GKW to GKDB data conversion

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Last update: June 4, 2018

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Chapter 1

Preamble

This document describes how to transform inputs and outputs from a GKW flux-tube simulation to match the format used in the GyroKinetic DataBase (GKDB).
The reader is assumed to have some knowledge of GKW [1, 2] and to have read the documentation of the GKDB [3].

Chapter 2

Conventions and normalisations

2.1 Coordinate systems

In GKW, the toroidal direction is defined to have the cylindrical coordinate system (R, Z, φ) right-handed whereas in the GKDB it is defined to have (R, φ, Z) right-handed, see Fig.2.1. In practice, it means that:

$$\varphi^{\texttt{GKDB}} = -\varphi^{\texttt{GKW}} \tag{2.1}$$

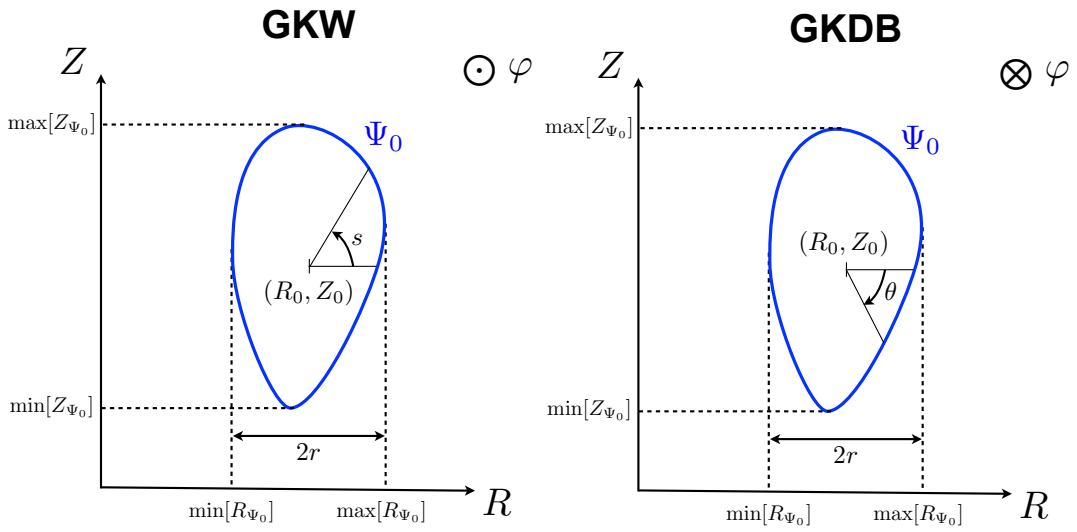

Figure 2.1: Cylindrical coordinate system used in GKW (left) and the GKDB (right).

The flux surface centre definition depends on how the magnetic equilibrium is specified. For `miller` geometry, the definition of R_0 is identical to that used in the GKDB and Z_0 is given as an input in the geometry namelist:

$$R_0^{\texttt{GKW-miller}} = R_0^{\texttt{GKDB}} \qquad Z_0^{\texttt{GKW-miller}} = \texttt{zmil} R_{\text{ref}}^{\texttt{GKW}} \tag{2.2}$$

For `chease` geometry, R_0 is taken to be the value of `ROEXP` specified in the `hamada.dat` file and Z_0 is the elevation of the magnetic axis.

$$R_0^{\texttt{GKW-chease}} = \texttt{ROEXP} \qquad Z_0^{\texttt{GKW-chease}} = Z_{\text{axis}} \tag{2.3}$$

The definition of the (dimensional) radial coordinate r is identical in GKW and the GKDB:

$$r^{\texttt{GKW}} = r^{\texttt{GKDB}} \tag{2.4}$$

The calculation of the poloidal angle θ used in the GKDB from GKW inputs is documented in section 3.1. At this stage, just notice that most of the time $Z_0^{\texttt{GKW}} \neq Z_0^{\texttt{GKDB}}$, therefore, the points $s = 0$ and $\theta = 0$ do not necessarily coincide.

2.2 Reference quantities

In GKW and the GKDB, all quantities are normalised and made dimensionless by making use of reference quantities. In what follows, normalised quantities are denoted with a "N" subscript. For instance, the normalised version of an arbitrary quantity $\mathcal{A}$ with the dimension of a length will be $\mathcal{A}_N^{\texttt{GKW}} = \mathcal{A}/R_{\text{ref}}^{\texttt{GKW}}$ in GKW and $\mathcal{A}_N^{\texttt{GKDB}} = \mathcal{A}/R_{\text{ref}}^{\texttt{GKDB}}$ in the GKDB. The conversion from GKW to the GKDB involves the ratio of reference quantities. For the example above:

$$\mathcal{A}_N^{\texttt{GKDB}} = \frac{R_{\text{ref}}^{\texttt{GKW}}}{R_{\text{ref}}^{\texttt{GKDB}}} \mathcal{A}_N^{\texttt{GKW}} \tag{2.5}$$

The ratio of the various reference quantities used in GKW and the GKDB are:

$$q_{\text{rat}} = \frac{q_{\text{ref}}^{\texttt{GKW}}}{q_{\text{ref}}^{\texttt{GKDB}}} = -\frac{1}{\texttt{z}_{e^-}^{\texttt{GKW}}} \qquad R_{\text{rat}}^{\texttt{miller}} = \frac{R_{\text{ref}}^{\texttt{GKW-miller}}}{R_{\text{ref}}^{\texttt{GKDB}}} = 1$$

$$m_{\text{rat}} = \frac{m_{\text{ref}}^{\texttt{GKW}}}{m_{\text{ref}}^{\texttt{GKDB}}} = \frac{m_e}{m_D} \frac{1}{\texttt{mass}_{e^-}^{\texttt{GKW}}} \qquad B_{\text{rat}}^{\texttt{miller}} = \frac{B_{\text{ref}}^{\texttt{GKW-miller}}}{B_{\text{ref}}^{\texttt{GKDB}}} = 1$$

$$T_{\text{rat}} = \frac{T_{\text{ref}}^{\texttt{GKW}}}{T_{\text{ref}}^{\texttt{GKDB}}} = \frac{1}{\texttt{temp}_{e^-}^{\texttt{GKW}}} \qquad R_{\text{rat}}^{\texttt{chease}} = \frac{R_{\text{ref}}^{\texttt{GKW-chease}}}{R_{\text{ref}}^{\texttt{GKDB}}} = \frac{\texttt{R0EXP}}{R_0^{\texttt{GKDB}}}$$

$$n_{\text{rat}} = \frac{n_{\text{ref}}^{\texttt{GKW}}}{n_{\text{ref}}^{\texttt{GKDB}}} = \frac{1}{\texttt{dens}_{e^-}^{\texttt{GKW}}} \frac{n_e(s=0)}{n_e(\theta=0)} \qquad B_{\text{rat}}^{\texttt{chease}} = \frac{B_{\text{ref}}^{\texttt{GKW-chease}}}{B_{\text{ref}}^{\texttt{GKDB}}} = \frac{\texttt{B0EXP}}{B_0^{\texttt{GKDB}}}$$

where the e^- subscript denotes the electron species and the electron to deuterium mass ratio is taken to be $\frac{m_e}{m_D} = 2.7237 \times 10^{-4}$ in the GKDB.
The reference charge, mass, temperature and density ratio can be computed from the electron species parameters in the `SPECIES` namelist of the GKW input file. The poloidal asymmetry factor for the electron density can be computed from data in the `cfdens` file (GKW output). With `chease` geometry, the ratios R_{rat} and B_{rat} can be computed from data in the `hamada.dat` file (GKW input).
The following derived quantities will also be used for the conversion:

$$v_{\text{thrat}} = \sqrt{\frac{T_{\text{rat}}}{m_{\text{rat}}}} \qquad \rho_{\text{rat}} = \frac{q_{\text{rat}} B_{\text{rat}}}{m_{\text{rat}} v_{\text{thrat}}}$$

Chapter 3

Inputs

3.1 Magnetic equilibrium

Only `miller` and `chease` magnetic equilibrium specifications are compatible with the GKDB format (`s-alpha` and `circ` are not an exact solution of the Grad-Shafranov equation).

3.1.1 Flux surface centre

Let's call $\{R_{\Psi_0}, Z_{\Psi_0}\}$ a set of points discretizing the flux surface of interest.
The values of $\{R_{\Psi_0}, Z_{\Psi_0}\}/R_{\text{ref}}^{\texttt{GKW}}$ are available in the `geom.dat` file (GKW output) and can be used to compute $\{R_0^{\texttt{GKDB}}, Z_0^{\texttt{GKDB}}\}/R_{\text{ref}}^{\texttt{GKW}}$.

3.1.2 Poloidal angle

With these values, one can then compute the GKDB poloidal angle θ:

$$\tan\theta = -\frac{Z_{\Psi_0}/R_{\text{ref}}^{\texttt{GKW}} - Z_0^{\texttt{GKDB}}/R_{\text{ref}}^{\texttt{GKW}}}{R_{\Psi_0}/R_{\text{ref}}^{\texttt{GKW}} - R_0^{\texttt{GKDB}}/R_{\text{ref}}^{\texttt{GKW}}} \tag{3.1}$$

As the discretisation of the flux surface in `geom.dat` is done on the GKW s grid, the equation above gives the relationship between θ and s.

3.1.3 Radial coordinate

$$r_N^{\texttt{GKDB}} = r_N^{\texttt{GKW}} \cdot R_{\text{rat}} = \texttt{eps} \cdot R_{\text{rat}} \tag{3.2}$$

3.1.4 Toroidal field and current direction

$$s_b^{\texttt{GKDB}} = -s_b^{\texttt{GKW}} = -\texttt{signb} \qquad \text{and} \qquad s_j^{\texttt{GKW}} = -s_j^{\texttt{GKW}} = -\texttt{signj} \tag{3.3}$$

3.1.5 Safety factor

$$q^{\texttt{GKDB}} = s_b^{\texttt{GKW}} s_j^{\texttt{GKW}} q^{\texttt{GKW}} = \texttt{signb} \cdot \texttt{signj} \cdot \texttt{q} \tag{3.4}$$

3.1.6 Magnetic shear

$$\hat{s}^{\texttt{GKDB}} = \hat{s}^{\texttt{GKW}} = \texttt{shat} \tag{3.5}$$

3.1.7 Pressure gradient (entering the curvature drift)

$$\beta_N'^{\texttt{GKDB}} = -\beta_N'^{\texttt{GKW}} \frac{B_{\text{rat}}^2}{R_{\text{rat}}} \tag{3.6}$$

The value of $\beta_N'^{\texttt{GKW}}$ is taken from `betaprime_ref` for `miller` geometry or from the `geom.dat` file for `chease` geometry.

3.1.8 Plasma shape

To compute the shaping Fourier coefficients and their radial derivatives, one first need to compute:

$$a_N^{\texttt{GKDB}}(r,\theta) = \frac{1}{R_{\text{ref}}^{\texttt{GKDB}}}\sqrt{\left[R_{\Psi_0}(r,\theta) - R_0^{\texttt{GKDB}}\right]^2 + \left[Z_{\Psi_0}(r,\theta) - Z_0^{\texttt{GKDB}}\right]^2} \tag{3.7}$$

For `miller` geometry, this can be done by computing $\{R_{\Psi_0}(r,\theta), Z_{\Psi_0}(r,\theta)\}/R_{\text{ref}}^{\texttt{GKW}}$ from the Miller parameters of the GKW input files and then perform the Fourier expansion.
For `chease` geometry $\{R_{\Psi_0}(r,s), Z_{\Psi_0}(r,s)\}$ is directly available in the `hamada.dat` file and can be used together with the relationship between θ and s to compute the Fourier coefficients.

3.2 Species

3.2.1 Charge

$$Z_{sN}^{\texttt{GKDB}} = Z_{sN}^{\texttt{GKW}} \cdot q_{\text{rat}} = \texttt{z}_s \cdot q_{\text{rat}} \tag{3.8}$$

3.2.2 Mass

$$m_{sN}^{\texttt{GKDB}} = m_{sN}^{\texttt{GKW}} \cdot m_{\text{rat}} = \texttt{mass}_s \cdot m_{\text{rat}} \tag{3.9}$$

3.2.3 Density

$$n_{sN}^{\texttt{GKDB}}(\theta=0) = n_{sN}^{\texttt{GKW}}(\theta=0) \cdot n_{\text{rat}} = \texttt{dens}_s \cdot n_{\text{rat}} \cdot \frac{n_{sN}^{\texttt{GKW}}(\theta=0)}{n_{sN}^{\texttt{GKW}}(s=0)} \tag{3.10}$$

In the presence of poloidal asymmetries, the density at $\theta = 0$ can be obtained from the `cfdens` output file. In this file, the first column is the s grid, then comes the logarithmic density gradient for each species and finally the density for each species (all with GKW normalisations).

3.2.4 Logarithmic density gradient

$$\frac{R_{\text{ref}}^{\texttt{GKDB}}}{L_{n_s}^{\texttt{GKDB}}}(\theta=0) = \frac{R_{\text{ref}}^{\texttt{GKW}}}{L_{n_s}^{\texttt{GKW}}}(\theta=0) \cdot R_{\text{rat}} = \texttt{rln}_s \cdot R_{\text{rat}} \cdot \frac{L_{n_s}^{\texttt{GKW}}(\theta=0)}{L_{n_s}^{\texttt{GKW}}(s=0)} \tag{3.11}$$

In the presence of poloidal asymmetries, the logarithmic density gradient at $\theta = 0$ can be obtained from the `cfdens` output file. In this file, the first column is the s grid, then comes the logarithmic density gradient for each species and finally the density for each species (all with GKW normalisations).

3.2.5 Temperature

$$T_{sN}^{\texttt{GKDB}} = T_{sN}^{\texttt{GKW}} \cdot T_{\text{rat}} = \texttt{temp}_s \cdot T_{\text{rat}} \tag{3.12}$$

3.2.6 Logarithmic temperature gradient

$$\frac{R_{\text{ref}}^{\texttt{GKDB}}}{L_{T_s}^{\texttt{GKDB}}} = \frac{R_{\text{ref}}^{\texttt{GKW}}}{L_{T_s}^{\texttt{GKW}}} \cdot R_{\text{rat}} = \texttt{rlt}_s \cdot R_{\text{rat}} \tag{3.13}$$

3.2.7 Toroidal velocity

$$u_N^{\texttt{GKDB}} = s_b^{\texttt{GKW}} \cdot u_N^{\texttt{GKW}} \cdot \frac{v_{\text{thrat}}}{R_{\text{rat}}} = \texttt{signb} \cdot \texttt{vcor} \cdot \frac{v_{\text{thrat}}}{R_{\text{rat}}} \tag{3.14}$$

3.2.8 Toroidal velocity gradient

$$u'^{\texttt{GKDB}}_{sN} = s_b^{\texttt{GKW}} \cdot u'^{\texttt{GKW}}_{sN} \cdot \frac{v_{\text{thrat}}}{R_{\text{rat}}^2} = \texttt{signb} \cdot \texttt{uprim}_s \cdot \frac{v_{\text{thrat}}}{R_{\text{rat}}^2} \tag{3.15}$$

3.2.9 Plasma beta

$$\beta_{eN}^{\texttt{GKDB}} = \beta_N^{\texttt{GKW}} \cdot n_{\rm rat} \cdot T_{\rm rat} \cdot B_{\rm rat}^2 \tag{3.16}$$

The value of $\beta_N^{\texttt{GKW}}$ is either taken from the input `beta_ref` of the `SPCGENERAL` namelist when the `beta_type='ref'` option is used or extracted from the output file `out` when the `beta_type='eq'` option is used.

3.2.10 Collisionality

$$\nu_{eN}^{\texttt{GKDB}} = \frac{e^4}{4\pi\varepsilon_0^2}\frac{1}{q_{\rm rat}^4}\frac{T_{\rm rat}^2}{n_{\rm rat}R_{\rm rat}}\frac{n_{\rm ref}^{\texttt{GKW}}R_{\rm ref}^{\texttt{GKW}}}{{T_{\rm ref}^{\texttt{GKW}}}^2} = \frac{e^4}{4\pi\varepsilon_0^2}\frac{1}{q_{\rm rat}^4}\frac{T_{\rm rat}^2}{n_{\rm rat}R_{\rm rat}}\frac{\texttt{nref}\cdot\texttt{rref}}{\texttt{tref}^2} \tag{3.17}$$

Note that the expression above assumes that the `freq_override` option is set to false.

3.2.11 Debye length

Always zero in GKW runs.

3.3 Wave vector

3.3.1 Radial wave vector

$$k_{r*}{\rho_{\rm ref}}^{\texttt{GKDB}} = \texttt{krrho}\cdot\frac{1}{\rho_{\rm rat}}\cdot\sqrt{\frac{g^{\psi\psi}(\theta=0)}{g^{\psi\psi}(s=0)}} \tag{3.18}$$

The quantity $g^{\psi\psi}$ is given on the s grid in `geom.dat`

3.3.2 Binormal wave vector

$$k_{\theta*}{\rho_{\rm ref}}^{\texttt{GKDB}} = \texttt{kthrho}\cdot\frac{1}{\rho_{\rm rat}}\cdot\sqrt{\frac{g^{\zeta\zeta}(\theta=0)}{g^{\zeta\zeta}(s=0)}} \tag{3.19}$$

The quantity $g^{\zeta\zeta}$ is given on the s grid in `geom.dat`

Chapter 4

Outputs

4.1 Mode amplitude

The normalised fields in GKW and the GKDB are related as follows:

$$\hat{\phi}_N^{\texttt{GKDB}} = \hat{\phi}_N^{\texttt{GKW}} \cdot \frac{T_{\rm rat}\rho_{\rm rat}}{q_{\rm rat}R_{\rm rat}}, \qquad \hat{A}_{\|N}^{\texttt{GKDB}} = \hat{A}_{\|N}^{\texttt{GKW}} \cdot \frac{B_{\rm rat}\rho_{\rm rat}^2}{R_{\rm rat}}, \qquad \hat{B}_{\|N}^{\texttt{GKDB}} = \hat{B}_{\|N}^{\texttt{GKW}} \cdot \frac{B_{\rm rat}\rho_{\rm rat}}{R_{\rm rat}}, \tag{4.1}$$

In GKW linear runs, the exponentially growing fields are further normalised with respect to the mode amplitude:

$$\hat{\phi}_{NN}^{\texttt{GKW}} = \frac{1}{\mathcal{A}_f^{\texttt{GKW}}}\hat{\phi}_N^{\texttt{GKW}}, \qquad \hat{A}_{\|\,NN}^{\ \texttt{GKW}} = \frac{1}{\mathcal{A}_f^{\texttt{GKW}}}\hat{A}_{\|\,N}^{\ \texttt{GKW}}, \qquad \hat{B}_{\|\,NN}^{\ \texttt{GKW}} = \frac{1}{\mathcal{A}_f^{\texttt{GKW}}}\hat{B}_{\|\,N}^{\ \texttt{GKW}} \tag{4.2}$$

with

$$\mathcal{A}_f^{\texttt{GKW}} = \sqrt{\int \left[|\hat{\phi}_N^{\texttt{GKW}}|^2 + |\hat{A}_{\|N}^{\texttt{GKW}}|^2 + |\hat{B}_{\|N}^{\texttt{GKW}}|^2\right] \mathrm{d}s \Big/ \int \mathrm{d}s} \tag{4.3}$$

The mode amplitude used to normalise linear runs and compute the mode growth rate in the GKDB is

$$\mathcal{A}_f^{\texttt{GKDB}} = \sqrt{\frac{1}{2\pi}\int \left[|\hat{\phi}_N^{\texttt{GKDB}}|^2 + |\hat{A}_{\|N}^{\texttt{GKDB}}|^2 + |\hat{B}_{\|N}^{\texttt{GKDB}}|^2\right] \mathrm{d}\theta} \tag{4.4}$$

and the ratio of the GKDB to GKW mode amplitudes is therefore given by:

$$\frac{1}{\mathcal{A}_{\rm rat}} = \frac{\mathcal{A}_f^{\texttt{GKDB}}}{\mathcal{A}_f^{\texttt{GKW}}} = \sqrt{\frac{1}{2\pi}\left[|\frac{T_{\rm rat}\rho_{\rm rat}}{q_{\rm rat}R_{\rm rat}} \cdot \hat{\phi}_{NN}^{\texttt{GKW}}|^2 + |\frac{B_{\rm rat}\rho_{\rm rat}^2}{R_{\rm rat}} \cdot \hat{A}_{\|NN}^{\texttt{GKW}}|^2 + |\frac{B_{\rm rat}\rho_{\rm rat}}{R_{\rm rat}} \cdot \hat{B}_{\|NN}^{\texttt{GKW}}|^2\right] \mathrm{d}\theta} \tag{4.5}$$

The mode amplitude ratio can therefore be computed from the GKW output file `parallel.dat` which contains $\hat{\phi}_{NN}^{\texttt{GKW}}(s)$, $\hat{A}_{\|\,NN}^{\ \texttt{GKW}}(s)$ and $\hat{B}_{\|\,NN}^{\ \texttt{GKW}}(s)$. Note that in this file, the fields may have been rotated in the complex plane, but this does not impact the mode amplitude calculation.

Bibliography

[1] A.G. Peeters, Y. Camenen, F.J. Casson, W.A. Hornsby, A.P. Snodin, D. Strintzi, G. Szepesi. *Comput. Phys. Commun.*, 180:2650, 2009.

[2] https://bitbucket.org/gkw/gkw/overview.

[3] https://github.com/gkdb/gkdb/wiki.