THREE-DIMENSIONAL FREE BOUNDARY CALCULATIONS USING A SPECTRAL GREEN'S FUNCTION METHOD*

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Abstract

The plasma energy $W_p = \int_{\Omega_p} (\frac{1}{2}B^2 + p)dV$ is minimized over a toroidal domain Ω_p using an inverse representation for the cylindrical coordinates $R = \sum R_{mn}(s) \cos(m\theta - n\zeta)$ and $Z = \sum Z_{mn}(s) \sin(m\theta - n\zeta)$, where (s, θ, ζ) are radial, poloidal, and toroidal flux coordinates, respectively. The radial resolution of the MHD equations is significantly improved by separating R and Z into contributions from even and odd poloidal harmonics which are individually analytic near the magnetic axis. A free boundary equilibrium results when Ω_p is varied to make the total pressure $\frac{1}{2}B^2 + p$ continuous at the plasma surface Σ_p and when the vacuum magnetic field $\mathbf{B}_v$ satisfies the Neumann condition $\mathbf{B}_v \cdot d\Sigma_p = 0$. The vacuum field is decomposed as $\mathbf{B}_v = \mathbf{B}_0 + \nabla\Phi$, where $\mathbf{B}_0$ is the field arising from plasma currents and external coils and Φ is a single-valued potential necessary to satisfy $\mathbf{B}_v \cdot d\Sigma_p = 0$ when $p \neq 0$. A Green's function method is used to obtain an integral equation over Σ_p for the scalar magnetic potential $\Phi = \sum \Phi_{mn} \sin(m\theta - n\zeta)$. A linear matrix equation is solved for Φ_{mn} to determine $\frac{1}{2}B_v^2$ on the boundary. Real experimental conditions are simulated by keeping the external and net plasma currents constant during the iteration. Applications to $\ell = 2$ stellarator equilibria are presented.

1. Introduction

There has been a recent emergence of accurate and efficient Lagrangian spectral codes for computing numerical three-dimensional fixed boundary magnetohydrodynamic (MHD) equilibria with nested magnetic surfaces [1,2]. Convergence problems, which previously limited the usefulness of numerical spectral methods, have been largely eliminated by using a radial discretization for the MHD forces which is accurate throughout the plasma volume and, in particular, near the coordinate singularity occurring at the magnetic axis [3]. Present spectral codes are rapid in comparison with the pioneering BETA code [4] (which uses finite differences in all three dimensions), so that they may be incorporated as part of a viable transport analysis scheme. The MOMCON spectral code [2] is being successfully used in a data analysis mode for both TFTR [5] and PBX [6] tokamak plasmas. It has also been recently adapted to an iteration scheme for obtaining stellarator pressure profiles which are globally stable to local resistive modes [7]. (This is possible in configurations with a global magnetic well.)

Concurrent with this progress, significant development of efficient methods for computing vacuum magnetic fields $\mathbf{B}_v = \mathbf{B}_0 + \nabla\Phi$ has also occurred. Here, $\mathbf{B}_0$ is the field arising from complex coil configurations and plasma currents, and Φ is a single-valued potential necessary (in general) to satisfy $\mathbf{B}_v \cdot d\mathbf{\Sigma} = 0$ on an arbitrary toroidal surface Σ . In the vacuum region interior (or exterior) to the coils, $\mathbf{B}_0 = \nabla\Phi_0$, where the magnetic potential Φ_0 may be expanded in Dommaschk potentials [8]. The resulting Dommaschk series converges rapidly for interior points when the coils are of moderate to large aspect ratio and when their winding law has only a small harmonic content. Vacuum boundary value problems have been analyzed using a Green's function method [9], which has been implemented for both the interior and exterior Neumann problems where $\nabla\Phi \cdot \mathbf{n} = -\mathbf{B}_0 \cdot \mathbf{n}$ is prescribed on the toroidal surface Σ . (Here, $\mathbf{n}$ is the unit normal vector to the surface Σ .) This method invokes Green's theorem to convert Laplace's equation into an integral equation for Φ over the surface Σ . When the surface is described by the inverse representation $R = \sum R_{mn} \cos(m\theta - n\zeta)$, $Z = \sum Z_{mn} \sin(m\theta - n\zeta)$, then Φ may also be expanded in a sine series to convert the integral equation to an algebraic matrix equation. This may be readily inverted to determine Φ on Σ , and it also yields the vacuum magnetic field throughout the entire vacuum region.

Synthesis of fixed boundary spectral codes and the vacuum Green's function code to produce a free boundary equilibrium code is appealing for several reasons. First, the plasma-vacuum boundary Σ_p , on which the integral equation for Φ is evaluated, is also the endpoint on the radial mesh (s) for the interior plasma coordinates. In the spectral decomposition of R and Z used in the plasma, $R_{mn}(s)$ and $Z_{mn}(s)$ are functions of $s = \psi/\psi(1)$, where $2\pi\psi$ is the toroidal flux, and thus $s = 1$ corresponds to Σ_p . Ultimately, force balance on Σ_p will yield boundary conditions determining $R_{mn}(1)$, $Z_{mn}(1)$, and Φ_{mn} . In a continuum limit, these boundary conditions are (i) the continuity of the total pressure, $p + \frac{1}{2}B^2 = \frac{1}{2}B_v^2$, on Σ_p and (ii) $\mathbf{B}_v \cdot \mathbf{n}_p = 0$. Condition (i) affects the plasma force equation by imposing an effective "flux" of magnetic pressure $\propto \mathbf{n}_p(\frac{1}{2}B_v^2)$ at the plasma edge. This represents the coupling of the plasma to the vacuum. Condition (ii) leads to an integral equation for Φ on Σ_p and represents the coupling of the vacuum to the plasma. Viewed from the vacuum, the plasma appears to be a perfect conductor with surface Σ_p . Note that only the value of $\frac{1}{2}B_v^2$ on Σ_p is required to evaluate the edge force balance. Thus, the Green's function technique is well adapted to this problem because it avoids superfluous computations of the vacuum field. Finally, the solution of the vacuum problem using the Green's function method is obtained by fixing the net plasma current and the external coil currents during the iteration of the MHD equations (which is required to obtain a self-consistent free boundary equilibrium). This corresponds closely to experimental conditions where coil currents are under direct external control.

This paper is organized as follows. Section 2 describes the spectral equilibrium code VMEC (Variational Moments Equilibrium Code). Section 3 describes NESTOR (NEumann Solver for TOroidal Regions), which is a code for computing the Neumann problem solution for the vacuum field. The treatment of the coupling between the plasma boundary and the vacuum field is discussed in Section 4. Finally, computed free boundary equilibria for an $\ell = 2$ stellarator configuration are presented in Section 5

2. VMEC – A Fixed-Boundary Lagrangian Spectral Code

2.1 Energy Principle and MHD Forces

The MHD energy principle and the numerical implementation used in VMEC to compute an equilibrium state are discussed in this section. Since VMEC is similar in many respects to the MOMCON code, the reader is referred to Ref. [2] for a discussion of code details.

The basic goal of VMEC is to minimize the total energy – magnetic plus thermal – of a plasma confined in a toroidal domain Ω_p :

$$W_p = \int_{\Omega_p} \left(\frac{1}{2} B^2 + p \right) dV . \quad (2.1)$$

Nontrivial solutions are selected by prescribing the magnetic fluxes on each surface and the mass (or pressure) profile. The magnetic field $\mathbf{B}$ in the plasma is written in a Clebsch representation [4],

$$\mathbf{B} = \nabla s \times \nabla \nu , \quad (2.2)$$

where $s \in (0, 1)$ is a radial flux variable [usually equal to the scaled toroidal flux $\psi(s)/\psi(1)$ in VMEC] and $\nu \equiv \psi'\theta - \chi'\zeta + \lambda$, where θ is the poloidal angle, ζ is the toroidal angle, $\lambda(s)$ is a periodic stream function, and the prime denotes d/ds . Here, $2\pi\chi(s)$ is the poloidal magnetic flux. The contravariant components of $\mathbf{B}$ are then $\mathbf{B} \cdot \nabla s = 0$, $\mathbf{B} \cdot \nabla \theta \equiv B^\theta = (\chi' - \lambda_\zeta)/\sqrt{g}$, and $\mathbf{B} \cdot \nabla \zeta \equiv B^\zeta = (\psi' + \lambda_\theta)/\sqrt{g}$, where $\sqrt{g} = (\nabla s \cdot \nabla \theta \times \nabla \zeta)^{-1}$ is the Jacobian of the transformation between real space and flux coordinates. Thus, $dV = |\sqrt{g}| ds d\theta d\zeta$ and $p = p(s)$ in Eq. (2.1), where $s = \text{const}$ are magnetic surfaces. For nested toroidal surfaces, $\sqrt{g}$ never vanishes. In the case $\lambda = 0$, the magnetic field lines are straight in $\theta - \zeta$ coordinates, since then $B^\theta/B^\zeta = \chi'/\psi' \equiv \iota(s)$, where ι is the rotational transform giving the mean pitch of the magnetic field lines.

The energy density may now be expressed in terms of the magnetic fluxes χ' and ψ' , λ , and the metric tensor elements $g_{\alpha\beta} = R_\alpha R_\beta + Z_\alpha Z_\beta + \delta_{\alpha\zeta} \delta_{\beta\zeta} R^2$ as follows:

$$B^2 = (B^\theta)^2 g_{\theta\theta} + 2B^\theta B^\zeta g_{\theta\zeta} + (B^\zeta)^2 g_{\zeta\zeta} . \quad (2.3)$$

Here, $\zeta = \phi$ and (R, ϕ, Z) are orthogonal cylindrical coordinates. The minimization of W_p in Eq. (2.1) is performed by varying the coordinates R and Z as well as the stream function λ , with either fixed magnetic fluxes or with no net toroidal current. This is then a Lagrangian description of MHD equilibria, which results in the determination of the metric

tensor elements that minimize W and thus describe the mapping between flux coordinate (s, θ, ζ) and cylindrical coordinates.

The dependence of R , Z , and λ on the flux coordinate angles may be expressed by Fourier series:

$$\begin{aligned} R &= \sum R_{mn}(s) \cos(m\theta - n\zeta) , \\ Z &= \sum Z_{mn}(s) \sin(m\theta - n\zeta) , \\ \lambda &= \sum \lambda_{mn}(s) \sin(m\theta - n\zeta) . \end{aligned} \tag{2.4}$$

Equation (2.4) describes magnetic surfaces which are symmetric about a horizontal axis in at least the two toroidal planes $\zeta = 0, \pi$. Since most existing stellarator coils produce surfaces with this symmetry, the use of Eq. (2.4) in VMEC does not pose a severe limitation in practice (and may be easily generalized).

When the series expansions in Eq. (2.4) are used to evaluate the metric tensor elements, the Jacobian $\sqrt{g} = R(R_\theta Z_s - R_s Z_\theta)$, and the contravariant components of $\mathbf{B}$, W_p becomes a functional of $R_{mn}(s)$, $R'_{mn}(s)$, $Z_{mn}(s)$, $Z'_{mn}(s)$, and $\lambda_{mn}(s)$. By varying W_p with respect to these Fourier amplitudes, there results [10,11] a set of mode equations which comprise the spectral decomposition of $\nabla R \cdot \mathbf{F}$, $\nabla Z \cdot \mathbf{F}$, and $\mathbf{J} \cdot \nabla s$, where $\mathbf{F} = \mathbf{J} \times \mathbf{B} - \nabla p$ is the MHD force (which vanishes in equilibrium) and $\mathbf{J} = \nabla \times \mathbf{B}$. When a finite number of modes in Eq. (2.4) is used to minimize W_p (as must be the case in practice), then only those Fourier modes appearing in Eq. (2.4) will be present in the resulting spectrum of $\nabla R \cdot \mathbf{F}$, etc. Thus, for a truncated spectral approximation for R , Z , and λ , the energy principle yields a set of spectral force equations which is optimal with respect to minimizing the energy W_p .

2.2 Boundary Conditions

Note that only λ_{mn} , but not its radial derivative, appears in W_p (through B^θ and B^ζ). Thus, no boundary conditions (other than periodicity in θ and ζ) are needed for the λ -force equation [1,12], $\mathbf{J} \cdot \nabla s = 0$. In contrast, the appearance of R'_{mn} and Z'_{mn} (through the R_s and Z_s terms in $\sqrt{g}$) implies that two boundary conditions in s are required for R and Z . One condition is provided by regularity of the solution [13] at the magnetic axis, $s = 0$, which is an interior singular curve of the flux coordinate system from which the lines $\theta = \text{const}$ emanate. The elliptic nature of flux surfaces in the neighborhood of the magnetic axis thus requires $R_{mn} \rightarrow 0$ and $Z_{mn} \rightarrow 0$ for $m \neq 0$, and $R_{0n} = R_{0n}(0) + O(s)$, $Z_{0n} = Z_{0n}(0) + O(s)$,

as $s \rightarrow 0$. This latter condition is equivalent to requiring that dR_{0n}/ds and dZ_{0n}/ds are finite at $s = 0$.

The remaining boundary condition is related to the shape of the plasma surface Σ_p at $s = 1$. Two possibilities exist, corresponding to fixed and free boundary equilibria. For the fixed boundary case, the shape of Σ_p is prescribed (and held constant during the variation of W). In general, this does not imply fixed values for both $R_{mn}(1)$ and $Z_{mn}(1)$, unless the stream function λ is retained in Eq. (2.4). One of the original motivations [10] for introducing λ was in fact to permit the flexibility to prescribe both $R_{mn}(1)$ and $Z_{mn}(1)$ while simultaneously satisfying the MHD equation $\mathbf{J} \cdot \nabla s = 0$ on the plasma boundary. Thus, the fixed boundary option in VMEC corresponds to fixed values for both $R_{mn}(1)$ and $Z_{mn}(1)$.

The second alternative is the free boundary option. For this case, which is discussed further in Section 4, the MHD force equations $\nabla R \cdot \mathbf{F} = 0$ and $\nabla Z \cdot \mathbf{F} = 0$ are solved at $s = 1$ to obtain equations for $R_{mn}(1)$ and $Z_{mn}(1)$, respectively. In contrast to the fixed boundary case, the values of the derivatives R'_{mn} and Z'_{mn} are (nonlinearly) determined by the edge force balance.

2.3 Role of λ as a Renormalization Parameter

It has been noted that the retention of λ allows prescribed values of $R_{mn}(1)$ and $Z_{mn}(1)$ on Σ_p . The following discussion attempts to indicate why this is a desirable numerical feature, therefore providing justification for retaining $\lambda \neq 0$ in Eq. (2.2). It should also be mentioned that while a term similar to λ appears in the BETA code [4], its role in the spectral code under discussion is quite different. Indeed, since the system of equations $\mathbf{F} \cdot \nabla R = 0$, $\mathbf{F} \cdot \nabla Z = 0$, and $\mathbf{J} \cdot \nabla s = 0$ is linearly dependent [10], the inclusion of λ introduces a degree of freedom which is not available in BETA and which can be exploited to accelerate the series convergence rate for R and Z in Eq. (2.4) on each magnetic surface, $s = \text{const}$. In this role, λ may be considered as a renormalization parameter.

An example shows the importance of λ . Suppose the plasma boundary is an ellipse described by $(R - R_0)^2/R_1^2 + (Z/Z_1)^2 = 1$. The optimal (most concise) spectral representation for this curve is $R = R_0 + R_1 \cos \theta$, $Z = Z_1 \sin \theta$, which contains only $m = 0, 1$ modes. This representation is not unique; indeed, the stretching transformation $\theta = \theta' + \tilde{\lambda}(\theta')$ yields a completely different, and generally much broader, spectrum in the θ' trigonometric expansion

for R and Z . Obviously, this process of spectral “pollution” 14 should be avoided: no additional information about the flux surface shape is included in the θ' coordinate system, and a much greater numerical effort will be required to determine the spectral coefficients by solving the additional nonlinear MHD modal force equations. The difference $\theta - \theta' = \tilde{\lambda}(\theta')$ does, however, convey information about the rate of traversal around the curve, which describes the variation with θ' of the volume element $\propto \sqrt{g}$.

The role of λ as a renormalization parameter for accelerating the Fourier series for R and Z should now be apparent. Without λ , the satisfaction of the equilibrium force equation $\mathbf{J} \cdot \nabla s = 0$ would be accomplished by a particular poloidal distribution of $\sqrt{g}$ which, in general, would be incompatible with an optimally convergent spectral representation for R and Z . Since variation of W with respect to λ guarantees that λ will be determined so that $\mathbf{J} \cdot \nabla s = 0$ is satisfied for any poloidal angle distribution, the relationship between R_{mn} and Z_{mn} for $m \geq 2$ (which ultimately determines the Lagrangian flux coordinate, θ) may be specified so that the spectrum $S_m \equiv \sum_n (R_{mn}^2 + Z_{mn}^2)$ is optimally convergent with respect to m .

For the simple elliptical shape considered previously, $S_m = 0$ for $m \geq 2$ is obviously the optimizing spectrum. In general, flux surfaces are noncircular. Moreover, their equilibrium shape is known only after the MHD force equations $F_R = 0 = F_Z$, together with $F_\lambda \equiv \mathbf{J} \cdot \nabla s = 0$, are solved, so that no *a-priori* optimization is generally possible. Thus, for example, while local constraints such as $R_{mn} = \pm Z_{mn}$ for $m \geq 2$ might be imposed on the basis of the boundary flux surface shape [1], there is no guarantee that the interior flux surfaces will be optimally represented by this prescription. In order to optimize S_m on each surface and for arbitrary flux surface shapes, it is necessary to minimize the mean curve mode number [15]

$$\langle M \rangle \equiv \sum_{m \geq 1} m^{p+1} S_m / \sum_{m \geq 1} m^p S_m \quad (2.5)$$

by considering tangential variations of the form $\delta R / \delta Z = R_\theta / Z_\theta$. In Eq. (2.5), $p > 1$ condenses S_m toward lower mode numbers. The result of this minimization is a set of quadratic equations relating R_{mn} and Z_{mn} :

$$F_c \equiv X(\theta, \zeta) R_\theta + Y(\theta, \zeta) Z_\theta = 0, \quad (2.6)$$

where $X = \sum m^p (m - \langle M \rangle) R_{mn} \cos(m\theta - n\zeta)$ and $Y = \sum m^p (m - \langle M \rangle) Z_{mn} \sin(m\theta - n\zeta)$. In VMEC, Eq. (2.6) is solved together with the MHD equilibrium equations by minimizing

$W_p = \sum \alpha_{mn} F_c^{mn}{}^2$, where α_{mn} are constants $\sim m^{-(p-1)}$ which normalize the eigenvalue spectrum arising from F_c to that of the MHD forces.

Some analytic insight into Eq. (2.6) follows from the formal solution:

$$\begin{aligned} X(\theta, \varsigma) &= Z_\theta \rho(\theta, \varsigma) , \\ Y(\theta, \varsigma) &= -R_\theta \rho(\theta, \varsigma) . \end{aligned} \tag{2.7}$$

Equation (2.7) shows that the optimal relation between the R and Z spectra is not generally a local one in Fourier space, but is like a polar (or “quasi-polar”) coordinate constraint, with ρ the effective polar radius. Since R_θ and Z_θ tend to be dominated by their $m = 1$ components, Eq. (2.7) is indeed a polar representation for X and Y .

2.4 Radial Discretization of the Energy

Equation (2.4) converts W_p into “exact” integrals over the angular coordinates. A remaining integral over s must be performed numerically. The radial discretization of B^2 not only affects the value of W_p computed on finite s -grids, but also directly influences the discrete representation of the MHD forces and the temporal convergence of the numerical scheme (basically, a conjugate gradient method) used to find the equilibrium state. Although adaptive grid techniques exist [16] for solving the coupled second-order ordinary differential equations in s for the mode amplitudes of R and Z (corresponding to an infinite s -grid), these methods have yet to be successfully applied to a configuration where many Fourier modes are present. Thus, VMEC employs a mesh in s .

The relative merits of various discretization schemes may be compared on the basis of the grid convergence properties of W_p . For second-order differencing schemes, it can be shown [1] that:

$$W_p = W_\infty + \sum_{n=1} \alpha_n (\Delta s)^{2n} \tag{2.8}$$

where $\Delta s = 1/(N_s - 1)$ and N_s is the number of radial grid points. Typically, $|\alpha_1| \geq |\alpha_n|$, so that the $n = 1$ term in Eq. (2.8) quickly dominates as $\Delta s \rightarrow 0$. Thus, a radial discretization is ranked better or worse depending on whether its $|\alpha_1|$ is smaller or larger. Factors of ten variation of $|\alpha_1|$ have been observed between different radial discretizations [3] .

The primary factor influencing $|\alpha_1|$ seems to be the radial discretization of the stream function λ . In the MOMCON [2] and BETA [4] codes, $\lambda_j \equiv \lambda(s_j)$ is represented on the same integer mesh as $R_j \equiv R(s_j)$ and $Z_j \equiv Z(s_j)$, so that the discretized covariant components

B_θ^j and B_z^j in the λ force equation are also on the integer mesh. This requires the quantity $(v^j)^2/\sqrt{g}^{j+\frac{1}{2}}$ to be averaged over adjacent half-grid points, a procedure which is inaccurate both near the magnetic axis, $s = 0$, and at the boundary, $s = 1$. It was recognized that a representation of the form $\lambda_{j+\frac{1}{2}} \equiv \lambda(s_{j+\frac{1}{2}})$ directly on the half-integer grid would overcome both these problems, but a numerical interchange instability near the axis seemed to render this approach unfeasible.

Schwenn [1] recognized that this numerical instability associated with λ differenced on the half-grid could be avoided by conservatively differencing the dominant toroidal field energy term, $B_z B_\theta \sqrt{g} \sim R^2/\sqrt{g}$, also on the half-grid. He was able to stabilize the axis interchange for many two- and three-dimensional configurations. However, for configurations with strong helical axes, his ansatz does not produce a convergent algorithm.

Consideration of such cases has led to an alternate differencing scheme for $\sqrt{g}$ which seems to be quite generally applicable [3]. The analytic properties of the Fourier coefficients in Eq. (2.4) near $s = 0$ leads to the following decomposition for R and Z :

$$\begin{aligned} R &= R_e + \sqrt{s}R_o, \\ Z &= Z_e + \sqrt{s}Z_o, \end{aligned} \tag{2.9}$$

where (R_e, Z_e) are the even poloidal mode number (m) terms in Eq. (2.4) and (R_o, Z_o) are $1/\sqrt{s}$ times the odd mode number terms. The advantage of Eq. (2.9) over Eq. (2.4) is that the even and odd Fourier harmonic terms separately possess Taylor series expansions in s and can therefore be summed or differenced to obtain accurate half-mesh values. For example, using Eq. (2.9) to evaluate $\tau \equiv \sqrt{g}/R$ yields $\tau^{j+\frac{1}{2}} = \tau_0^{j+\frac{1}{2}} + \tau_1^{j+\frac{1}{2}}$, where

$$\tau_0^{j+\frac{1}{2}} = \frac{1}{2}(R_{o\theta}Z_o - R_oZ_{o\theta})^{j+\frac{1}{2}} \tag{2.10}$$

gives the dominant contribution near $s \rightarrow 0$, and $\tau_1^{j+\frac{1}{2}} = 0(\sqrt{s})\tau_0^{j+\frac{1}{2}}$ is given in Ref.[3]. The product sum rule, $(XY)^{j+\frac{1}{2}} = \frac{1}{2}[(XY)^j + (XY)^{j+1}]$, is used to evaluate Eq. (2.10). Together with a half-mesh representation for λ , this yields a numerically stable and spatially accurate algorithm. Equations (2.9) and (2.10) form the basis of the radial differencing used in VMEC.

3: NESTOR – A Spectral Green's Function Code for the Vacuum Boundary Value Problem

The vacuum magnetic field $\mathbf{B}_v$ confining the toroidal plasma can be written as $\mathbf{B}_v = \mathbf{B}_0 - \nabla \Phi$, where $\mathbf{B}_0$ is the field arising from the net toroidal plasma current and external coil currents and Φ is a single-valued potential necessary to satisfy the Neumann condition

$$(\mathbf{B}_0 - \nabla \Phi) \cdot \mathbf{n}_p = 0 \quad (3.1)$$

on the plasma boundary. Fixing the external field $\mathbf{B}_0$, the vacuum field solution is obtained by solving the exterior Neumann problem for Φ . The potential Φ satisfies the Laplace equation $\Delta \Phi = 0$ in the exterior of the plasma domain and its normal derivative $\partial \Phi / \partial n = -\mathbf{B}_0 \cdot \mathbf{n}_p$ assumes a prescribed value on the plasma boundary.

The Laplace equation for Φ can be converted into an integral equation,

$$\Phi(\mathbf{x}) + \frac{1}{2\pi} \int_{\Sigma_p} d\Sigma'_p \frac{\partial G(\mathbf{x}, \mathbf{x}')}{\partial n'} \Phi(\mathbf{x}') = \frac{1}{2\pi} \int_{\Sigma_p} d\Sigma'_p G(\mathbf{x}, \mathbf{x}') \frac{\partial \Phi(\mathbf{x}')}{\partial n'}, \quad (3.2)$$

where $\mathbf{x}$ and $\mathbf{x}'$ are points on the boundary Σ_p and $G(\mathbf{x}, \mathbf{x}') = 1/|\mathbf{x} - \mathbf{x}'|$ is the Green's function. With condition (3.1), the right side of the integral equation may be explicitly evaluated and is therefore considered to be a source term.

The free boundary problem requires only the value of B_θ^2 on the boundary, which is obtained from $\mathbf{B}_0$ and $\Phi(\mathbf{x})$ on the boundary. Treating the vacuum problem by solving the integral equation (3.2) appears to be an appropriate approach, both because the solution yields $\Phi(\mathbf{x})$ on Σ_p and because no extraneous values of $\Phi(\mathbf{x})$ in the vacuum region are ever needed or computed.

In Ref.[9] a solution method for the integral equation for the interior and exterior Neumann problem in toroidal domains is described. When the boundary is given by Eq. (2.4) evaluated at $s = 1$, then the periodic potential Φ on Σ_p can be expressed as a sine Fourier series

$$\Phi(\theta, \zeta) = \sum \Phi_{mn} \sin(m\theta - n\zeta). \quad (3.3)$$

With this ansatz for Φ , the Fourier transform of Eq. (3.2) leads to an infinite set of linear equations for the Fourier coefficients Φ_{mn} , which is solved by truncation of the higher modes $|m| > M, |n| > N$.

The main difficulty inherent to the Green's function method is the calculation of the Fourier transform of the singular Green's function and its normal derivative. This is solved by the following regularization procedure. Appropriate functions with the same singularity and periodicity are subtracted from the kernels, and their analytically calculated Fourier transforms are added to the Fourier transformed integral equation.

The NESTOR computer code solves the integral equation by the technique just described. It has been previously applied to solving the interior Neumann problem in toroidal vacuum field studies [17] to find fields with "good" magnetic surfaces, as well as other desired properties, which may serve as suitable starting configurations for stellarator plasma equilibrium studies.

4. Free Boundary Equations

In the continuum limit defined as $\Delta s \rightarrow 0$ and the number of Fourier modes $\rightarrow \infty$, the shape of the free boundary surface Σ_p between the plasma (where $p \neq 0$) and the vacuum (where $p = 0$) is determined by the pressure balance, $p + \frac{1}{2}B^2 = \frac{1}{2}B_v^2$, and the normality of $\mathbf{B}_v$, $\mathbf{B}_v \cdot \mathbf{n}_p = 0$. These boundary conditions may be obtained from a variational principle for the combined plasma-vacuum configuration [4, 10].

A discrete version of the free boundary equations, which is used for subsequent numerical computations, is derived in this section. The present formulation of the discrete free boundary equations differs in several respects from previous ones. First, the continuity of pressure across Σ_p appears as a natural boundary condition for the discrete plasma force equations derived here. Thus, the discrete force equations determining Σ_p are derived consistently from the same variational procedure used to obtain the interior plasma forces. This is in contrast to the method in Ref.[4] where, because of the particular coordinate mapping used for R and Z , an exception to the variational principle was made to obtain free boundary equations which would yield a stable iteration scheme.

A second respect in which the present procedure departs from existing methods is through the use of a spectral Green's function approach for computing the scalar magnetic potential Φ and hence the self-consistent vacuum magnetic field, which is normal to Σ_p . Green's functions have been previously used [18] in plasmas with toroidal symmetry to compute the axisymmetric component of the vector potential, $\psi = -RA_\zeta$. Compared with a relaxation scheme for computing the vacuum potential [4], there are at least two advantages to a Green's

function approach when the vacuum field is coupled with the moving plasma boundary: (i) the vacuum potential needs to be computed only on Σ_p , since only $\frac{1}{2}B_v^2$ on Σ_p is required to move the free boundary; (ii) the *exact* vacuum field satisfying $\mathbf{B} \cdot \mathbf{n}_p = 0$ is obtained for any instantaneous position of the free boundary. Feature (i) is desirable, since superfluous calculations of Φ throughout the entire vacuum region are avoided. Nevertheless, the Green's function integral equation for determining Φ on Σ_p is complicated (cf. Section 3), involving four-dimensional Fourier transforms (a feature which somewhat diminishes its advantage over the simple iterative approach). Attribute (ii) is important from the viewpoint of numerical stability of the coupled plasma-vacuum system of equations. In practice, it is found that it is not necessary to compute the vacuum solution at each iteration of the plasma equations. Rather, linear interpolation of $\frac{1}{2}B_v^2$ in time over 10 – 20 plasma iterations is sufficient to maintain numerical stability. The scaling of this interpolation interval (N_v) with the number of Fourier modes remains to be determined. The anticipation is that $N_v \sim M_F$, where M_F is the total number of Fourier modes used in Eq. (2.4).

4.1 Discrete Plasma Force Equations on Σ_p

The plasma forces obtained from the variation of W_p are in a conservative form. Thus, it is possible to obtain their discrete representations by integrating the continuum forces between half-radial mesh points $s_{j+\frac{1}{2}} \equiv (j + \frac{1}{2})\Delta s$. At the boundary $s = 1$, this procedure fails and is replaced by an integration between $s_{N-\frac{1}{2}} = 1 - \frac{1}{2}\Delta s$ and $s_N = 1$. For example, the result for the leading-order term (in Δs^{-1}) comprising F_R^N is:

$$\begin{aligned} F_R^N &= \frac{2}{\Delta s} \int_{s_{N-\frac{1}{2}}}^{s_N} -\frac{\partial}{\partial s}(Z_\theta P) ds \\ &= \frac{-2}{\Delta s} (Z_\theta^N P^N - Z_\theta^{N-\frac{1}{2}} P^{N-\frac{1}{2}}) \end{aligned} \quad (4.1)$$

where $P = R(p + \frac{1}{2}B^2)$ and therefore $P^N = R^N(\frac{1}{2}B_v^2)$. Thus, only the total magnetic pressure of the vacuum ($\propto P^N$), and no other individual components of $\mathbf{B}_v$, affects the motion of the free-boundary coordinate R^N (and Z^N). When Eq. (4.1) is combined with a similar equation for F_Z^N , with $-Z_\theta$ replaced by R_θ , the result is that P/R must be continuous on Σ_p as $\Delta s \rightarrow 0$. Thus, the jump in P/R on Σ_p occurring for finite values of Δs (and finite numbers of Fourier modes) gives an indication of the numerical convergence of a free-boundary solution. Typically, rms values for $\Delta(P/R)$ of less than 10^{-3} are obtained.

The remaining lower order terms composing F_R^N are obtained by evaluating them either on Σ_p or at $s_{N-\frac{1}{2}}$. The resulting discretization for F_R^N can also be derived from a variational principle in which the continuum limit $\Delta s = 0$ is taken for the vacuum energy $W_v = \int \frac{1}{2} B_v^2 dV$.

4.2 Current Constraints for the Vacuum

The integral form of Maxwell's equations can be used to relate the secular pieces of the external potential to the net plasma and coil currents [10]. To recover the free-boundary equations, the variation of the vacuum energy is performed with these currents held constant. Thus, $I^\theta = \oint \mathbf{B} \cdot d\ell_\phi$ and $I^\phi = \oint \mathbf{B} \cdot d\ell_\theta$ are fixed during the equilibrium iterations. When there is no toroidal plasma current, $I^\phi = 0$. Note that $\mathbf{B}_\phi = (I^\theta/2\pi)\nabla\phi$ is the mean toroidal field. For a fixed value of the toroidal flux $2\psi = AB_\phi$, the effective plasma cross sectional area A can be increased (decreased) by decreasing (increasing) I^θ .

5. Numerical Examples

Numerical free-boundary stellarator equilibria obtained using the method described in the previous sections are now presented. For the external magnetic field, an analytical $\ell = 2$ stellarator vacuum field was chosen. The field $\mathbf{B}_0 = \nabla\Phi_{ext}$ is generated by Dommaschk potentials [8,9]:

$$\Phi_{ext}(R, \phi, Z) = \frac{I}{2\pi} \left[\phi + \left(a \frac{\partial}{\partial Z} + \frac{b}{N_F} \frac{\partial}{\partial \phi} \right) (\Phi_s \sin N_F \phi + \Phi_c \cos N_F \phi) \right], \quad (5.1)$$

where

$$\begin{aligned} \Phi_c &= \frac{Z^2}{2} C_{N_F,0} + C_{N_F,1} \\ \Phi_s &= \frac{Z^3 R}{6} \frac{\partial C_{N_F,0}}{\partial R} + Z R^3 \frac{\partial}{\partial R} \left(\frac{C_{N_F,1}}{R^2} \right) \\ C_{N_F,0} &= (R^{N_F} - R^{-N_F})/2N_F, \\ C_{N_F,1} &= [-(N_F - 1)R^{N_F+2} + (N_F + 1)R^{N_F} \\ &\quad - (N_F + 1)R^{-N_F+2} + (N_F - 1)R^{-N_F}] / [8N_F(N_F^2 - 1)]. \end{aligned} \quad (5.2)$$

The number of toroidal field periods is $N_F = 5$ and the constants are $a = -1.495873$ and $b = -3.270651$. The current producing the toroidal field is denoted by I . The potential Φ_{ext} produces a field with a large domain of "good" magnetic surfaces. In Fig. 1, Poincaré plots of the vacuum field are shown at four different toroidal positions.

As a first test of the free-boundary equilibrium code, the magnetic surfaces of the analytic vacuum field $\mathbf{B}_0$ were reproduced as solutions with $p, B_0^2 \rightarrow 0$. Starting from an axisymmetric boundary with circular cross section and running the equilibrium code with no net toroidal current on each flux surface, the shape of the boundary converged to a magnetic surface of the analytic vacuum field. The flux surfaces of the interior plasma region are in good agreement with the analytic vacuum magnetic surfaces. The solid curve in Fig. 1 gives the plasma boundary of the equilibrium solution. The flux surfaces of the free-boundary solution are plotted in Fig. 2. The coincident iota-profiles of the equilibrium solution and the analytic field are shown in Fig. 3. By varying the initial plasma boundary, the computed equilibrium solutions are found to be independent of the initial shape of the boundary. The deformation of an initially circular plasma boundary (dashed line) into the final elliptic boundary is illustrated in Fig. 4 for several iteration steps. The particular magnetic surface to which the boundary corresponds depends only on the strength of the external field and the total toroidal flux in the plasma domain. Here, the toroidal flux is $2\pi\psi = \pi$ and the strength of the external field is chosen so that $I = 790$.

The effect of a finite plasma pressure on the equilibrium is shown in Figs. 5 and 6. Keeping the external field fixed, free-boundary equilibria were computed for different values of β . The flux surfaces of a $\beta = 0.02$ free-boundary equilibrium are plotted in Fig. 5. For comparison, the corresponding fixed-boundary equilibrium is shown in Fig. 6. While for both solutions the shift of the magnetic axis relative to the boundary is comparable, an additional radial shift of the boundary for the free-boundary equilibrium is obtained. The change of the iota-profile due to the finite value of β is shown in Fig. 7. The value of iota increases with β at the magnetic axis and decreases in the outer plasma region.

The radial shift of the plasma boundary due to finite β can be compensated by imposing a vertical magnetic field, B_z . The mean radial shift of the plasma cross section at the toroidal angle $\phi = 0$ is plotted versus the normalized vertical magnetic field strength B_z/B_ϕ in Fig. 8. The dashed line indicates the position of the $\beta = 0$ plasma for comparison. The shape and position of the flux surfaces for a $\beta = 0.02$ plasma are shown for two different values of the vertical field in Fig. 9. For a vertical field $B_z/B_\phi = 0.03$ the radial shift is overcompensated and the boundary of the plasma is considerably deformed, while for the moderate value of $B_z/B_\phi = 0.007$ the radial shift due to the finite β is almost exactly compensated. The

shape of the boundary and the flux surfaces nearly coincide with those of the corresponding fixed-boundary equilibrium.

All numerical results presented were obtained with $n_\rho = 17$ radial mesh points in the plasma, with $n_\theta = 20$ poloidal and $n_\zeta = 8$ toroidal mesh points per period in the plasma and on the boundary for the vacuum. The poloidal (m) and toroidal (n) Fourier mode amplitudes used were $0 \leq m \leq 4$ and $|n| \leq 2$ in the plasma. Fourier mode amplitudes $0 \leq m \leq 7$, $|n| \leq 3$ were taken for the external vacuum field contribution.

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Figure Captions

- Fig.1 Poincaré plots of vacuum magnetic flux surfaces for $l = 2$ stellarator field obtained using Dommaschk potentials. The solid boundary curve is computed from the free-boundary code using $\mathbf{j} \cdot \nabla \zeta = 0$ and $p = 0$.
- Fig.2 Vacuum magnetic surfaces (same configuration as Fig.1) obtained from the free-boundary code.
- Fig.3 Comparison of iota-profile $\iota_p = \iota/N_F$ versus $s = \psi/\psi(1)$ for $\beta = 0$. Solid curve is from Dommaschk potentials, dashed curve is from free-boundary code.
- Fig.4 Deformation of initial circular plasma boundary (dashed line) into stellarator ellipse (for $\zeta = 0$). Curves are drawn at every 50 equilibrium iterations.
- Fig.5 Free-boundary $\beta = 0.02$ stellarator equilibrium.
- Fig.6 Fixed-boundary $\beta = 0.02$ stellarator equilibrium.
- Fig.7 Iota-profiles for $\beta = 0, 0.01, 0.02$ free-boundary equilibria.
- Fig.8 Mean shift of plasma cross-section (for $\zeta \approx 0$) versus applied vertical field for $\beta = 0.01, 0.02$.
- Fig.9 Free-boundary equilibria for $\beta = 0.02$ and $B_Z/B_\phi = 0.007$ and 0.03 .

Fig.1 Poincaré plots of vacuum magnetic flux surfaces for $l=2$ stellarator field obtained using Dommaschk potentials. The solid boundary curve is computed from the free-boundary code using $\langle \vec{r} \cdot \nabla \rangle = 0$ and $p=0$.

Fig.2 Vacuum magnetic **sur**faces (same configuration as Fig.1) obtained from the free-boundary code.

Fig.3 Comparison of iota profiles $i_p = i/N$ vs. $s = \phi/\phi(1)$ for $\beta=0$. Solid curve is from Dommaschk potentials, dashed curve is from free-boundary code.

Fig.4 Deformation of initial circular plasma boundary into stellarator ellipse (for $\beta=0^\circ$). Curves are drawn at every 50 equilibrium iterations.

Fig.5 Free-boundary, $\langle \beta \rangle = 0.02$ stellarator equilibrium.

Fig.6 Fixed-boundary, $\langle \beta \rangle = 0.02$ stellarator equilibrium.

Fig.7 Iota profiles for $\langle \beta \rangle = 0$, 0.01, 0.02
free-boundary equilibria.

Fig.8 Mean shift of plasma cross section (for $\zeta=0^\circ$)
vs. applied vertical field for $\langle\beta\rangle=0.01, 0.02$.

Fig.9 Free-boundary equilibria for $\langle \beta \rangle = 0.02$
and $B_z/B_\phi = 0.007$ and 0.03 .