

which yields

$$\sum_s Z_s n_{s1} - \Phi_1 \sum_s \frac{Z_s^2 e}{T_s} n_{s0} = 0. \tag{47}$$

With kinetic ions, adiabatic electrons ($n_{e1} = 0$) and neglecting impurities we obtain

$$\Phi_1 = \frac{T_e}{e}\left[\frac{T_e}{T_i}n_{i0} + n_{e0}\right]^{-1} n_{i1}. \tag{48}$$

We need to make sure that the adiabatic species and only one kinetic species are used, and that the input densities fulfill quasi-neutrality:

$$Z_i\hat{n}_i + Z_e\hat{n}_e = 0 \tag{49}$$

(Here species i would be the kinetic species and e the adiabatic).

Implementation in SFINCS

For a first benchmark, we want to implement the same equations as EUTERPE in SFINCS.
In the code we add an adiabatic species which only enters into the quasi-neutrality equation, and neglect its collisional impact on the kinetic species (the effect of ion-electron collisions is small compared to ion-ion collisions). Moreover, we will only consider the first of the kinetic species in quasi-neutrality and neglect the rest. This is implemented by modifying the LHS of the row corresponding to quasi-neutrality in the block-matrix structure of Matt's ISHW poster, adding the adiabatic term to the Φ_1-column and removing all kinetic species except the first.
The equation we will implement in SFINCS is thus

$$Z_i n_{i1} - \Phi_1\left[\frac{Z_i^2 e}{T_i}n_{i0} + \frac{Z_e^2 e}{T_e}n_{e0}\right] = 0. \tag{50}$$

We note that

$$n_s = n_{s0}(\psi)\exp\left(-q_s\Phi_1/T_s\right) + n_{s1} = \int d^3v f_{Ms}\exp\left(-q_s\Phi_1/T_s\right) + \int d^3v f_{1s} = \\ = d^3v f_{0s} + d^3v f_{1s}. \quad (51)$$

The velocity integration is SFINCS is done in $(x,\xi) = \left(v/v_s, v_\parallel/v\right)$, and

$$\int d^3v = 2\pi v_s^3 \int_0^\infty dx\, x^2 \int_{-1}^1 d\xi \quad (52)$$

(note that $v_s^2 = 2T_s/m_s$ differs from Jose's notation $v_{\mathrm{th}}^2 = T/m$). Using SFINCS normalizations $n_s = \bar{n}\hat{n}_s$, $T_s = \bar{T}\hat{T}_s$, $v_s/\bar{v} = \sqrt{\hat{T}_s/\hat{m}_s}$, $f_s = \bar{n}\hat{f}_s/\bar{v}^3$, we find

$$\hat{n}_s = 2\pi\left(\hat{T}_s/\hat{m}_s\right)^{3/2}\int_0^\infty dx\, x^2 \int_{-1}^1 d\xi \hat{f}_s. \quad (53)$$

Also using $\Phi_1 = \bar{\Phi}\hat{\Phi}_1$ and $\alpha = e\bar{\Phi}/\bar{T}$ we can write Eq. 50

$$Z_i\hat{n}_{i1} - \alpha\hat{\Phi}_1\left[\frac{Z_i^2}{\hat{T}_i}\hat{n}_{i0} + \frac{Z_e^2}{\hat{T}_e}\hat{n}_{e0}\right] = 0 \quad (54)$$

and finally obtain

$$\left[2\pi Z_i\left(\hat{T}_i/\hat{m}_i\right)^{3/2}\int_0^\infty dx\, x^2\int_{-1}^1 d\xi \hat{f}_{i1}\right] - \alpha\hat{\Phi}_1\left[\frac{Z_i^2}{\hat{T}_i}\hat{n}_{i0} + \frac{Z_e^2}{\hat{T}_e}\hat{n}_{e0}\right] = 0. \quad (55)$$

This is the equation we will implement in the code, but adding a λ to make the system square.

Additional changes

Decide which output fluxes should be possible to obtain, i.e. which combinations of

$$\langle \int d^3v \, f \boldsymbol{v} \cdot \nabla X \rangle, \tag{56}$$

should be possible? Here f can be f_0, f_1 or $f_0 + f_1$. $\boldsymbol{v}$ can be $\boldsymbol{v}_E$, $\boldsymbol{v}_m$ or $\boldsymbol{v}_E + \boldsymbol{v}_m$. X can be any of the radial coordinates, r, r_N, ψ or ψ_N.

Allow for the output fluxes in SI units.

Files to change:

`diagnostics.F90`

Appendix A. Check of Matt's former implementation of $\frac{Ze}{T} f_M v_\parallel \nabla_\parallel \Phi_1$

This section is only to compare to what has already been implemented in SFINCS, to see that we understand the normalizations.

Looking at Matt's ISHW poster, since Φ_1 is an unknown this term is in the LHS of the square block matrix system. The term is accessed by "rowIndex = BLOCK_F" and "colIndex = BLOCK_QN". We use

$$\nabla_\parallel \Phi_1 = \boldsymbol{b} \cdot \nabla \Phi_1 = \frac{1}{B}\left[B^\theta \frac{\partial \Phi_1}{\partial \theta} + B^\zeta \frac{\partial \Phi_1}{\partial \zeta}\right] = \frac{\bar{\Phi}}{\hat{B}\bar{R}}\left[\hat{B}^\theta \frac{\partial \hat{\Phi}_1}{\partial \theta} + \hat{B}^\zeta \frac{\partial \hat{\Phi}_1}{\partial \zeta}\right],$$

$$f_M = n_0(\psi) \frac{m^{3/2}}{(2\pi T)^{3/2}} \exp\left[-\frac{v^2}{v_s^2}\right] = \hat{n}\bar{n} \frac{\hat{m}^{3/2}}{\left(2\pi\hat{T}\right)^{3/2}} \left(\frac{\bar{m}}{\bar{T}}\right)^{3/2} \exp\left[-x^2\right],$$

$v_\parallel = v_s x \xi = v_s x P_1 = x P_1 \sqrt{2\hat{T}/\hat{m}}\sqrt{\bar{T}/\bar{m}}$ and $x = v/v_s$. With $\alpha = e\bar{\Phi}/\bar{T}$ we obtain

$$\begin{aligned}\frac{Ze}{T} f_M v_\parallel \nabla_\parallel \Phi_1 &= \frac{Ze}{\hat{T}\bar{T}} \hat{n}\bar{n} \frac{\hat{m}^{3/2}}{\left(2\pi\hat{T}\right)^{3/2}} \left(\frac{\bar{m}}{\bar{T}}\right)^{3/2} \exp\left[-x^2\right]\, x P_1 \sqrt{2\hat{T}/\hat{m}}\sqrt{\bar{T}/\bar{m}}\, \frac{\bar{\Phi}}{\hat{B}\bar{R}}\left[\hat{B}^\theta \frac{\partial \hat{\Phi}_1}{\partial \theta} + \hat{B}^\zeta \frac{\partial \hat{\Phi}_1}{\partial \zeta}\right] = \\ &= \frac{Z\alpha}{2\pi^{3/2}} x P_1 \exp\left[-x^2\right]\, \frac{\hat{n}\hat{m}}{\hat{B}\hat{T}^2}\, \frac{\bar{n}\bar{m}}{\bar{R}\bar{T}}\left[\hat{B}^\theta \frac{\partial}{\partial \theta} + \hat{B}^\zeta \frac{\partial}{\partial \zeta}\right]\hat{\Phi}_1. \qquad (57)\end{aligned}$$

In SFINCS the kinetic equation is made dimensionless by multiplying with

$$\frac{\bar{v}^3 \bar{R}}{\bar{n}\bar{v}} = \frac{2\bar{T}\bar{R}}{\bar{m}\bar{n}},$$

which implies that the RHS of Eq. 57 becomes

$$\frac{Z\alpha}{\pi^{3/2}} x P_1 \exp\left[-x^2\right]\, \frac{\hat{n}\hat{m}}{\hat{B}\hat{T}^2}\left[\hat{B}^\theta \frac{\partial}{\partial \theta} + \hat{B}^\zeta \frac{\partial}{\partial \zeta}\right]\hat{\Phi}_1 \qquad (58)$$

in the implementation.

Appendix B. Temporary page

Implementation of $f_0 \dfrac{q}{T} \nabla \Phi_0 \cdot \boldsymbol{v}_{E1}$

$$\begin{aligned}
&\left(f_0 \frac{q}{T} \nabla \Phi_0 \cdot \boldsymbol{v}_{E1}\right)_{\text{SFINCS}} = \\
&\qquad = \frac{Z\alpha^2\Delta}{2\pi^{3/2}} \frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{5/2}\hat{B}^2\hat{\psi}_a} \frac{\partial\hat{\Phi}_0}{\partial\psi_N} \exp\left(-x^2\right) \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right) \left[\hat{B}_\theta \frac{\partial}{\partial\zeta} - \hat{B}_\zeta \frac{\partial}{\partial\theta}\right] \hat{\Phi}_1
\end{aligned} \tag{59}$$

Implementation of $f_0 \dfrac{q}{T} \Phi_1 \dfrac{\nabla T}{T} \cdot \boldsymbol{v}_d$

$$\begin{aligned}
&\left(f_0 \frac{q}{T} \Phi_1 \frac{\nabla T}{T} \cdot \boldsymbol{v}_d\right)_{\text{SFINCS}} = \\
&= \frac{\alpha\Delta}{3\pi^{3/2}} \frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{5/2}\hat{B}^3\hat{\psi}_a} \hat{\Phi}_1 \frac{\partial\hat{T}}{\partial\psi_N} x^2 \left(P_2\left(\xi\right) + 2\right) \exp\left(-x^2\right) \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right) \left[\hat{B}_\theta \frac{\partial\hat{B}}{\partial\zeta} - \hat{B}_\zeta \frac{\partial\hat{B}}{\partial\theta}\right]
\end{aligned} \tag{60}$$

Implementation of $f_0 \dfrac{q}{T} \Phi_1 \dfrac{\nabla T}{T} \cdot \boldsymbol{v}_{E1}$

$$\begin{aligned}
&\left(f_0 \frac{q}{T} \Phi_1 \frac{\nabla T}{T} \cdot \boldsymbol{v}_{E1}\right)_{\text{SFINCS}} = \\
&\qquad = \frac{Z\alpha^2\Delta}{2\pi^{3/2}} \frac{\hat{n}\hat{m}^{3/2}\hat{D}}{\hat{T}^{7/2}\hat{B}^2\hat{\psi}_a} \frac{\partial\hat{T}}{\partial\psi_N} \hat{\Phi}_1 \exp\left(-x^2\right) \exp\left(-\frac{Z\alpha\hat{\Phi}_1}{\hat{T}}\right) \left[\hat{B}_\theta \frac{\partial}{\partial\zeta} - \hat{B}_\zeta \frac{\partial}{\partial\theta}\right] \hat{\Phi}_1
\end{aligned} \tag{61}$$

References

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[4] M. Landreman, *Technical Documentation for version 3 of SFINCS* (2014).