Free-Boundary Axisymmetric MHD Equilibrium

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June 29, 2018

Abstract

The calculation of equilibrium conditions is a common task in the study and modeling of magnetic-confinement experiments for controlled nuclear fusion, in which a high-temperature plasma is confined in a finite region of space by magnetic fields. Given the plasma shape, for toroidal devices with axial symmetry, such as tokamaks, the equilibrium calculation reduces to the solution of an elliptic PDE. In several circumstances, the plasma shape may not be known a priori, or one may desire to also compute the magnetic fields in the volume surrounding the plasma through the calculation of a free-boundary equilibrium. This requires either the coil currents or the magnetic poloidal flux on a curve in the vacuum region to be known ab initio. It is well known how to calculate both, but surprisingly until the introduction of the FREE-FIX code no general tools were available in the fusion community for this task. FREE-FIX is a general tool for calculating coil currents to be used as the input for a free-boundary equilibrium. A new formulation is presented, which considerably reduces the computational cost of the calculation. FREE-FIX performs well for different geometries and experiments. Some possible future applications are also suggested.

1 Introduction and Problem Definition

Equilibrium calculation is commonly the first task that needs to be performed in the analysis of nuclear fusion experiments in the magnetic confinement field of research. Equilibrium calculations can be and are used, both in experiment analysis and in the design phase, as a necessary input

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for evaluating properties such as transport and stability against macroscopic and microscopic modes. In this context, the simplest physical model for the analysis of equilibrium is the ideal magnetohydrodynamic (MHD) model. In general, the properties of a magnetic confinement experiment will be in MHD equilibrium during most of any discharge, highlighting the importance of equilibrium calculations.

Tokamaks are the most advanced line of experiments for reaching controlled nuclear fusion. One of the defining characteristic of the tokamak concept is (with very good approximation) the symmetry of its geometry with respect to the axis located at the geometrical center of the donut-shaped device. Under the assumption of symmetry, the equilibrium problem can be reduced to a two-dimensional elliptic PDE for the magnetic poloidal flux, which can assume different forms depending on the details of the equilibrium model. Small hyperbolic regions may be present in the plasma in special circumstances, [1, 2] which will not be discussed in this work. In many tokamak equilibrium calculations the plasma shape and the value of the magnetic poloidal flux (the main unknown of the problem) at the plasma edge are assigned from input and one solves the equilibrium problem only in the plasma region. We will indicate this type of calculation as “fixed-boundary” equilibrium calculations.

Given a “fixed-boundary” equilibrium, one may be interested in determining a posteriori the magnetic fields in the vacuum region surrounding the plasma. In principle, this could be accomplished by somehow extrapolating the vacuum fields from the fixed-boundary equilibrium. We will not consider this approach (numerically ill posed) in the present work. As an alternative, one could solve the equilibrium problem again, but this time in a region involving both the plasma and the vacuum surrounding it. In this case, the plasma shape will need to be determined self-consistently as part of the solution of the equilibrium problem. We will denote this type of calculation as “free-boundary” equilibrium calculation in the remainder of this work.

A different strategy, namely using the virtual casing principle [3,4], could also be used to determine the vacuum field. The reason why this strategy was not pursued in this work is that a virtual casing calculation requires the accurate knowledge of the poloidal magnetic field on the plasma boundary. Due to the Cartesian grid implementation of FLOW, [5, 6] (the code used for equilibrium calculations in this work) no grid points are situated on the plasma boundary and edge fields can be computed only with a lower accuracy than the fields inside the plasma. In a sense, the approach followed in this work is the most universal approach, as it only requires knowledge of the magnetic fields and current density inside the plasma, i.e. of quantities that any equilibrium code, regardless of the formulation and implementation, will certainly be able to provide.

It is noted that the "fixed-boundary" and "free-boundary" names for the equilibrium calculations described in this work are commonly used in the fusion community. The names come from the fact that the boundary between the plasma and vacuum regions is assigned ("fixed") from input in the first case and determined as part of the problem solution in the second.

It is implied in the definition of the problem that the plasma shape obtained from the free-boundary equilibrium should match the shape defined in the fixed-boundary equilibrium. It is also assumed that any interested user will have access to an equilibrium code capable of solving the free-boundary equilibrium problem.

The input required by a free-boundary solver will depend on the solver, but can in general be reduced to two options: first, the value of the coil currents for each coil surrounding the plasma, or second, the value of the magnetic poloidal flux on a closed curve in the vacuum region. The FREE-FIX code, described in this work, is written to solve the problem described above, that is, calculate coil currents and vacuum magnetic flux on an assigned curve given a fixed-boundary equilibrium. The FREE-FIX code was first introduced in a more compact for in Ref. [7]. Users can then use their free-boundary equilibrium codes to calculate the free-boundary equilibrium.

A few points are worth mentioning before proceeding with the details of the code implementation and results.

First, as posed above this is a standard problem that has been formally solved in the past. However, no general tool exists in the fusion community to obtain a numerical solution for the problem. That means that any scientist needing a tool such as FREE-FIX needs to implement a solution, uselessly multiplying research efforts. We hope that FREE-FIX will become a universal useful tool for the calculation of coil currents and thus for equilibrium calculations. As detailed later, FREE-FIX also contains an innovative solution approach that has not been considered before. As such, it is more than a tool implementing a known solution to a problem of general interest (which we believe to be of value on itself).

Second, FREE-FIX can be used in conjunction with *any* axisymmetric equilibrium code, regardless of the model used to describe the plasma. That is due to the fact that the equations governing the magnetic field in the vacuum, which, as discussed later, are used in FREE-FIX are the same *regardless of the plasma model*. Indeed, the development of FREE-FIX was undertaken to provide the input for the equilibrium solver in the code HYM [8, 9], which includes energetic particles. Moreover, the equilibrium code FLOW [5, 6], which includes macroscopic plasma rotation in the magnetohydrodynamic (MHD) and kinetic models, was used for testing during the code development.

Third, we believe that FREE-FIX may be of value to the community for two additional application.

First, FREE-FIX could benefit real-time equilibrium reconstructions and plasma shape and position control [10]. Typical control schemes assume that the plasma evolves through a series of MHD equilibria [11]. Both position and shape are determined by the coil currents, which are adjusted in real time with feedback controls. Since the calculation speed is crucial for this application, a faster processing of the current corrections given an input in position or shape error, which can be obtained with FREE-FIX innovative approach, will allow for better real-time control.

A second envisioned application has the coil shape and positions as unknowns. In the design of experiments, one needs to determine the positions and currents of coils given, once again, a desired range of plasma shapes and positions. This requires an optimization calculation, given constraints such as the number of coils and their maximum currents. A fast tool for calculating the necessary currents given a plasma shape and a guess for the coil geometry could benefit this type of calculation. It is acknowledged that the speed of calculation for design is not as important as for real-time control; however, a tool for accelerating any numerical calculation can only be beneficial. Some modifications (e.g., modeling coils as finite-size conductors, possibly with non-uniform current distributions, rather than wires, adding probes and hardware of arbitrary shape to the model) would be required in FREE-FIX, which would need to be used as a module for a larger optimization code.

We will now proceed to define the numerical problem in detail (Section 2); in Section 3 the solution method, including details on FREE-FIX's innovative approach is presented; in Section 4 some sample and test calculations are described; a discussion including possible applications and future work is presented in Section 5 and conclusions are given in Section 6.

2 Problem Definition

The present work only considers axisymmetric geometries, i.e., geometries symmetric with respect to rotation around the axis of a cylindrical (R, φ, Z) system of coordinates. In this system of coordinates, it is customary to define the magnetic field as

$$\underline{B} = \underline{B}_p + B_\varphi \hat{e}_\varphi, \tag{1}$$

where the toroidal field B_φ is in the direction of symmetry and the poloidal field $\underline{B}_p$ is the remaining part of the magnetic field. Using the symmetry assumption,

$$\frac{\partial}{\partial \varphi} = 0 \tag{2}$$

and the $\nabla \cdot \underline{B} = 0$ condition, the poloidal component of the magnetic field $\underline{B}_p$ is written as

$$\underline{B}_p = \nabla \psi \times \nabla \varphi, \tag{3}$$

where the poloidal magnetic flux ψ is related to the toroidal component of the vector potential $\underline{A}$ by $\psi = RA_\varphi$. It is important to stress at this point that Eq. (3) only requires the assumption of symmetry, but no other assumption or specific form of the momentum equation governing force-balance.

To fix ideas, the simplest equilibrium model for tokamak plasmas, which is governed by the Grad-Shafranov (GS) equation, [12,13] is briefly discussed. If one assumes that the axisymmetric plasma is described by static ideal MHD equations, the momentum equation is written as

$$\nabla p = \underline{J} \times \underline{B}, \tag{4}$$

where p is the plasma pressure and $\underline{J} = (\nabla \times \underline{B})/\mu_0$ the electric current density. A short manipulation gives the GS equation:

$$\Delta^* \psi \equiv R \frac{\partial}{\partial R}\left(\frac{1}{R}\frac{\partial \psi}{\partial R}\right) + \frac{\partial^2 \psi}{\partial Z^2} = -\mu_0 R^2 \frac{dp}{d\psi} - F\frac{dF}{d\psi} = -RJ_\varphi, \tag{5}$$

where $F(\psi) = RB_\varphi$ and the pressure $p(\psi)$ are functions of the poloidal magnetic flux ψ that need to be assigned from input. Notice that the left hand side of Eq. (5) is the toroidal component of the current density as obtained from Maxwell's equations and will be the same regardless of the equilibrium model and that the poloidal magnetic field is completely determined once the poloidal flux ψ is known. On the other hand, the right hand side of Eq. (5) will depend on the equilibrium model (including e.g. macroscopic rotation, multi-fluid or multi-species effects, gravity) and may assume many different forms. It will be assumed in the remainder of this work that, regardless of the equilibrium model, in the vacuum region the poloidal flux is obtained from

$$\Delta^* \psi = 0, \tag{6}$$

i.e. that no toroidal current flows in the vacuum region.

In order to calculate ψ in a free-boundary equilibrium calculation, one needs to assign (1) the input necessary to calculate the right hand side of Eq. (5) inside the plasma and (2) either the currents in the coils around the plasma or the value of ψ, which is determined from Maxwell's equations once the currents in the coils are known, on a closed curve surrounding the plasma (the computational boundary). The calculation of the coil currents and vacuum ψ on the computational boundary is the purpose of FREE-FIX. The methods implemented for this calculation are described in the next section.

3 Solution Method, Old and New

The calculation of coil currents and vacuum ψ on the computational boundary is based on the Green's function method. The problem has in fact a well-known solution, which is discussed in detail e.g. in Ref. [14][p111]. The starting point of the method is to determine the Green's function of the Δ^* operator introduced in Eq. (5). The expression of the Green's function is found in the literature [14]:

$$G(R, Z; R', Z') = \frac{1}{2\pi}\frac{\sqrt{RR'}}{k}\left[\left(2 - k^2\right) K(k) - 2E(k)\right], \tag{7}$$

where $E(k)$ and $K(k)$ are complete elliptic integrals [15] and

$$k^2 \equiv \frac{4RR'}{(R + R')^2 + (Z - Z')^2}. \tag{8}$$

In this work, Green's functions are calculated using the Numerical Recipes [16] routines *rf*, *elle* and *ellf*. Then, if the position of the coils, the coil currents I_i and the plasma shape and current density are known, ψ can be expressed at any point in the vacuum as

$$\psi(R', Z') = \int_P G(R, Z; R', Z')J_\varphi(R, Z)dRdZ + \sum_{i=1}^{N_c} G(R_i^c, Z_i^c; R', Z')I_i, \tag{9}$$

where the integral is taken over the plasma region, the sub- or super-script "c" indicates the N_c coils, which have been represented as wires of infinitesimal cross section for simplicity.

In order to calculate the coil currents, Eq. (9) is applied to points on the (prescribed) plasma boundary, under the reasonable assumption that no singular currents are present on the plasma boundary. The integral in Eq. (9) is evaluated with a simple mid-point integration, which proved to be sufficient for our purposes. Since the plasma boundary is defined by a curve Γ over which $\psi = const.$ (assumed to be $\psi = 0$ in this work as is standard practice in equilibrium calculations), Eq. (9) evaluated in any (R', Z') point on the plasma boundary becomes a linear equation in the N_c unknowns corresponding to the coil currents.

Intuitively, one may try to calculate the N_c unknowns by evaluating Eq. (9) on N_c distinct point on the plasma boundary Γ. We will call this the "direct method". This method is implemented in FREE-FIX using the Numerical Recipes [16] routines *ludcmp* and *lubksb* and is included mainly for reference, as it invariably fails to return appropriate values for the coil currents. Indeed, free-boundary equilibria calculated using the coil currents obtained with the direct method produce plasma shapes very different from the prescribed one.

The known successful method uses a minimization approach, evaluating Eq. (9) in a number of points on the plasma boundary $N_{fit} \gg N_c$ and finding the N_c currents that minimize the difference between the calculated and prescribed values of ψ on the N_{fit} points. Both a least square fit (LSF) and a singular value decomposition (SVD) method were implemented in FREE-FIX. The Numerical Recipes [16] routines *lfit*, *gaussj* and *svdfit*, *svdcmp*, *svbksb* were used for the LSF and SVD solution respectively. Direct calculation shows that there is no noticeable difference between the LSF and the SVD solution. If enough points are used for the minimization both methods succeed in providing the input, i.e. the set of coil currents, needed to reproduce the desired plasma shape. In the cases tested in this work, which have a number of coils $N_c \sim 10 - 15$, a few tens to ~ 100 points were needed for satisfactory results.

Even though the method does in general return satisfactory results, not every desired plasma shape can be reproduced with the same set of coils and the method may still fail if the desired shape is experimentally unfeasable.

The work described so far amounts to creating a universal tool for the community, which solves a known problem with known techniques. The innovative part of this work is in the new method, which allows the solution of the numerical problem considered in this work with a reduced amount of computational cost.

We start by observing that the methods described above impose (in an exact or least-square fit sense) the calculated $\psi = 0$ curve Γ_c to *intersect* the desired curve Γ in a finite number of points. A stronger condition is to require Γ_c to be *tangent* to Γ. This was implemented in FREE-FIX, resulting in a method, which imposes two conditions in each selected point on Γ, namely that for the calculated ψ first $\psi = 0$ on Γ and second $\nabla\psi$ be perpendicular to Γ. The second condition is assigned by calculating the unit vector $\hat{\tau}$ tangent to Γ and imposing

$$\nabla\psi \cdot \hat{\tau} = 0. \tag{10}$$

An advantageous property of Eq. (10) is seen by observing that

$$\begin{aligned} \nabla'\psi(R', Z') = \int_P & \nabla' G(R, Z; R', Z') J_\varphi(R, Z) dR dZ + \\ & + \sum_{i=1}^{N_c} \nabla' G(R_i^c, Z_i^c; R', Z') I_c \end{aligned} \tag{11}$$

and that the necessary derivatives of the Green's function are given by

$$\begin{aligned} \frac{\partial G}{\partial R'} = \sqrt{R} \Bigg(& \frac{\partial k}{\partial R'} R' (4K + k(2(E - 2K) + k(-kK + K + E)) - 4E) \\ & -2(k-1)k \left(k^2 K - 2K + 2E\right) \Bigg) \Big/ \left(4\pi(k-1)k^2\right) \end{aligned} \tag{12}$$

and

$$\begin{aligned} \frac{\partial G}{\partial Z'} = \sqrt{R} \Bigg(& E((k(k+2) - 4) \frac{\partial k}{\partial R'} R' - 4(k-1)k) - (k-1) \\ & \left(\left(k^2 + 4\right) \frac{\partial k}{\partial R'} R' + 2k \left(k^2 - 2\right) \right) K \Bigg) \Big/ \left(4\pi(k-1)k^2\right), \end{aligned} \tag{13}$$

where the argument k has been omitted from the elliptic integrals E and K for brevity. Remarkably, no derivatives of the equilibrium quantities are needed and the only elliptic integrals that need to be evaluated are the same elliptic integrals that are needed in the calculation of the Green's function used in Eq. (9). This is especially useful because most of the computational cost in the calculation of the unknown coil currents I_c is in the evaluation of the elliptic integrals E and K. Thus, by imposing the two conditions $\psi = 0$ and Eq. (10) in each of N_{fit} points on Γ one needs about half the computational cost needed to impose $\psi = 0$ in $2N_{fit}$ points.

The FREE-FIX implementation proved that the method just described allows to reproduce the desired plasma shape with a number of fit points much smaller than what is needed by the standard approach. In fact, a number of points smaller than the number of unknowns (i.e. of coil currents) can be sufficient.

The positioning of the fit points on the boundary influences the minimum number of points needed to obtain a good approximation of the desired shape. Two different strategies were found to produce similarly good results. First, the "equal distance" approach, which requires that the distance between two consecutive points be the same for any couple of consecutive points. The distance d between two points is simply defined as

$$d \equiv \sqrt{(R_1 - R_2)^2 + (Z_1 - Z_2)^2}, \tag{14}$$

where the subscripts 1 and 2 refer to any two consecutive points. Second, the "equal arc length" approach, which requires consecutive points to be equally spaced in the length of the curve surrounding the plasma (meaning that the distance between any two consecutive points measured along the curve surrounding the plasma is the same). If the number of test points is sufficiently large, typically a few tens, differences between the various strategies often become negligible. A summary of the different methods and options used in this work is contained in B.

Before proceeding with testing the performance of the various methods, it is useful to define a quantitative measure of the difference between the desired and calculated curve.

Given the desired and calculated curves Γ and Γ_c, both of them can be parametrized with the same angle θ, defined as a standard angular coordinate measured from the horizontal axis, with the axis origin fixed at geometric the center of the desired plasma shape. For any value of θ, the distance

$$\delta = \sqrt{(R_\Gamma - R_{\Gamma_c})^2 + (Z_\Gamma - Z_{\Gamma_c})^2}, \tag{15}$$

is taken as a local error measure for the assigned value of θ. A normalized value $\hat{\delta}$ is obtained dividing by the (desired) local minor radius of the plasma, $r(\theta)$, which is simply the distance between the point on Γ and the geometric center of the plasma, $R = R_0$, $Z = Z_0$ ($Z_0 = 0$ in this work, as is common in tokamak calculations). We define the $< L_2 >$ and $< \hat{L}_2 >$ norms as the average values of δ and $\hat{\delta}$ over a number of points uniformly distributed in θ. Similarly, the L_∞ and $\hat{L}_\infty$ norms are given by the maximum values of δ and $\hat{\delta}$ over the same test points. These norms will test for both the shape and position of the plasma and may return somewhat pessimistic results because of the way the parametrization is defined. This will happen for example in case of a slight horizontal shift of the top or bottom of the calculated boundary with respect to the desired one, which will cause a larger mismatch in the vertical direction. An example is shown in Fig. 1, where three different plasma shapes are plotted. The original plasma shape

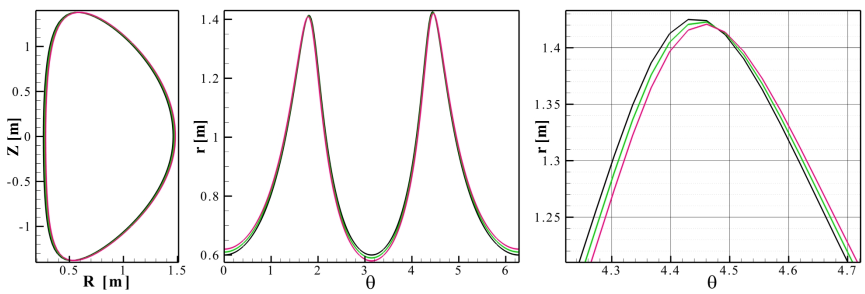

Figure 1: Left: original plasma shape (black) and shifted plasma shapes (colors); center: radius vs. θ; right: zoom of radius vs. θ.

is shown in black, the same shape shifted by 1 cm to the right is in green and still the same shape, but shifted by 2 cm to the right in red. Shapes are shown on the left, radii $r(\theta)$ in the center and a zoom of $r(\theta)$ around the maximum value of r on the right. The plot on the right in particular shows how a small horizontal mismatch in the plasma shape can cause a larger difference in radius for a given θ, since the segment connecting the point on the top of the plasma to the plasma center is close to vertical.

Before proceeding with testing FREE-FIX for actual tokamak equilibrium calculations, another few considerations are necessary.

First, it is observed that the plasma shape in experiments can be measured only with a finite amount of precision and error bars of the order of a cm are typically included when the plasma shape is measured in an experiment [17, 18]. Thus, inaccuracies in the plasma shape obtained from free-boundary calculations of the order of the experimental uncertainties are not going to be particularly meaningful for the problem considered in this work.

Second, it should be recognized that any inaccuracies in free-boundary calculations can be due to errors in the coil currents calculated by FREE-FIX or errors in the equilibrium calculations themselves, which depend on the equilibrium code and not on the input provided by FREE-FIX. The equilibrium calculations presented in this work were performed using an extension of the code FLOW [5] developed to calculate free-boundary equilibria. Since no other equilibrium solvers were available to us at the time of this study, it was not possible to evaluate the accuracy of the free-boundary solver implemented in FLOW. A detailed description of FLOW is contained in Ref. [5], but a brief summary of its numerical solver is included in Appendix A for completeness.

All calculations presented in this work were performed with uniform Cartesian grids with 128 point in each direction. Increasing the spatial resolution to 512 points in each direction does not produce any noticeable variation in plasma shape or errors as defined by the norms introduced above.

4 Sample Application

FREE-FIX was used to calculate the input for free-boundary equilibria of two of the major US tokamaks, NSTX [19] and DIII-D [20, 21]. For each of the equilibria shown in this section, a fixed-boundary equilibrium with an assigned boundary shape was computed first. The calculated equilibrium ψ was then used as an input for FREE-FIX to produce the value of ψ on a closed "box" around the plasma needed as boundary condition by FLOW in the fashion described in section 3. A new free-boundary equilibrium was computed and compared to the desired (fixed-boundary) one.

For each experiment a set of coils approximating the real coil geometry was used. The coil geometry was determined in part by trial and error, with the purpose to keep the coil geometry as close as possible to the experimental one and the number of coils as small as possible for simplicity, but still be able to obtain reasonably accurate plasma shapes. No limitation on the number or position of the coils is hardwired into FREE-FIX. As mentioned earlier, coils are represented as wires of infinitesimal cross section. This reduces the accuracy of the resulting magnetic field near the coils. However, preliminary studies performed during the development of FREE-FIX showed that this has little effect close to the plasma. The input used for all the calculations presented in this section is available from FREE-FIX' website. [22]

The main findings of a sample "spherical-tokamak" NSTX equilibrium calculation are collected in Fig. 2. The figure shows the plasma shape determined by four free-boundary equilibria (in color) and compares them with the desired plasma shape (black). The slightly jagged appearance of the target shape is due to the limited number of grid points used in the shape representation. A smooth profile is used as input and in all calculations. The free-boundary equilibria are obtained using the different methods described in Section 3. Figure 2(a) shows the result obtained using the "direct method", i.e. by using a number of points on the prescribed boundary equal

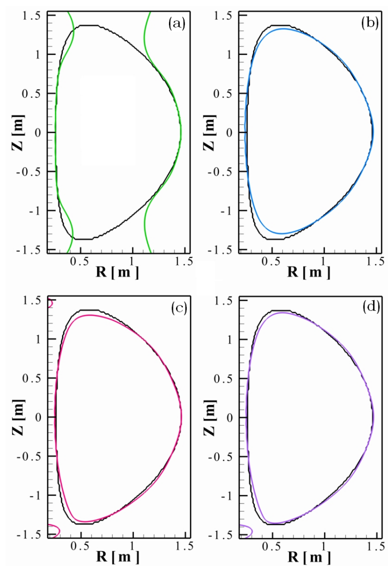

Figure 2: Desired plasma shape (black) and plasma shapes calculated with FREE-FIX input for an NSTX equilibrium. Input is calculated with the direct method (a), an LSF with 100 points uniformly distributed in θ (b), an SVD including gradients of ψ and 7 points (c), an LSF with 100 equidistant points on the desired boundary (d). All equilibria were calculated with FLOW.

to the number of coils and solving the linear system for the coil currents without any fitting. The results confirm what was anticipated in Section 3, i.e. that the direct method does not produce satisfactory results. Figure 2(b) is obtained from an LSF FREE-FIX calculation using 100 points uniformly distributed in θ. It is seen that the desired plasma shape is reproduced with reasonable accuracy. A good approximation of the desired shape is also obtained in Fig. 2(c), which corresponds to a FREE-FIX SVD calculation using only 7 points, in which both the $\psi = 0$ condition and Eq. (10) are imposed. We stress that the number of coil currents in this calculation is 9 plus the central solenoid's, meaning that a number of points smaller than the number of unknowns is sufficient to reproduce the desired plasma shape. Finally, Fig. 2(d) is obtained with the same method and number of points as Fig. 2(b), but using points determined with the "equal distance" approach, more uniformly distributed on the plasma shape.

The same methods are tested for a "standard-tokamak" DIII-D equilibrium and the results, qualitatively similar to the ones shown in Fig. 2, are shown in Fig. 3. The slightly jagged appearance of the target shape is due

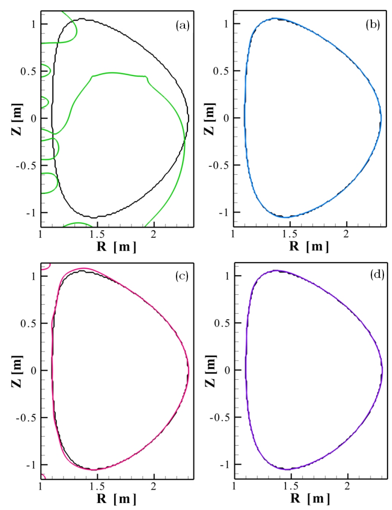

Figure 3: Desired plasma shape (black) and plasma shapes calculated with FREE-FIX input for a DIII-D equilibrium. Input is calculated with the direct method (a), an SVD with 100 points uniformly distributed in θ (b), an LSF including gradients of ψ and 14 points (c), an SVD with 100 equidistant points on the desired boundary (d). All equilibria were calculated with FLOW.

to the limited number of grid points used in the shape representation. A smooth profile is used as input and in all calculations. The direct method, shown in Fig. 3(a) fails again to reproduce a satisfactory plasma shape. A very good match between the desired and calculated shapes is obtained using an SVD calculation with 100 points on the plasma boundary distributed using two different strategies, Fig. 3(b) and 3(d). In this case, the strategy used to select the point positions does not have a noticeable effect on the quality of the result. If the calculation is repeated also including gradients of the target ψ, a good approximation of the desired shape is obtained with little more than 10 points [14 in Fig. 3(c)]. For all calculations shown in Fig. 3, 16 coil currents plus the central solenoid current need to be calculated. Thus, using gradients to impose Eq. (10) once again allows to obtain a reasonable approximation to the target shape with a number of points smaller than the number of unknowns.

Some more quantitative details on the accuracy with which the desired plasma shape is reproduced by the various methods are given in Table 1. The table shows, for different methods as defined in Appendix B (see in particular Table 3) and different numbers of N_{fit} points on the plasma boundary, distributed at either "constant-θ" ("coords"=1) or constant-distance ("coords"=10), four different figures of merit. Those are the average and maximum distance between the desired and obtained shape, with or without normalization with respect to the radius length. For each of methods 2, 4

Method	N_{fit}	coords	$< L_2 >$	$< \hat{L}_2 >$	L_∞	$\hat{L}_\infty$
2	30	1	3.04×10^{-4}	3.23×10^{-4}	1.66×10^{-2}	1.70×10^{-2}
2	50	1	1.77×10^{-4}	2.11×10^{-4}	8.10×10^{-3}	8.00×10^{-3}
2	75	1	1.78×10^{-4}	2.11×10^{-4}	8.17×10^{-3}	8.07×10^{-3}
2	100	1	1.78×10^{-4}	2.11×10^{-4}	8.18×10^{-3}	8.08×10^{-3}
2	25	10	1.48×10^{-4}	1.88×10^{-4}	6.73×10^{-3}	6.76×10^{-3}
2	30	10	1.62×10^{-4}	1.98×10^{-4}	7.49×10^{-3}	7.05×10^{-3}
2	50	10	1.61×10^{-4}	1.98×10^{-4}	7.56×10^{-3}	7.20×10^{-3}
2	75	10	1.61×10^{-4}	1.98×10^{-4}	7.60×10^{-3}	7.21×10^{-3}
2	100	10	1.61×10^{-4}	1.98×10^{-4}	7.60×10^{-3}	7.21×10^{-3}
3	100	1	1.78×10^{-4}	2.11×10^{-4}	8.18×10^{-3}	8.08×10^{-3}
4	12	10	1.44×10^{-3}	1.56×10^{-3}	6.00×10^{-2}	5.79×10^{-2}
4	13	10	2.54×10^{-3}	2.78×10^{-3}	1.05×10^{-1}	1.03×10^{-1}
4	15	10	9.36×10^{-4}	1.05×10^{-3}	5.43×10^{-2}	5.41×10^{-2}
4	20	10	6.27×10^{-4}	6.93×10^{-4}	2.62×10^{-2}	2.69×10^{-2}
4	50	10	2.21×10^{-4}	2.73×10^{-4}	9.13×10^{-3}	9.05×10^{-3}
4	100	1	1.64×10^{-4}	2.15×10^{-4}	7.20×10^{-3}	8.37×10^{-3}
11	20	10	4.50×10^{-4}	4.86×10^{-4}	3.32×10^{-2}	3.07×10^{-2}
12	13	10	2.39×10^{-3}	2.54×10^{-3}	1.32×10^{-1}	1.39×10^{-1}
12	14	10	7.17×10^{-4}	7.73×10^{-4}	4.32×10^{-2}	3.99×10^{-2}
12	15	10	5.08×10^{-4}	5.58×10^{-4}	2.22×10^{-2}	1.99×10^{-2}
12	20	10	7.54×10^{-4}	8.21×10^{-4}	3.45×10^{-2}	3.33×10^{-2}
12	50	10	2.77×10^{-4}	3.30×10^{-4}	1.29×10^{-2}	1.25×10^{-2}

Table 1: DIII-D error table. Four different measures of error in the obtained shape are shown for several methods and number of boundary points.

and 12, the first entry corresponds to the minimum number of points needed to obtained a closed plasma boundary. The main message to be taken from Table 1 is that "good results" (as identified in Fig. 3) have average distances from the desired shape of the order of 10^{-4} (typical radii are ~ 1 meter, so normalized figures are similar to unnormalized ones) and maximum distances slightly less than 10^{-2}. Methods using Eq. (10) (4 and 12) can provide a reasonable approximation to the desired shape with a much smaller number of points than needed by the standard method. A point distribution evenly spaced in θ (1) does not perform as well as other strategies (10 for equal-distance). Also, no difference is seen between SVD and LSF (compare methods 2 and 3). Our conclusion from this application is that FREE-FIX performs well in reproducing the shape of standard tokamaks plasmas.

After considering a highly shaped spherical tokamak and a standard tokamak shape, it is worthwhile to briefly consider other possible shapes to gain some insight on the versatility of the code. Four additional equilibria are considered and presented in Fig. 4. The equilibria represented in the

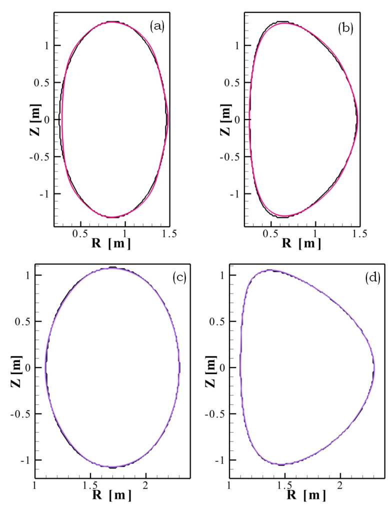

Figure 4: Desired plasma shape (black) and plasma shapes calculated with FREE-FIX input (color) for an NSTX-like elliptical equilibrium (a), a symmetric, mildly shaped NSTX equilibrium (b), a DIII-D-like elliptical equilibrium (c) and a DIII-D equilibrium with flow (d). Input is calculated with the same normalized SVD method with 100 points uniformly distributed in θ for all equilibria. All equilibria were calculated with FLOW.

figure correspond to (a) an NSTX-like elliptical equilibrium, (b) a symmetric, mildly shaped NSTX equilibrium, (c) a DIII-D-like elliptical equilibrium and (d) a DIII-D equilibrium with flow. The DIII-D elliptical equilibrium is calculated using a reduced set of coils (9 instead of 16), to highlight how in some cases good results can be obtained with relatively simple coil arrangements. FREE-FIX was ran for all four equilibria with the same method, number of points and point distribution strategy.

For both NSTX and DIII-D an elliptical shape is fairly non-standard, but can be reproduced with the standard set of coils (or even a reduced one). The NSTX shaped equilibrium is less elongated than the one used earlier. This results in a more accurate match between desired and obtained plasma shapes than for the more highly shaped one (see Table 2 and compare Figs. 2 and 2). The DIII-D equilibrium with flow has the same shape and coils as the reference DIII-D equilibrium. The resulting accuracy is very similar, but not identical. This is due to the fact that the two equilibria have different current density distributions, which are determined by the right hand side of the (modified) Grad-Shafranov equation, in turn determined by the input information on the equilibrium type.

A summary of the error evaluation for the equilibria described above is shown in Table 2. The two equilibria introduced earlier in this work are included for reference. free-boundary equilibria are successfully obtained

Equilibrium	$< L_2 >$	$< \hat{L}_2 >$	L_∞	$\hat{L}_\infty$
NSTX ellipse	1.20×10^{-3}	1.68×10^{-3}	3.04×10^{-2}	5.06×10^{-2}
NSTX shaped	8.28×10^{-4}	8.57×10^{-4}	2.90×10^{-2}	2.44×10^{-2}
DIII-D ellipse	3.43×10^{-4}	4.39×10^{-4}	1.05×10^{-2}	1.28×10^{-2}
DIII-D with flow	1.64×10^{-4}	2.16×10^{-4}	6.86×10^{-3}	8.53×10^{-3}
NSTX	1.96×10^{-3}	1.74×10^{-3}	1.07×10^{-1}	7.61×10^{-2}
DIII-D	1.64×10^{-4}	2.15×10^{-4}	7.20×10^{-3}	8.37×10^{-3}

Table 2: Error table for NSTX and DIII-D equilibria. All calculations are performed with the same approach and number of points. The NSTX and DIII-D equilibria described earlier are included for reference.

with FLOW using FREE-FIX to generate the necessary input for all the shapes considered in Fig. 4. It can be remarked that shapes that are close to the shape for which the coil system was designed (e.g., mildly shaped plasmas) can be reproduced with better accuracy than shapes different from the experimental shapes, even if the shape itself is simple (e.g. an ellipse).

As a final note, we did not include any detailed comparison of the plasma property for the input (fixed-boundary) and output (free-boundary) equilibria. The reason is that if the plasma shape (the $\psi = 0$ curve) is fixed, the solution of the equilibrium inside the plasma is also fixed, since it is the solution of the same elliptic differential equation given the value of the unknown on a closed curve. Therefore, a good match for the plasma shape will automatically result in a good match of the solution inside the plasma. In conclusion, the errors in the plasma shape used above are the best metrics for the quality of the free-boundary equilibrium. Even if we did not show that explicitly, it was verified that all meaningful plasma parameters are matched well if the plasma shape is reproduced accurately.

5 Discussion and Future Expansions

Some additional extensions of the code that would be helpful to the community can be envisioned.

One point of general interest is the possibility to impose the location of X-points on the plasma surface. From the point of view of the standard method, an X-point is no different from any other point of the plasma boundary. However, the poloidal magnetic field, and thus $\nabla\psi$, vanish in the X-point and the plasma surface has a non-smooth shape, meaning that the unit vector $\hat{\tau}$ tangent to the plasma surface assumes different values if one approaches the X-point from two different directions along the plasma boundary.

An option for the presence of a single X-point was included in FREE-FIX. The approach is to impose two sets of conditions in the X-point using two different unit vectors $\hat{\tau}$ in imposing Eq. (10). This will automatically result in two distinct equations for linear combinations of the components of $\nabla\psi$ in the same point, which will be satisfied only if both components of $\nabla\psi$ are independently vanishing. The equation for the value of ψ is repeated, but this does not cause any issue in the minimization process.

Since the code FLOW does not explicitly allow for an X-point on the boundary, the option was tested by modifying ad hoc the direction of $\hat{\tau}$ in the assigned X-point. The resulting equilibrium (not shown) is very similar to the original one, but with the shape of the plasma being "pulled" in the direction of the assigned X-point. The method can trivially be extended to a double-null geometry. It is emphasized that a proper treatment of X-points requires a self-consistent equilibrium calculation that includes X-points. Thus, the treatment will be further pursued when users' need arises. However, the structure of the treatment is already in place and will only require a minimal effort to be adapted to a different equilibrium description.

A further point worth a brief discussion is the presence of structures in the "vacuum region", such as probes or other hardware, including the first wall. Any physical object that needs to be included in the calculation will have a finite resistivity, which will allow the magnetic field to penetrate into it in a finite amount of time. Considering that resistive diffusion times are typically large with respect to MHD times, [23] it is reasonable to approximate the shapes under consideration as made of superconductive materials, in which the magnetic field cannot penetrate and ψ = constant. Any additional piece of hardware included in the calculation will provide one more condition (ψ = constant on the surface of each object) and one more unknown (the value of ψ on the surface) to be included in the minimization calculation. The shapes of the ψ = constant surfaces then need to be included in the free-boundary equilibrium calculation. Any other reasonable condition involving ψ and possibly $\nabla\psi$ on the structures present in the vacuum region can be included in the model in a similar way. Since the presence of structures in the vacuum region is not allowed by FLOW, we could not explore this issue in FREE-FIX.

6 Conclusions

In this work, the code FREE-FIX was presented in more detail than in Ref. [7]. FREE-FIX calculates the coil currents and the value of $\psi(R, Z)$ on an assigned closed curve outside the plasma to be used as input for free-boundary equilibrium codes. The required input for FREE-FIX is a desired plasma shape and plasma equilibrium properties (i.e., a fixed-boundary equilibrium). This is a well-known problem, but no universal tools are available to the community for its solution, a gap that FREE-FIX is designed to fill.

The main unknowns are the coil currents, obtained using a Green's function method to enforce numerical conditions to be satisfied. Green's function are known from the literature and expressed in terms of elliptic integrals. The required numerical conditions are that the poloidal magnetic flux due to the plasma and coil currents should have an assigned, fixed value on the plasma boundary, typically $\psi = 0$. The standard procedure is to use a least square fit or singular value decomposition to minimize the difference between the desired and resulting shape in a finite number of points, a standard numerical problem.

Numerical tests for the DIII-D tokamak and the NSTX spherical tokamak were performed with the FLOW equilibrium code, showing good agreement between the desired and obtained shape. A variety of shapes, coil configurations and equilibrium models was tested with success. Remarkably, good agreement can be found with a small number of points, even smaller than the number of unknowns. That is made possible by the innovative idea introduced in FREE-FIX for matching the desired shape. The new condition is to require that $\nabla\psi$ be normal to the desired plasma shape, i.e. that the $\psi = 0$ curve be tangent to it. The advantage of this numerical method is that the condition on the poloidal magnetic flux gradient only depends on the same elliptic integral as the $\psi = 0$ condition. Since almost all of the computational cost is in calculating elliptic integrals, this results in a computational cost that is only about half of what would be required by imposing the same number of conditions, but only using the $\psi = 0$ requirement. Moreover, the condition on the derivative proves to be "stronger" than the condition on the value of ψ, in the sense that for the same (small) number of equations a satisfactory result may be obtained when two conditions are imposed in each point, while no good solution is found if only one condition per point is imposed. It was shown that the choice for the location of the points where the conditions are enforced is of critical importance for small numbers of points. Various error estimates were introduced to give quantitative evaluations of the accuracy of the result.

FREE-FIX is freely distributed to the community and it is our hope that other scientists will benefit from its use. An impact may also be made for applications different from the ones described in this work. In particular, it is suggested that the fast algorithm introduced in this work for determining the boundary condition needed for a free-boundary equilibrium could benefit real-time equilibrium reconstructions used for plasma shape and position control and optimization calculations in the design of experiments.

7 Acknowledgments

This work was performed under DOE grant DE-FG02-93ER54215 and PPPL subcontract S013799-F. Our thanks go to E. Belova for bringing the problem to our attention, to S. Gerhardt for his help with NSTX data, to S. Jardin, A. Cerfon, J. Hanson and J.P. Freidberg for useful discussion and to C. Sovinec for his encouragement.

A Brief Description of FLOW

The equilibrium code FLOW was used for all equilibrium calculations in this work. FLOW is written in Cartesian coordinates and uses a finite-difference, red-black, multi-grid SOR solver to calculate the magnetic poloidal flux $\psi(R, Z)$. When needed (i.e. in the presence of macroscopic rotation) the plasma mass density is calculated from a Bernoulli-type algebraic equation with a combination of bisection and Newton-Raphson methods.

The free-boundary version of the code, although in existence for several years, has not been documented elsewhere and is in fact the main topic of a future publication. For the purpose of the present work, it suffices to say that an assigned value of ψ (typically $\psi = 0$, although the choice of a different value is allowed from input) is used to separate the plasma ($\psi > 0$) from the vacuum ($\psi < 0$) region. In the plasma region the RHS of the GS-like equation solved by FLOW is assigned using input "free-functions" of the poloidal magnetic flux ψ. In the vacuum region, the RHS (proportional to the toroidal current density J_φ) is identically set to 0. Note that with this definition J_φ can be discontinuous at the free-boundary interface.

Since it is possibile to have positive values of ψ outside the last closed flux surface (i.e. the plasma edge), FLOW calculates the $\psi = 0$ curve at each iteration and defines all points outside the curve to be vacuum points. The curve is obtained by interpolating ψ over the domain with a two-dimensional spline approximation, then a secant, false-position root finder is used to calculate the value $r(\theta)$, for which $\psi = 0$ in a finite number of points. Here r is a radial coordinate measured from the geometric center of the plasma and θ is the usual standard angle variable. In the case where a closed $\psi = 0$ curve is not found [see Figs. 2(a) and 3(a)], the plasma extends to the edge of the computational domain.

B Summary of Solution Methods

For convenience, all the numerical methods and options referenced elsewhere in this work are summarized here. The methods and corresponding option number are listed in Table 3.

The first solution method (1) implemented in FREE-FIX is the "direct method", in which the number of points on the boundary and thus of equations is equal to the number of currents that need to be determined. This method only assigns the value of ψ on the boundary as condition. Currents are calculated from the exact solution of the linear system formed by the $\psi = 0$ equation repeated in the appropriate number of distinct points. The next methods available to users are a singular value decomposition (2) and a least square fit method (3) that assign the value of ψ on the boundary in a number of points larger than the number of coil currents to be calculated. The major innovation introduced in this work for the calculation of coil currents is the use of the condition that the calculated $\psi = 0$ curve be tangent to the desired $\psi = 0$ curve. An LSF calculation is used to impose both the value of ψ and the tangent condition on a number of points larger than half the number of coil currents (4). If one imposed the two conditions per point in a number of points equal to half the number of unknowns, a linear system that can be solved exactly is again obtained (5). In this case, only the $\psi = 0$ condition is imposed in one of the points if the number of unknowns is odd. We observe at this point that the two conditions imposed

Method	Description
1	exact
2	singular value decomposition
3	linear least square fit
4	linear least square fit with gradients
5	exact with gradients
11	weighted SVD fit
12	weighted SVD fit with gradients

Table 3: Solution method options

in methods (4) and (5) as expressed by $\psi = 0$ and Eq. (10) have different physical dimensions. Moreover, in regions where the gradient of the unknown is small, a small mismatch in the numerical value of ψ can cause a relatively large difference in plasma shape. These two ideas are used for the next two methods, method (11), in which only the $\psi = 0$ equation is used and all equations are normalized to the local value of $|\nabla\psi|$ and method (12), in which Eq. (10) is also used and normalized to $|\nabla\psi|/r$ to obtain equations with the same physical dimensions.

All methods are summarized in Table 3. In general, methods (4), (11) and (12) give the best results. For highly shaped plasmas such as NSTX, typically method (12) performs better than method (4) for the L_∞ norm, but it may do so at the expense of the L_2 performance. Users should consider using, introducing, or requesting the performance metric that best represents the goal of the calculation (e.g., most similar plasma volume, best match for desired elongation, best match for position etc.).

Performance also depends on the strategy chosen to distribute points on the boundary, the more so for smaller numbers of points. The available options are described in Table 4. In general, options 10 and 11 give the best

Value	Description
1	Inserts points at constant θ spacing.
10	(Approximately) calculates the length of the boundary, then distributes points at equal distances. **Computationally expensive!** Does not work well if number of points is low.
11	(Approximately) calculates the length of the boundary, then distributes points at equal arc length distances.

Table 4: Main options for point distribution on the $\psi = 0$ curve

and similar results. Typically, differences between the options become less meaningful as the number of points increases. However, different strategies for the point distribution will not necessarily converge to the same free-boundary equilibrium.

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