CONSISTENT RECALCULATION OF MHD EQUILIBRIA FROM VMEC[*]

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1. Introduction

The Variational Moments Equilibrium Code (VMEC [1]) provides data of magnetic field configurations in flux coordinates. However, for different applications one needs input data in a different representation, e.g., the stochastic mapping code [2] uses input data in real space coordinates, or the neoclassical transport code [3] uses input data in Boozer coordinates [4]. Therefore, the output data of VMEC need to be postprocessed, in particular they have to be transformed to different coordinate systems. However, such coordinate transformations are sensitive to the ill behaved VMEC output data near the magnetic axis, in particular to the spectral representation of the cylindrical coordinates $R = \sum R_{mn}(s)\cos(m\theta - n\varphi)$ and $Z = \sum R_{mn}(s)\sin(m\theta - n\varphi)$ where (s, θ, φ) are radial, poloidal and toroidal flux coordinates.

A way to cure this problem is to smooth all Fourier amplitudes of R and Z using a specially designed smoothing spline method while enforcing a leading dependence on small values of the flux surface label s. Any smoothing procedure causes at least a slight variation of the equilibrium. Therefore, the equilibrium is recalculated in a consistent way based on the rotational transform ι and smoothed Fourier amplitudes for R and Z.

2. Basics

VMEC solves the MHD equilibrium equations for nested flux surfaces[7]. The geometric coordinates R and Z are expanded in Fourier series in both a poloidal angle variable and a toroidal angle variable. The coefficients R_{mn} and Z_{mn} are functions of the normalized toroidal flux s, where $s = 0$ represents the magnetic axis and $s = 1$ gives the outermost closed flux surface. But there is a well known convergency problem near the magnetic axis which cause ill behaved Fourier amplitudes of the coordinates R and Z. This behavior may cause problems in particular if one needs a transformation from flux surface coordinates which are used in VMEC to other coordinates. Therefore, it is necessary to postprocess the output of VMEC.

The basic quantities R_{mn} and Z_{mn} for reconstructing the equilibrium are splined with a specially designed smoothing spline (see 3). The recalculation of equilibrium quantities is shown in 4. These quantities together with ι allow the calculation of the components of the magnetic field in cylindrical coordinates (see 5) and Boozer coordinates (see 6).

3. Spline

The near axis expansion causes integer powers of $\sqrt{s}$ in the coefficients R_{mn} and Z_{mn}. Due to this, an ordinary 3rd or 5th order spline can not reproduce the function with high

accuracy. In fact, this gives unphysical magnetic fields, e.g. with oscillations around the magnetic axis (see Fig. 2). Therefore, a test function $t(s)$ is added to the spline. The coefficients R_{mn} and Z_{mn} may contain kinks near $s = 0$. This problem can be solved with the use of a smoothing spline. To create a spline with all these properties, one starts with a usual 3rd order spline $P(s)$. Multiplication with a test function $t(s)$ gives $Sp(s) = t(s)P(s)$ with $t(s) = s^{m/2}$ and $m = 0, 1, \ldots$, which is given from the near axis expansion. Now a smoothing term like $\xi\left(P'''(s)\right)^2$ and a least squares approximation $\frac{1}{2}\sum_{i=1}^{N-1}\left\{\sum_j\left[t(s_j)\left(a_i + b_ih_j + c_ih_j^2 + d_ih_j^3\right) - y_j\right]^2\right\} + \frac{1}{2}\left[t(s_N)a_N - y_N\right]^2$ in between the nodes are added. This gives the following function, which has to be minimized:

$$
\begin{aligned}
Sp \;=\; & \frac{1}{2}\sum_{i=1}^{N-1}\left\{\sum_j\left[t(s_j)\left(a_i + b_ih_j + c_ih_j^2 + d_ih_j^3\right) - y_j\right]^2\right\} + \frac{1}{2}\left[t(s_N)a_N - y_N\right]^2 \\
& + \frac{1}{2}\sum_{i=1}^{N-1}\xi_id_i^2 + \sum_{i=1}^{N-1}\left[\alpha_i\left(a_i + b_ih_i + c_ih_i^2 + d_ih_i^3 - a_{i+1}\right)\right. \\
& + \beta_i\left(b_i + 2c_ih_i + 3d_ih_i^2 - b_{i+1}\right) + \gamma_i\left(c_i + 3d_ih_i - c_{i+1}\right)\left.\right] \\
& + \chi_1\left(\mu_1b_1 + \nu_1c_1 + \sigma_1b_N + \rho_1c_N - \kappa_1\right) + \chi_2\left(\mu_2b_1 + \nu_2c_1 + \sigma_2b_N + \rho_2c_N - \kappa_2\right)
\end{aligned}
$$

The last two terms give a complete flexibility in using boundary conditions. It should be noted, that it is quite difficult to find a proper value for the smoothing parameter ξ_i. If the values for ξ_i are too large, the equilibrium will be changed too much, and for too small values the smoothing is not strong enough to obtain a good equilibrium. For comparison of the results, the same procedure was also done for a 5th order spline. It has been seen that the spline reacts more sensitive to the smoothing parameter and that there has been no improvement of the equilibrium.

4. Recalculation of Equilibrium Quantities

The starting point for recalculating the equilibrium is the Clebsch representation of the magnetic field $\mathbf{B} = \nabla s \times \nabla\nu$ [1], with $\nu = \psi'\theta - \chi'\varphi + \lambda$. Here ψ and χ are the toroidal and the poloidal flux, respectively, the prime denotes the derivative with respect to s, and λ is the so called stream function.

Internally, VMEC computes an additional stream function λ to optimize, dynamically and at every radial surface, the convergency rate in Fourier space for the spectral sum $\sum(R_{mn}^2 + Z_{mn}^2)$. In VMEC however, λ is not fully consistent. For consistent recalculation of this internally computed λ, one has to ensure $(\nabla \times \mathbf{B}) \cdot \nabla s = 0$. This says that the current-density lines lie in constant s surfaces. This gives a linear elliptic second order differential equation for λ. This equation is solved using the technique of Fourier transformation. The comparison of a particular Fourier coefficient for λ from VMEC output and the consistently calculated one is shown in Fig. 1. With given λ and $\mathbf{B}$, the poloidal current $J = \int_{longway}\mathbf{B}d\mathbf{l} = \int B_\varphi d\varphi$ and the toroidal current $I = \int_{shortway}\mathbf{B}d\mathbf{l} = \int B_\theta d\theta$ can be calculated [6]. The radial force balance gives $p' = (I'\chi' - J'\Psi')/V'$ where the prime denotes the derivative with respect to normalized toroidal flux s. Integration gives the pressure profile $p(s)$.

5. B-Field Components in Real Space Coordinates

After transformation to cylindrical coordinates the components of the magnetic field are $B_R = [(\chi' - \lambda_{,\varphi})R_{,\theta} + (\psi' + \lambda_{,\theta})R_{,\varphi}]/\sqrt{g}$, $B_\varphi = (\psi' + \lambda_{,\theta})R/\sqrt{g}$ and $B_Z = [(\chi' - \lambda_{,\varphi})Z_{,\theta} + (\psi' + \lambda_{,\theta})Z_{,\varphi}]/\sqrt{g}$ with $\sqrt{g} = R(R_{,\theta}Z_{,s} - R_{,s}Z_{,\theta})$ and $\chi'(s) = \iota(s)\psi'$. When $|\mathbf{B}|$ is computed with the smoothing spline including the test function $t(s)$ for
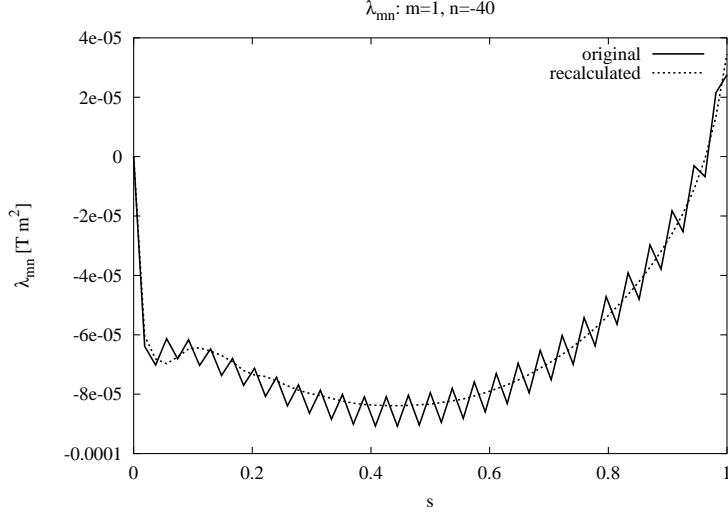
Figure 1: Comparison of a bad mode of stream function λ from VMEC output (solid) with consistent calculated λ (dashed).

R_{mn} and Z_{mn} and the consistently calculated stream function λ, $|\mathbf{B}|$ is well behaved and smooth, as can be seen in Fig. 2. If $|\mathbf{B}|$ is computed without the test function $t(s)$ strong oscillation around the magnetic axis appear.
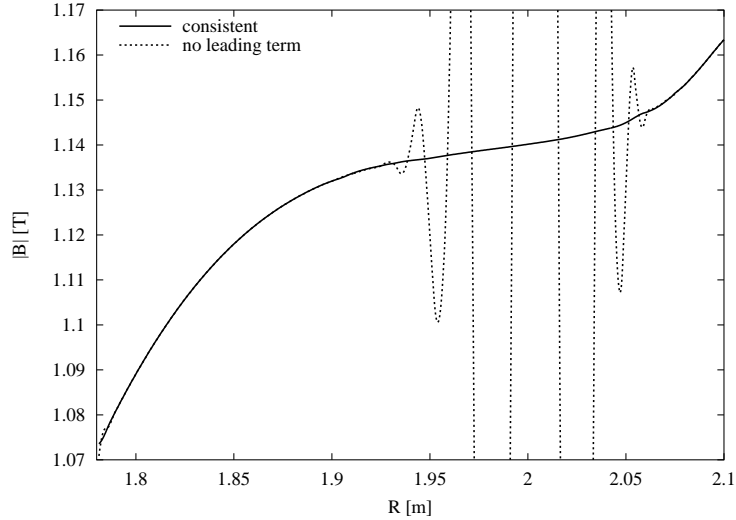

Figure 2: Comparison of the field calculated with consistent stream function λ and splines for R_{mn} and Z_{mn} with (solid) and without (dashed) test function $t(s)$ for a high β-field of W7-AS.

6. Transformation to Boozer Coordinates

To do the transformation from flux coordinates (s, θ, φ) to the Boozer coordinate system [5], the following relations $\theta_B - \iota\varphi_B = \theta - \iota\varphi + \lambda$ and $I\theta_B + J\varphi_B = I\theta + J\varphi + \omega$ have to be solved. The single valuedness of the magnetic field $\mathbf{B}$ with respect to θ and φ has to be taken into account, it is expressed through $\theta_B = \theta + \tilde{\theta}(s, \theta, \varphi)$ and $\varphi_B = \varphi + \tilde{\varphi}(s, \theta, \varphi)$. $\tilde{\theta}$ and $\tilde{\varphi}$ are periodic functions with respect to θ and φ. Substituting the equation for θ_B and φ_B into the first equations in this paragraph, one finds that the functions $\tilde{\theta}$ and

$\tilde{\varphi}$ are given by $\tilde{\theta} = (\iota\omega + J\lambda)/(J + \iota I)$ and $\tilde{\varphi} = (\omega - I\lambda)/(J + \iota I)$. These equations provide the prescription for a transformation from the general magnetic coordinate system (s, θ, φ) to the Boozer coordinate system (s, θ_B, φ_B).

7. Summary
If a **B**-field, based on an equilibrium calculated with VMEC, is to be transformed to real space coordinates, unphysical effects appear around the magnetic axis. To avoid these effects a specially designed spline is used for splining the coefficients R_{mn} and Z_{mn}. This causes slight variations of the equilibrium. Therefore, the stream function λ has to be recalculated consistently before other quantities like currents, components of the **B**-field and the pressure profile may be computed. Further on, R and Z as well as $|\mathbf{B}|$ are transformed to Boozer coordinates. Now a tool is available, which allows a postprocessing of the VMEC output and provides improved equilibria in three coordinate systems. The code is useful in various applications where a representation of the magnetic field in real space is desired, such as ray-tracing or computation of high energy ion orbits with taking Larmor gyration into account.

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