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

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

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

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

and

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

The new equations are

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

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

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

and

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

Here we have the definitions

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

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

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

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

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

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Firstly, f_M has been replaced by f_0 containing the $\exp\left(-q\Phi_1/T\right)$ factor.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

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

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.

Implementation 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

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

REMARK: In EUTERPE Φ_1 is only an unknown in the quasi-neutrality equation, in the kinetic equation it is an input which means that there are no nonlinearities. It also means that the exponential in f_0 is not expanded in the kinetic equation. Are all terms in Eq. 17 feasible to implement in SFINCS? E.g. is it a problem that the $\Phi_1\frac{\nabla T}{T}\cdot\boldsymbol{v}_E$-term contains 3 factors with Φ_1?

REMARK: Because of f_0 it seems as all terms which contain Φ_1 are now nonlinear. Does it make sense to have both switches includePhi1 and nonlinear available in SFINCS?

Quasi-neutrality equation

In EUTERPE Φ_1 is calculated from quasi-neutrality by expanding the exponential, assuming adiabatic electrons and neglecting the impurities:

$$n_s = n_{s0}(\psi)\exp(-q_s\Phi_1/T_s) + n_{s1}, \tag{19}$$

$$\sum_s Z_s n_s = 0, \tag{20}$$

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

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

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

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

which yields

$$\sum_s Z_s n_{s1} - \Phi_1 \sum_s \frac{Z_s^2 e}{T_s} n_{s0} = 0. \tag{21}$$

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

$$\Phi_1 = \frac{T_e}{e}\left[\frac{T_e}{T_i}n_{i0} + n_{e0}\right]^{-1} n_{i1}. \tag{22}$$

Implementation in SFINCS

For a first benchmark, we want to implement the same equations as EUTERPE in SFINCS.

REMARK: This is not a very generic quasi-neutrality equation so it is possible that we might want to change it in SFINCS later.

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.

REMARK: It feels a bit weird to remove species from quasi-neutrality, even if the impurity density is small. Does this mean that we should removed the check that the input densities are quasi-neutral and instead check that $n_{i0}(\psi) = n_{e0}(\psi)$ in the input?

The equation we will implement in SFINCS is thus

$$Z_i n_{i1} - \Phi_1\left[\frac{Z_i^2 e}{T_i}n_{i0} + \frac{Z_e^2 e}{T_e}n_{e0}\right] = 0. \tag{23}$$

We note that

$$n_s = n_{s0}(\psi)\, \exp\left(-q_s \Phi_1 / T_s\right) + n_{s1} = \int d^3 v f_{Ms} \exp\left(-q_s \Phi_1 / T_s\right) + \int d^3 v f_{1s} = \\ = d^3 v f_{0s} + d^3 v f_{1s}. \quad (24)$$

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

$$\int d^3 v = 2\pi v_s^3 \int_0^\infty dx\, x^2 \int_{-1}^{1} d\xi \quad (25)$$

(note that $v_s^2 = 2T_s/m_s$ differs from Jose's notation $v_{\rm th}^2 = T/m$). 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

$$\hat{n}_s = 2\pi \left(\hat{T}_s/\hat{m}_s\right)^{3/2} \int_0^\infty dx\, x^2 \int_{-1}^{1} d\xi \hat{f}_s. \quad (26)$$

Also using $\Phi_1 = \bar{\Phi}\hat{\Phi}_1$ and $\alpha = e\bar{\Phi}/\bar{T}$ we can write Eq. 23

$$Z_i \hat{n}_{i1} - \alpha\hat{\Phi}_1 \left[\frac{Z_i^2}{\hat{T}_i}\hat{n}_{i0} + \frac{Z_e^2}{\hat{T}_e}\hat{n}_{e0}\right] = 0 \quad (27)$$

and finally obtain

$$\left[2\pi Z_i \left(\hat{T}_i/\hat{m}_i\right)^{3/2} \int_0^\infty dx\, x^2 \int_{-1}^{1} d\xi \hat{f}_{i1}\right] - \alpha\hat{\Phi}_1 \left[\frac{Z_i^2}{\hat{T}_i}\hat{n}_{i0} + \frac{Z_e^2}{\hat{T}_e}\hat{n}_{e0}\right] = 0. \quad (28)$$

This is the equation we will implement in the code, but adding a λ to make the system square.
REMARK: Is the 2π factor correct in Eq. 28? It is not in the former implementation of quasi-neutrality, but in that situation it could be divided away.

References

[1] J. M. García-Regaña, R. Kleiber, C. D. Beidler, Y. Turkin, H. Maaßberg and P. Helander, *Plasma Phys. Control. Fusion* **55** (2013) 074008.

[2] J. M. García-Regaña, C. D. Beidler, Y. Turkin, R. Kleiber, P. Helander, H. Maaßberg, J. A. Alonso and J. L. Velasco, *arXiv:1501.03967* (2015).

[3] Landreman M, Smith H M, Mollén A and Helander P 2014 *Phys. Plasmas* **21** 042503