

Notes on DKES

First let us introduce some DKES notation. The perturbed distribution function is written as

$$f_1 = \left[\frac{mv}{q} (A_{1,\text{DKES}} + K A_{2,\text{DKES}}) \hat{f}_1 + A_{3,\text{DKES}} \hat{f}_3 \right] f_M \quad (1)$$

and the functions \hat{f}_i satisfy

$$(\tilde{C} - \tilde{V}) \hat{f}_i = S_i, \quad (2)$$

for $i = 1$ and $i = 3$. The pitch-angle diffusion operator is defined as

$$\tilde{C} = \frac{\sqrt{g}}{v} C = \text{CMUL} \sqrt{g} \frac{1}{2} \frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial}{\partial \xi}, \quad (3)$$

and the Vlasov operator as

$$\tilde{V} = \frac{\sqrt{g}}{v} V = \quad (4)$$

$$= \frac{\xi}{B} \frac{d\Psi}{d\rho} \left(\iota \frac{\partial}{\partial \theta} + \frac{\partial}{\partial \zeta} \right) + \quad (5)$$

$$+ \frac{1}{2} (1 - \xi^2) \frac{d\Psi}{d\rho} \left(\iota \frac{\partial B^{-1}}{\partial \theta} + \frac{\partial B^{-1}}{\partial \zeta} \right) \frac{\partial}{\partial \xi} + \quad (6)$$

$$- \text{EFIELD} \ll B^{-2} \gg \left[G \frac{\partial}{\partial \theta} - I \frac{\partial}{\partial \zeta} \right], \quad (7)$$

where

$$S_1 = -\frac{1 + \xi^2}{2B^3} \left[G \frac{\partial B}{\partial \theta} - I \frac{\partial B}{\partial \zeta} \right], \quad (8)$$

$$S_3 = \xi \sqrt{g} B, \quad (9)$$

$$\sqrt{g} = \frac{d\Psi}{d\rho} \frac{G + \iota I}{B^2}, \quad (10)$$

$$\text{CMUL} = \frac{\nu}{v}, \quad (11)$$

$$\text{EFIELD} = -\frac{1}{v} \frac{d\Phi_0}{d\rho}, \quad (12)$$

$$\ll \cdot \gg = \int_0^{2\pi} \int_0^{2\pi} \cdot d\theta d\zeta. \quad (13)$$

The quantity ρ is the flux surface label used in defining the thermodynamic forces

$$A_{1,\text{DKES}} = \frac{d \ln n}{d\rho} - \frac{3}{2} \frac{d \ln T}{d\rho} + \frac{q}{T} \frac{d\Phi_0}{d\rho} \quad (14)$$

$$A_{2,\text{DKES}} = \frac{d \ln T}{d\rho} \quad (15)$$

$$A_{3,\text{DKES}} = -\frac{q}{T} \frac{\langle \mathbf{E} \cdot \mathbf{B} \rangle}{\langle B^2 \rangle}. \quad (16)$$

Normally, we use $\rho = a\sqrt{\Psi/\Psi_a}$ in the DKES calculations, and if the r used in Beidler et al. (2011) is equal to ρ we get $d\rho/dr = 1$.

The output from DKES stored in the .dk files is the three diffusion coefficients

$$\hat{\Gamma}_{ij} = \left\langle \frac{1}{\sqrt{g}} \int_{-1}^1 d\xi S_i \hat{f}_j \right\rangle. \quad (17)$$

For practical reasons, the .dk files are always produced with the input equilibrium magnetic field scaled so that the $(0, 0)$ component $\bar{B}_0 = 1$ T. To indicate that the magnetic fields are the scaled ones used in the DKES calculation, in this section we mark all magnetic fields with an overbar.

We want to relate $\hat{\Gamma}_{ij}$ to the D_{ij}^* coefficients defined in Beidler et al. (2011). In Beidler et al. (2011) the perturbed distribution function is written as

$$f_1 = R_0 \bar{B}_0 A_{3,\text{DKES}} \hat{f}_{\text{I}} f_{\text{M}} + \frac{mv}{2q\bar{B}_0} \frac{d\rho}{dr} (A_{1,\text{DKES}} + K A_{2,\text{DKES}}) \hat{f}_{\text{II}} f_{\text{M}}, \quad (18)$$

so that eq. (1) gives us

$$\hat{f}_{\text{II}} = 2\bar{B}_0 \frac{dr}{d\rho} \hat{f}_1, \quad (19)$$

$$\hat{f}_{\text{I}} = \frac{1}{R_0 \bar{B}_0} \hat{f}_3. \quad (20)$$

Beidler et al. (2011) also defines

$$\frac{dr}{dt} = \frac{mv^2(1+\xi^2)}{2q\bar{B}^3} (\bar{\mathbf{B}} \times \nabla \bar{B}) \cdot \nabla r = \frac{mv^2}{q} \frac{dr}{d\rho} \left(-\frac{1+\xi^2}{2\bar{B}^3\sqrt{g}} \right) \left[\bar{G} \frac{\partial \bar{B}}{\partial \theta} - \bar{I} \frac{\partial \bar{B}}{\partial \zeta} \right], \quad (21)$$

and $v_d = mv^2/2qR_0\bar{B}_0$, so that

$$\frac{1}{v_d} \frac{dr}{dt} = 2R_0 \bar{B}_0 \frac{dr}{d\rho} \left(-\frac{1+\xi^2}{2\bar{B}^3\sqrt{g}} \right) \left[\bar{G} \frac{\partial \bar{B}}{\partial \theta} - \bar{I} \frac{\partial \bar{B}}{\partial \zeta} \right] \quad (22)$$

. The coefficient D_{11}^* is defined in Beidler et al. (2011) as

$$D_{11}^* = \frac{4}{\pi} \frac{v\iota}{v_d^2 R_0} \left(-\frac{v_d^2 R_0}{2v} \right) \left\langle \int_{-1}^1 d\xi \frac{1}{v_d} \frac{dr}{dt} \hat{f}_{\text{II}} \right\rangle = \quad (23)$$

$$= -\frac{2\iota}{\pi} 2R_0 \bar{B}_0 \frac{dr}{d\rho} 2\bar{B}_0 \frac{dr}{d\rho} \left\langle \int_{-1}^1 d\xi \left(-\frac{1+\xi^2}{2\bar{B}^3\sqrt{g}} \right) \left[\bar{G} \frac{\partial \bar{B}}{\partial \theta} - \bar{I} \frac{\partial \bar{B}}{\partial \zeta} \right] \hat{f}_1 \right\rangle = \quad (24)$$

$$= -\frac{8\iota}{\pi} R_0 \bar{B}_0^2 \left(\frac{dr}{d\rho} \right)^2 \hat{\Gamma}_{11}. \quad (25)$$

The coefficient D_{31}^* is defined as

$$D_{31}^* = \frac{3}{2 \cdot 1.46} \frac{\iota \sqrt{\epsilon_t}}{v_d R_0} \left(-\frac{v_d R_0}{2} \right) \left\langle \int_{-1}^1 d\xi \xi \frac{\bar{B}}{B_0} \hat{f}_{II} \right\rangle = \quad (26)$$

$$= -\frac{3\iota \sqrt{\epsilon_t}}{4 \cdot 1.46} 2\bar{B}_0 \frac{dr}{d\rho} \frac{1}{B_0} \left\langle \frac{1}{\sqrt{g}} \int_{-1}^1 d\xi \xi \sqrt{g} \bar{B} \hat{f}_I \right\rangle = \quad (27)$$

$$= -\frac{3\iota \sqrt{\epsilon_t}}{2 \cdot 1.46} \frac{dr}{d\rho} \hat{\Gamma}_{31}. \quad (28)$$

The coefficient D_{33}^* is defined as

$$D_{33}^* = \frac{3\nu}{v^2} \frac{\bar{B}_0^2}{\langle \bar{B}^2 \rangle} \left(-\frac{v R_0}{2} \right) \left\langle \int_{-1}^1 d\xi \xi \frac{\bar{B}}{B_0} \hat{f}_I \right\rangle = \quad (29)$$

$$= -\frac{3\nu}{2v} \frac{\bar{B}_0^2 R_0}{\langle \bar{B}^2 \rangle} \frac{1}{B_0^2 R_0} \left\langle \frac{1}{\sqrt{g}} \int_{-1}^1 d\xi \xi \sqrt{g} \bar{B} \hat{f}_3 \right\rangle = \quad (30)$$

$$= -\frac{3\nu}{2v} \frac{1}{\langle \bar{B}^2 \rangle} \hat{\Gamma}_{33}. \quad (31)$$

Notes on DKES – SFINCS comparison

After having translated the DKES code outputs to the normalised mono-energetic transport coefficients D_{11}^*, D_{31}^* and D_{33}^* , we can relate these to the coefficients D_{ij} and $\hat{\Gamma}_{ij}$ by (assuming $dr/d\rho = 1$)

$$D_{11} = D_{11}^* \frac{\pi}{4} \frac{R_0}{v\iota} \left(\frac{mv^2}{2qR_0 B_0} \right)^2 = D_{11}^* \frac{\pi}{16} \frac{m^2 v^3}{\iota R_0 B_0^2 q^2} = -\frac{m^2 v^3}{2q^2} \frac{\bar{B}_0^2}{B_0^2} \hat{\Gamma}_{11}, \quad (32)$$

$$D_{31} = D_{31}^* 1.46 \frac{2}{3} \frac{R_0}{\iota \sqrt{\epsilon_t}} \frac{mv^2}{2qR_0 B_0} = D_{31}^* \frac{1.46}{3} \frac{mv^2}{q B_0 \iota \sqrt{\epsilon_t}} = -\frac{mv^2}{2q B_0} \hat{\Gamma}_{31}, \quad (33)$$

$$D_{33} = D_{33}^* \frac{v^2}{3\nu} \frac{\langle B^2 \rangle}{B_0^2} = -\frac{v}{2\bar{B}_0^2} \hat{\Gamma}_{33}. \quad (34)$$

Note that magnetic fields without overbar here and in the following denotes the actual field and not the scaled one as in the previous section.

Performing the integral on page 3 in Beidler et al. (2011), we obtain

$$L_{11}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{11}(K) = \frac{\pi}{16} \frac{m^2 v_T^3}{\iota R_0 B_0^2 q^2} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K^2 e^{-K} D_{11}^*(K)}_{I_{11}^*} \quad (35)$$

$$L_{12}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K \sqrt{K} e^{-K} D_{12}(K) = \frac{\pi}{16} \frac{m^2 v_T^3}{\iota R_0 B_0^2 q^2} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K^3 e^{-K} D_{11}^*(K)}_{I_{12}^*} \quad (36)$$

$$L_{22}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K^2 \sqrt{K} e^{-K} D_{22}(K) = \frac{\pi}{16} \frac{m^2 v_T^3}{\iota R_0 B_0^2 q^2} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K^4 e^{-K} D_{11}^*(K)}_{I_{22}^*} \quad (37)$$

$$L_{31}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{31}(K) = \frac{1.46}{3} \frac{m v_T^2}{q B_0 \iota \sqrt{\epsilon_t}} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K^{3/2} e^{-K} D_{31}^*(K)}_{I_{31}^*} \quad (38)$$

$$L_{32}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K \sqrt{K} e^{-K} D_{32}(K) = \frac{1.46}{3} \frac{m v_T^2}{q B_0 \iota \sqrt{\epsilon_t}} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K^{5/2} e^{-K} D_{31}^*(K)}_{I_{32}^*} \quad (39)$$

$$L_{33}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{33}(K) = \frac{v_T}{3} \frac{\langle B^2 \rangle}{B_0^2} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K e^{-K} \left(\frac{v}{\nu} D_{33}^*(K) \right)}_{I_{33}^*} \quad (40)$$

In the last integral, $\frac{v}{\nu} D_{33}^*(K)$ is grouped together because this is the quantity most directly related to the DKES outputs. Alternatively, we can express L_{ij}^B directly in the DKES output quantities,

$$L_{11}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{11}(K) = -\frac{m^2 v_T^3}{2q^2} \frac{\bar{B}_0^2}{B_0^2} \hat{I}_{11} \quad (41)$$

$$L_{12}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K \sqrt{K} e^{-K} D_{12}(K) = -\frac{m^2 v_T^3}{2q^2} \frac{\bar{B}_0^2}{B_0^2} \hat{I}_{12} \quad (42)$$

$$L_{22}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K^2 \sqrt{K} e^{-K} D_{22}(K) = -\frac{m^2 v_T^3}{2q^2} \frac{\bar{B}_0^2}{B_0^2} \hat{I}_{22} \quad (43)$$

$$L_{31}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{31}(K) = -\frac{m v_T^2}{2q B_0} \hat{I}_{31} \quad (44)$$

$$L_{32}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK K \sqrt{K} e^{-K} D_{32}(K) = -\frac{m v_T^2}{2q B_0} \hat{I}_{32} \quad (45)$$

$$L_{33}^B = \frac{2}{\sqrt{\pi}} \int_0^\infty dK \sqrt{K} e^{-K} D_{33}(K) = -\frac{v_T}{2\bar{B}_0^2} \underbrace{\frac{2}{\sqrt{\pi}} \int_0^\infty dK K e^{-K} \hat{\Gamma}_{33}(K)}_{\hat{I}_{33}} \quad (46)$$

where \hat{I}_{ij} are defined analogously to I_{ij}^* with $D_{ij}^*(K)$ replaced by $\hat{\Gamma}_{ij}(K)$.

Following Matt's notes, we can calculate the Sfincs matrix elements as

$$L_{11}^S = - \left(\frac{d\Psi}{dr} \right)^2 \frac{q^2 B_0 v_T (G + \iota I)}{(m v_T^2 / 2)^2 G^2} L_{11}^B = - \frac{\pi}{4} \left(\frac{d\Psi}{dr} \right)^2 \frac{G + \iota I}{G^2 \iota R_0 B_0} I_{11}^* = \left(\frac{d\Psi}{dr} \right)^2 \frac{2 \bar{B}_0^2 (G + \iota I)}{B_0 G^2} \hat{I}_{11} \quad (47)$$

$$L_{21}^S = L_{12}^S = - \frac{\pi}{4} \left(\frac{d\Psi}{dr} \right)^2 \frac{G + \iota I}{G^2 \iota R_0 B_0} I_{12}^* = \left(\frac{d\Psi}{dr} \right)^2 \frac{2 \bar{B}_0^2 (G + \iota I)}{B_0 G^2} \hat{I}_{12} \quad (48)$$

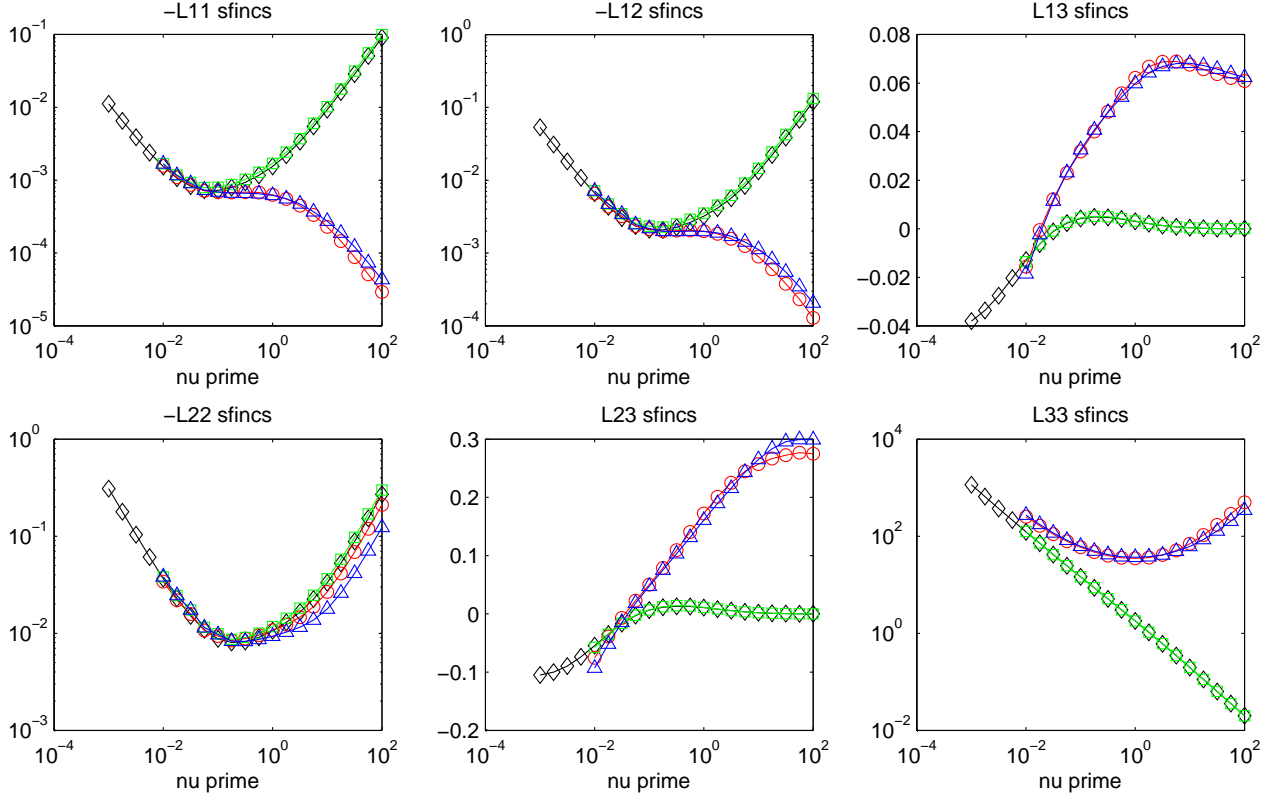
$$L_{22}^S = - \frac{\pi}{4} \left(\frac{d\Psi}{dr} \right)^2 \frac{G + \iota I}{G^2 \iota R_0 B_0} I_{22}^* = \left(\frac{d\Psi}{dr} \right)^2 \frac{2 \bar{B}_0^2 (G + \iota I)}{B_0 G^2} \hat{I}_{22} \quad (49)$$

$$L_{13}^S = L_{31}^S = - \frac{2q B_0}{m v_T^2 G} \frac{d\Psi}{dr} L_{31}^B = - \frac{1.46}{3} \frac{2}{\iota G \sqrt{\epsilon_t}} \frac{d\Psi}{dr} I_{31}^* = \frac{1}{G} \frac{d\Psi}{dr} \hat{I}_{31} \quad (50)$$

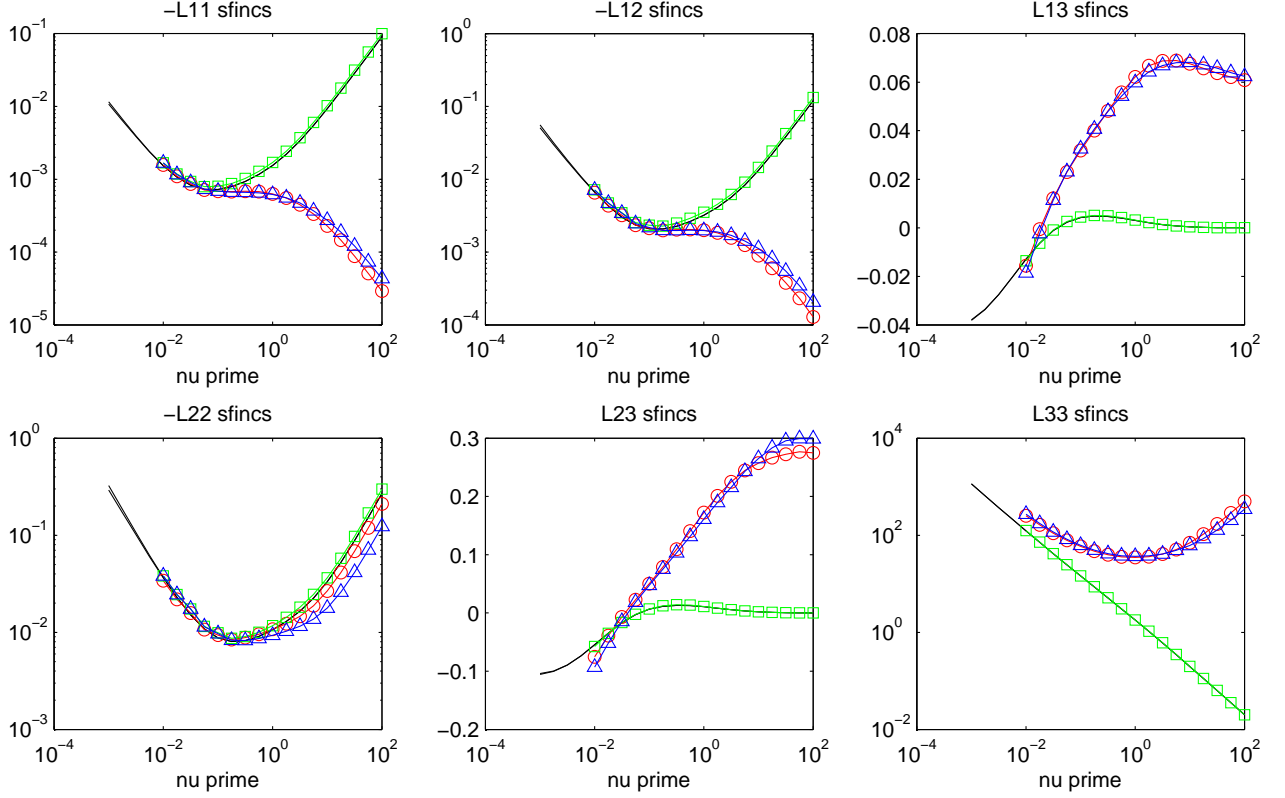
$$L_{23}^S = L_{32}^S = - \frac{1.46}{3} \frac{2}{\iota G \sqrt{\epsilon_t}} \frac{d\Psi}{dr} I_{32}^* = \frac{1}{G} \frac{d\Psi}{dr} \hat{I}_{32} \quad (51)$$

$$L_{33}^S = \frac{B_0}{v_T (G + \iota I)} L_{33}^B = \frac{\langle B^2 \rangle}{3 B_0 (G + \iota I)} I_{33}^* = - \frac{B_0}{2 \bar{B}_0^2 (G + \iota I)} \hat{I}_{33} \quad (52)$$

The L_{ij} from DKES are plotted in black with diamonds below (in the figure 5 of the manuscript).



The following figure shows the error bounds on the DKES results. The spread is very small. Only for L22 at small nuPrime can it be clearly seen in the figure.



REFERENCES

Beidler, C. D., et al. 2011, Nucl. Fusion, 51, 076001