

1 Generation of Boozer file from EFIT output

1.1 Magnetic field from EFIT data

Code EFIT provides axisymmetric equilibrium field which can be written as a sum of poloidal and toroidal field as follows,

$$\mathbf{B} = \nabla \times (A_\varphi \nabla \varphi) + B_\varphi \nabla \varphi, \quad (1)$$

where the toroidal covariant vector-potential component $A_\varphi = \psi$ is the poloidal flux specified in the nodes of rectangular grid in cylindrical coordinates, $\psi = \psi(R, Z)$, and the toroidal covariant magnetic field component $B_\varphi = B_\varphi(\psi)$ is a flux function equal up to a factor to a poloidal current, $B_\varphi = 2I_{\text{pol}}c^{-1}$. Interface to EFIT data, “field_divB0”, uses 2D splines of 5-th order to interpolate ψ and provides physical cylindrical components of the magnetic field as functions of cylindrical variables (R, φ, Z) according to (1),

$$\hat{B}_R = -\frac{1}{R} \frac{\partial \psi}{\partial Z}, \quad \hat{B}_Z = \frac{1}{R} \frac{\partial \psi}{\partial R}, \quad \hat{B}_\varphi = \frac{B_\varphi}{R}. \quad (2)$$

These components as well as their derivatives over all coordinates are available via formal arguments of subroutine “field”. In addition, function ψ and its first and second derivatives are available via module “field_eq_mod”.

1.2 Symmetry flux coordinates by field line integration

Equations of field line in cylindrical coordinates are

$$\begin{aligned} \frac{dR}{d\varphi} &= \frac{B^R}{B^\varphi} = \frac{R\hat{B}_R}{\hat{B}_\varphi}, \\ \frac{dZ}{d\varphi} &= \frac{B^Z}{B^\varphi} = \frac{R\hat{B}_Z}{\hat{B}_\varphi}, \end{aligned} \quad (3)$$

while the same equations in symmetry (and any other straight field line) flux coordinates are

$$\begin{aligned} \frac{dr}{d\varphi} &= \frac{B^r}{B^\varphi} = 0, \\ \frac{d\vartheta}{d\varphi} &= \frac{B^\vartheta}{B^\varphi} = \iota, \end{aligned} \quad (4)$$

where $\iota = \iota(r)$. Integrating Eqs. (3) over one poloidal turn what requires finding the periodic boundary upon integrating over φ from 0 to this boundary, φ_{max} , we obtain safety factor $q = \iota^{-1}$ as $q = \varphi_{\text{max}}(2\pi)^{-1}$. Repeating the integration with a fixed step $\Delta\varphi = 2\pi q K^{-1}$ where K is the number of steps we obtain the data on equi-distant grid of symmetry flux angle ϑ ranging in $[0, 2\pi]$, i.e. a set of array elements $(\vartheta_k, R_k, Z_k, B_k, \sqrt{g_k})$ belonging to the same point $\vartheta_k = 2\pi k K^{-1}$. Metric determinant here is obtained from

$$\nabla \cdot \mathbf{B} = 0 \quad \Rightarrow \quad \frac{\partial}{\partial \vartheta} \sqrt{g} B^\vartheta + \frac{\partial}{\partial \varphi} \sqrt{g} B^\varphi = \frac{\partial}{\partial \vartheta} \sqrt{g} B^\vartheta = \iota \frac{\partial}{\partial \vartheta} \sqrt{g} B^\varphi = 0 \quad (5)$$

as

$$\sqrt{g} = \frac{C_s}{B^\varphi} = \frac{C_s R}{\hat{B}_\varphi}, \quad (6)$$

where constant $C_s = C_s(r)$ is a flux function. The value of this constant is not important since it cancels in neoclassical averages. Note that Eq. (6) is valid for general 3D field geometries.

Repeating the integration for a set of flux surfaces $r = r_j$ we obtain the data on the rectangular grid equidistant in ϑ . This data is interpolated over ϑ with help of periodic splines and over r with help of Lagrange polynomials. Thus, continuous functions $R = R(r, \vartheta)$, $Z = Z(r, \vartheta)$, $B = B(r, \vartheta)$ and $\sqrt{g} = \sqrt{g(r, \vartheta)}$ are available everywhere in plasma volume together with their derivatives computed from splines and Lagrange polynomials.

1.3 Boozer transformation function from field line integration

For Boozer coordinates radial variable r is unchanged. Then, the Jacobian \sqrt{g} of symmetry flux coordinates (r, ϑ, φ) is expressed through the Jacobian $\sqrt{g_B}$ of Boozer coordinates $(r, \vartheta_B, \varphi_B)$ as follows

$$\sqrt{g} = \frac{\partial(\vartheta_B, \varphi_B)}{\partial(\vartheta, \varphi)} \sqrt{g_B} \equiv J_B \sqrt{g_B}. \quad (7)$$

Substituting in (7) Boozer angles from direct transformation via transformation function $G = G(r, \vartheta, \varphi)$,

$$\vartheta_B = \vartheta + \iota G, \quad \varphi_B = \varphi + G, \quad (8)$$

magnetic differential equation for G is obtained as

$$\frac{dG}{d\varphi} \equiv \frac{1}{B^\varphi} \mathbf{B} \cdot \nabla G \equiv \iota \frac{\partial G}{\partial \vartheta} + \frac{\partial G}{\partial \varphi} = \frac{\sqrt{g}}{\sqrt{g_B}} - 1 = J_B - 1. \quad (9)$$

The Jacobian of Boozer coordinates for the particular choice of radial variable $r = \psi_{\text{tor}}$ is

$$\sqrt{g_B} = \frac{\iota B_\vartheta + B_\varphi}{B^2}, \quad (10)$$

where $B_\vartheta = B_\vartheta(r)$ and $B_\varphi = B_\varphi(r)$ are flux functions. Therefore, for arbitrary choice of r this Jacobian is

$$\sqrt{g_B} = \frac{C_B}{B^2}, \quad (11)$$

with $C_B = C_B(r)$ being a flux function too. Substituting (11) and (6) in (9) this equation is transformed to

$$\frac{dG}{d\varphi} = \frac{RB^2}{C\hat{B}_\varphi} - 1, \quad (12)$$

where $C = C_B C_s'^{-1}$ is also a flux function. Particular expression for this function is not needed because it can be evaluated from the condition that transformation function G is a single-valued function on the flux surface,

$$\lim_{L_\varphi \rightarrow \infty} \frac{1}{L_\varphi} \int_0^{L_\varphi} d\varphi \left(\frac{RB^2}{C\hat{B}_\varphi} - 1 \right) = \left\langle B^\varphi \left(\frac{RB^2}{C\hat{B}_\varphi} - 1 \right) \right\rangle \langle B^\varphi \rangle^{-1} = 0. \quad (13)$$

In axisymmetric field where $G = G(r, \vartheta)$ it is sufficient to set the upper integration limit over φ not to infinity but to $L_\varphi = \varphi_{\text{max}} = 2\pi q$ what results in

$$C = \frac{1}{2\pi q} \int_0^{2\pi q} d\varphi \frac{RB^2}{\hat{B}_\varphi}. \quad (14)$$

Thus, constant C can be determined during the first field line integration together with safety factor q . Second integration of field line equations (3) extended by Eq. (12) will result in additional quantity G_k

in the set of array elements $(\vartheta_k, R_k, Z_k, B_k, \sqrt{g_k}, G_k)$ such that subsequent 2D interpolation provides G continuously everywhere together with necessary derivatives.

This primary information from field line integration is already sufficient for computation of mod-B spectrum, B_{mn} , which for axisymmetric field contains finite amplitudes only for $n = 0$,

$$B_{m0} = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta_B B e^{-im\vartheta_B} = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta \left(1 + \iota \frac{\partial G}{\partial \vartheta} \right) B e^{-im(\vartheta + \iota G)}. \quad (15)$$

Here, one can express derivative of G via (12) which taking into account (9) and axisymmetry of G results in the explicit form of the transformation Jacobian from symmetry flux to Boozer coordinates,

$$J_B = 1 + \iota \frac{\partial G}{\partial \vartheta} = \frac{RB^2}{C\hat{B}_\varphi}. \quad (16)$$

Integrals (15) of periodic sub-integrand are efficiently evaluated on an equidistant grid of ϑ ,

$$\vartheta_k = \frac{2\pi k}{K}, \quad k = 1, 2, \dots, K. \quad (17)$$

Denoting values of different function at the nodes of the grid as follows,

$$J_B^{(k)} = \frac{R(r, \vartheta_k) B^2(r, \vartheta_k)}{C(r) \hat{B}_\varphi(r, \vartheta_k)}, \quad B_{(k)} = B(r, \vartheta_k), \quad \mathcal{E}_{(k)} = \exp(-i(\vartheta_k + \iota(r)G(r, \vartheta_k))), \quad (18)$$

Fourier amplitudes (15) are obtained as

$$B_{m0} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=1}^K J_B^{(k)} B_{(k)} \mathcal{E}_{(k)}^m. \quad (19)$$

The same is done also for cylindrical coordinates,

$$R_{m0} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=1}^K J_B^{(k)} R_{(k)} \mathcal{E}_{(k)}^m, \quad Z_{m0} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=1}^K J_B^{(k)} Z_{(k)} \mathcal{E}_{(k)}^m, \quad (20)$$

including transformation function λ defined via $2\pi\lambda = \varphi - \varphi_B = -G$,

$$\lambda_{m0} = -\frac{1}{2\pi} \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=1}^K J_B^{(k)} G_{(k)} \mathcal{E}_{(k)}^m. \quad (21)$$

Note that NEO-2 needs these coordinates for two purposes. First, it computes effective plasma radius defined as $dV = Sdr$ where V is volume limited by flux surface and S is flux surface area. Second, it uses R and Z for computation of radial covariant component of the magnetic field B_r via metric tensor so that this component computed by VMEC directly, which is discussed also in the next subsection, is not used.

1.4 Covariant field components

For computation of covariant field components in Boozer coordinates we use the fact that we know cylindrical coordinates R and Z as functions of symmetry flux coordinates $\mathbf{x} = (r, \vartheta, \varphi)$ everywhere together with their derivatives over x^i . Thus, we can assume that we know the covariant unit vectors $\partial \mathbf{r} / \partial x^i$ of symmetry flux coordinates since transformation from cylindrical to Cartesian coordinates is straightforward.

Radial covariant component is obtained as

$$B_r^B = \mathbf{B} \cdot \left(\frac{\partial \mathbf{r}}{\partial r} \right)_B = \mathbf{B} \cdot \frac{\partial(\mathbf{r}, \vartheta_B, \varphi_B)}{\partial(r, \vartheta_B, \varphi_B)} = \mathbf{B} \cdot \frac{\partial(\mathbf{r}, \vartheta_B, \varphi_B)}{\partial(r, \vartheta, \varphi)} \frac{\partial(\vartheta, \varphi)}{\partial(\vartheta_B, \varphi_B)} = \mathbf{B} \cdot \frac{\partial(\mathbf{r}, \vartheta_B, \varphi_B)}{\partial(r, \vartheta, \varphi)} \frac{1}{J_B}. \quad (22)$$

For more explicit expressions we use axial symmetry in order to obtain

$$\begin{aligned} B_r^B &= \mathbf{B} \cdot \frac{\partial \mathbf{r}}{\partial r} - \mathbf{B} \cdot \frac{\partial \mathbf{r}}{\partial \vartheta} \frac{1}{J_B} \frac{\partial}{\partial r} \iota G - \mathbf{B} \cdot \frac{\partial \mathbf{r}}{\partial \varphi} \frac{1}{J_B} \left(\frac{\partial G}{\partial r} - G \frac{\partial \iota}{\partial r} \frac{\partial G}{\partial \vartheta} \right) \\ &= \hat{B}_R \frac{\partial R}{\partial r} + \hat{B}_Z \frac{\partial Z}{\partial r} - \left(\hat{B}_R \frac{\partial R}{\partial \vartheta} + \hat{B}_Z \frac{\partial Z}{\partial \vartheta} \right) \frac{1}{J_B} \frac{\partial}{\partial r} \iota G - \hat{B}_\varphi \frac{R}{J_B} \left(\frac{\partial G}{\partial r} - G \frac{\partial \iota}{\partial r} \frac{\partial G}{\partial \vartheta} \right), \end{aligned} \quad (23)$$

where J_B is given by (16). Cylindrical coordinates R and Z and function G and their derivatives in the last expression (23) are known from the interpolation of field line integration result. Physical cylindrical components of the magnetic field in this expression should be computed by “field” routine for known R and Z . Therefore, covariant radial component (23) is known at equidistant grid nodes ϑ_k ,

$$B_{r(k)}^B = B_r^B(r, \vartheta_k), \quad (24)$$

and its Fourier amplitudes can be computed in analogy to (19) as

$$B_{r,m0} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{k=1}^K J_B^{(k)} B_{r(k)}^B \mathcal{E}_{(k)}^m. \quad (25)$$

Component over poloidal angle is computed in a similar way to (22),

$$B_\vartheta^B = \mathbf{B} \cdot \left(\frac{\partial \mathbf{r}}{\partial \vartheta_B} \right)_B = \mathbf{B} \cdot \frac{\partial(r, \mathbf{r}, \varphi_B)}{\partial(r, \vartheta_B, \varphi_B)} = \mathbf{B} \cdot \frac{\partial(\mathbf{r}, \varphi_B)}{\partial(\vartheta, \varphi)} \frac{1}{J_B} = \mathbf{B} \cdot \left(\frac{\partial \mathbf{r}}{\partial \vartheta} - \frac{\partial G}{\partial \vartheta} \frac{\partial \mathbf{r}}{\partial \varphi} \right) \frac{1}{J_B}. \quad (26)$$

Eliminating poloidal derivative of G with help of (16) and using then explicit expression for J_B we get

$$B_\vartheta^B = \frac{1}{J_B} \left(B_\vartheta + \frac{B_\varphi}{\iota} (1 - J_B) \right) = \frac{\iota B_\vartheta + B_\varphi}{\iota J_B} - \frac{B_\varphi}{\iota} = \frac{B^2}{\iota J_B B^\varphi} - \frac{B_\varphi}{\iota} = q(C - B_\varphi). \quad (27)$$

Obviously B_ϑ^B is a flux function because both, B_φ and constant C are flux functions known already after the first field line integration. In order to see that this is a toroidal current we rewrite (14) from the form of field line integral to the form of integral over the poloidal angle using the axial symmetry,

$$C = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta \frac{RB^2}{\hat{B}_\varphi} = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta \frac{B^2}{B^\varphi}. \quad (28)$$

Substituting this in the last expression (27) we get

$$B_\vartheta^B = \frac{q}{2\pi} \int_0^{2\pi} d\vartheta \left(\frac{B^2}{B^\varphi} - B_\varphi \right) = \frac{q}{2\pi} \int_0^{2\pi} d\vartheta \frac{B_\vartheta B^\vartheta}{B^\varphi} = \frac{1}{2\pi} \int_0^{2\pi} d\vartheta B_\vartheta = \frac{2}{c} I_{\text{tor}}, \quad (29)$$

where the last expression follows from Ampere’s law and Stokes theorem.

We do not need to repeat the ansatz for the toroidal component because in axisymmetric field both flux coordinate systems have the same toroidal covariant vector (since G is independent of φ),

$$\frac{\partial \mathbf{r}}{\partial \varphi_B} = \frac{\partial \mathbf{r}}{\partial \varphi}. \quad (30)$$

Respectively, toroidal covariant field component is also unchanged,

$$B_\varphi^B = B_\varphi = R \hat{B}_\varphi = \frac{2}{c} I_{\text{pol}}. \quad (31)$$

1.5 Computation of the cross-section area and of the toroidal flux

Cross-section area is given by the following contour integral

$$S_{pol} = \oint dZ R(Z) = \int_0^{2\pi} d\vartheta \frac{\partial Z(r, \vartheta)}{\partial \vartheta} R(r, \vartheta) = \int_0^{2\pi q} d\varphi \frac{dZ}{d\varphi} R = \int_0^{2\pi q} d\varphi \frac{R^2 \hat{B}_Z}{\hat{B}_\varphi}, \quad (32)$$

where last two expressions correspond to the integration along the field line (see (3)). Equivalently, one can switch R and Z in the contour integral in order to obtain

$$S_{pol} = - \oint dR Z(R) = - \int_0^{2\pi q} d\varphi \frac{RZ \hat{B}_R}{\hat{B}_\varphi}. \quad (33)$$

Both formulas result in positive area in AUG cases where toroidal field is in mathematically positive direction and poloidal field points up at the outer midplane or if both fields are reversed. In a general case, results of Eqs. (32) and (33) should be multiplied with $\text{sign}(\hat{B}_\varphi \hat{B}_Z)$ in the outer midplane.

In absence of finite- β effect, covariant toroidal magnetic field component B_φ is constant in plasma volume. Respectively, physical component \hat{B}_φ is a function of R only, and, therefore, toroidal flux can be computed as follows,

$$\Psi_{tor} = - \oint dR Z(R) \hat{B}_\varphi(R) = - \int_0^{2\pi q} d\varphi RZ \hat{B}_R, \quad (34)$$

which is a straightforward consequence of (33).

In presence of finite- β effect, single field line integration is not sufficient, and the flux should be integrated over flux surface label in symmetry flux coordinates,

$$\Psi_{tor}(r) = \int_{r_{axis}}^r dr' \int_0^{2\pi} d\vartheta \frac{\partial \mathbf{r}}{\partial r} \times \frac{\partial \mathbf{r}}{\partial \vartheta} \cdot \mathbf{B} = \int_{r_{axis}}^r dr' \int_0^{2\pi} d\vartheta \sqrt{g} B^\varphi = 2\pi \int_{r_{axis}}^r dr' \sqrt{g} B^\varphi, \quad (35)$$

where we used the fact that $\sqrt{g} B^\varphi$ is a flux function. Starting field line integration from the outer midplane $Z = Z_b$ and using the starting major radius value R_b as a flux surface label, $r = R_b$, we can express cylindrical coordinates in the vicinity of the starting point via flux coordinates as follows,

$$R = R_b + \frac{R_b \hat{B}_R \vartheta}{\iota \hat{B}_\varphi} + O(\vartheta^2), \quad Z = Z_b + \frac{R_b \hat{B}_Z \vartheta}{\iota \hat{B}_\varphi} + O(\vartheta^2), \quad (36)$$

what results for metric determinant in

$$\sqrt{g} = R \frac{\partial(R, \varphi, Z)}{\partial(r, \vartheta, \varphi)} = -R \frac{\partial(R, Z)}{\partial(r, \vartheta)} = -\frac{R_b^2 \hat{B}_Z}{\iota \hat{B}_\varphi} + O(\vartheta). \quad (37)$$

Substituting this expression evaluated exactly at the midplane, $\vartheta = 0$, in (35) we get

$$\Psi_{tor}(R_b) = -2\pi \int_{R_{axis}}^{R_b} dR'_b q(R'_b) R'_b \hat{B}_Z(R'_b, Z_b). \quad (38)$$

Since safety factor is always positive in field line integration, sign of the flux in Eq. (38) is correct for AUG cases and should be multiplied with $\text{sign}(\hat{B}_\varphi \hat{B}_Z)$ in a general case.

1.6 Sign conventions

Field line integration procedure determines q as a positive quantity. Therefore, direction of the poloidal angle corresponds to Erika's definition for positive $\sigma = \text{sign}(\hat{B}_\varphi \hat{B}_Z)$ where \hat{B}_Z is computed at the outer midplane.

Poloidal current J according to Erika's Fig.2 points downwards if this current is defined as a current through a circle centered at the main axis of the torus. This means that $J = -I_{\text{pol}}$ with I_{pol} defined by (31) as a current in positive direction with respect to Z -axis.

Toroidal current I according to Erika's Fig.2 points in mathematically positive toroidal direction. In case $\sigma = 1$ flux coordinate system (s, ϑ, φ) is left-handed, and, therefore, current I_{tor} in Eq. (29) points in negative direction with respect to the toroidal angle, and, respectively, $I = -I_{\text{tor}}$.

If Both currents are switch the sign flux coordinate system remains left-handed, $\sigma = 1$. In this case both, B_φ and B_ϑ switch signs. If only one current switches sign, system becomes right-handed, $\sigma = -1$. Since toroidal angle is always counted in mathematically positive toroidal direction of cylindrical coordinates, poloidal angle changes direction in both such cases in order to keep q positive. In the first such case where the poloidal current I_{pol} switches sign, direction of toroidal field B_φ is switched. Since poloidal current is defined independently of coordinate system as current through the circle centered at Z -axis it does not change sign but the poloidal field B_ϑ does together with the direction of poloidal angle. In the second such case where the toroidal current I_{tor} switches sign, sign of the toroidal field B_φ is unchanged and sign of the poloidal field B_ϑ is also unchanged because change in the direction of the poloidal field is compensated by the change of the poloidal angle direction. Thus, in the general case of positively defined q relation between currents and covariant field components can be written as

$$I = -\sigma I_{\text{tor}}, \quad J = -I_{\text{pol}}, \quad (39)$$

where I_{tor} and I_{pol} are defined by Eqs. (29) and (31), respectively. Besides that, we note that toroidal flux (38) is in mathematically positive direction only for the right-handed flux coordinate system, $\sigma = -1$. For the left-handed system it is counted in mathematically negative direction. In order count it in mathematically positive direction of cylindrical coordinates in all cases we re-define the sign of the normalized toroidal flux $\psi_{\text{tor}} = \Psi_{\text{tor}}(2\pi)^{-1}$ as follows,

$$\psi_{\text{tor}}(R_b) = \sigma \int_{R_{\text{axis}}}^{R_b} dR'_b q(R'_b) R'_b \hat{B}_Z(R'_b, Z_b). \quad (40)$$

1.7 Pressure gradient

For completeness of Boozer file let us compute pressure gradient. Although it is not used by NEO-2, it might be useful for linearized ideal MHD model of RMP's. Using force balance and Ampere's law,

$$c\nabla p = \mathbf{j} \times \mathbf{B}, \quad 4\pi\mathbf{j} = c\nabla \times \mathbf{B}, \quad (41)$$

one obtains flux coordinates

$$\frac{4\pi}{B^\varphi} \frac{\partial p}{\partial r} = \left(\frac{\partial}{\partial \varphi} + \iota \frac{\partial}{\partial \vartheta} \right) B_r - \frac{\partial B_\varphi}{\partial r} - \iota \frac{\partial B_\vartheta}{\partial r}. \quad (42)$$

Averaging this expression over the angles eliminates B_r . In Boozer coordinates and axisymmetric field result is particularly simple,

$$\begin{aligned}
\frac{\partial p}{\partial r} &= -\frac{1}{2} \left(\frac{\partial B_\varphi^B}{\partial r} + \iota \frac{\partial B_\vartheta^B}{\partial r} \right) \left(\int_0^{2\pi} \frac{d\vartheta_B}{B_B^\varphi} \right)^{-1} = -\frac{1}{2 (B_\varphi^B + \iota B_\vartheta^B)} \left(\frac{\partial B_\varphi^B}{\partial r} + \iota \frac{\partial B_\vartheta^B}{\partial r} \right) \left(\int_0^{2\pi} \frac{d\vartheta_B}{B^2} \right)^{-1} \\
&= -\frac{1}{4\pi (B_\varphi^B + \iota B_\vartheta^B)} \left(\frac{\partial B_\varphi^B}{\partial r} + \iota \frac{\partial B_\vartheta^B}{\partial r} \right) \left(\frac{1}{B^2} \right)_{00}^{-1}, \tag{43}
\end{aligned}$$

where $(\dots)_{00}$ means Fourier amplitude for $(m, n) = (0, 0)$. Last expression is valid in a general 3D case.