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A High Performance Spectral Code for Nonlinear MHD Stability

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ABSTRACT

A new spectral code, NSTAB, has been developed to do nonlinear stability and equilibrium calculations for the magnetohydrodynamic (MHD) equations in three dimensional toroidal geometries. The code has the resolution to test nonlinear stability by calculating bifurcated equilibria directly. These equilibria consist of weak solutions with current sheets near rational surfaces and other less localized modes. Bifurcated equilibria with a pronounced current sheet where the rotational transform crosses unity are calculated for the International Thermonuclear Experimental Reactor (ITER). Bifurcated solutions with broader resonances are found for the the LHD stellarator currently being built in Japan and an optimized configuration like the Wendelstein VII-X proposed for construction in Germany. The code is able to handle the many harmonics required to capture the high mode number of these instabilities.

NSTAB builds on the highly successful BETAS code, which applies the spectral method to a flux coordinate formulation of the variational principle associated with the MHD equilibrium equations. However, a new residue condition for the location of the magnetic axis has been developed and implemented. This condition is based on the weak formulation of the equations and imposes no constraints on the inner flux surfaces.

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The NSTAB code was developed on CRAY computers running the UNICOS operating system. The manuscript was prepared with the AMS-TEX typesetting package. The graphics were produced with the help of the Mathematica, Matlab and NCARGKS software packages.

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NOTATION

E	energy
$\mathbf{B}$	magnetic field
$\mathbf{J}$	current density
p	pressure
β	plasma beta parameter
A	aspect ratio
s	toroidal flux coordinate
ψ	Clebsch flux function
ι	rotational transform
I	net toroidal current
$\mathbf{X}$	position vector
u	poloidal angle
v	toroidal angle, cylindrical coordinate
r, z	cylindrical coordinates
r_0, z_0	position of the magnetic axis
r_1, z_1	coordinates of the plasma boundary
R	distance of a flux surface from the magnetic axis
K	Jacobian from Cartesian to cylindrical coordinates
H	inner product characterizing the Jacobian
U	vector of unknowns
L_j	nonlinear differential operators
M_j	preconditioner for L_j
δ	displacement operator
m, n	indices of the Fourier coefficients
$L_j^{m,n}$	Fourier coefficients of the differential operators
$R^{m,n}, \psi^{m,n}$	Fourier coefficients of R and ψ
$\Delta_{m,n}$	Fourier coefficients of the plasma boundary
$Z_{m,n}$	Fourier coefficients for rezoning the plasma boundary
a, e	acceleration parameters in the iterative scheme
λ	eigenvalue of a differential operator
ω	rate of exponential decay of the error
N_s	number of radial mesh points
N_u	degree of the trigonometric polynomials in u
N_v	degree of the trigonometric polynomials in v

CHAPTER 1

Introduction

1.1 The Physical Problem and Computational Model

Controlled nuclear fusion proposes to provide us with an abundant source of energy. A fusion reactor might produce substantially smaller amounts of pollution or radioactive waste than alternatives such as burning fossil fuels and nuclear fission. The international effort to harness fusion energy has produced steady progress in the last forty years [7]. It remains to be seen if a working reactor can be built, as existing experiments still require far more energy for their operation than they produce. One of the main areas of research is magnetic confinement fusion, which uses strong magnetic fields to confine a plasma in a vacuum chamber. A plasma is a completely ionized gas that can be treated as an electrically neutral collection of ions and electrons. The goal is to confine the plasma long enough at high enough temperatures so that the deuterium ions will fuse into heavier elements. The resultant release of energy would be used to heat a coolant and ultimately produce electricity.

Two types of experiments are of interest here, the tokamak and the stellarator, both of which confine the plasma inside a torus. Magnetic confinement works on the principle that the motion of a charged particle tends to follow a magnetic field line. Thus the first priority for good confinement is to have a strong toroidal magnetic field (the long way around the torus) whose field lines do not leave the torus. Perfect confinement would be achieved if the particles truly followed the field lines. However, in addition to the fast motion of the particles along the field lines, there are slower particle drifts across the field lines due to the

curvature of the torus, oscillations of the electric field, and Coulomb collisions with other charged particles.

To control outward drift of the plasma, it is necessary to add a poloidal magnetic field (the short way around the torus), which produces a helical twist in the field lines. The difference between the tokamak and stellarator consists in how this poloidal field is produced. In the tokamak, the strong toroidal magnetic field is created by passing a large current through coils wound poloidally around the torus. The poloidal component of the magnetic field is generated by inducing a net toroidal current in the plasma itself. The plasma column forms an axially symmetric torus with circular or D-shaped cross sections (see Fig. 2). Stellarators produce the poloidal magnetic field directly from helically wound coils which are required to have a more complicated shape. Stellarators are not axisymmetric, so in general the individual cross sections are all different. They can have elliptical, triangular or even crescent like shapes (see Fig. 1). In addition there may be a large helical excursion so that the plasma column looks like a deformed, stretched out corkscrew that is joined at both ends. These complicated shapes make stellarators hard to build, but the lack of any induced toroidal current allows for steady state operation.

The magnetohydrodynamic (MHD) equations describe the behavior of the magnetic field in the plasma. They have been used successfully to model many aspects of these devices. The BETA code [2, 3] implemented one of the first numerical methods to solve these equations in three-dimension toroidal geometries like those mentioned above. This finite difference code introduced a flux coordinate formulation of the variational principle associated with the time averaged, ideal MHD equilibrium equations, and it also exploited a the second order Richardson iterative scheme. BETA has been used extensively for designing stellarators, performing parameter studies, and studying nonlinear stability and Monte

Carlo transport in both stellarators and tokamaks [4, 9, 10, 18].

More accurate results have been made possible by the development of the spectral codes VMEC [14, 15] and BETAS [6]. These codes use Fourier series expansions in the two periodic angles on the torus and finite differences in the radial direction. VMEC was one of the first successful spectral codes, and is the most widely used today. The BETAS code improved the speed of the computational method with the development of a preconditioner for the iterative scheme. This feature has since been incorporated into VMEC [13]. BETAS uses a coordinate system, an arrangement of the unknowns, and a radial difference scheme which gives it the resolution to find bifurcated equilibrium solutions with current sheets and other less localized modes of physical interest.

1.2 Numerical Implementation

This thesis describes a new equilibrium code called NSTAB and demonstrates how it is used to test nonlinear stability. The code implements the spectral method in the flux coordinate form of the variational principle to solve the MHD equations. The flux coordinate formulation presupposes the existence of a family of nested KAM surfaces [4], the innermost one being a simple closed curve called the magnetic axis (see Fig. 2). The location of the magnetic axis must be computed, which is difficult because of a singularity in the coordinate system.

In the earlier BETA code, the energy integral was written as a finite sum after a suitable quadrature formula was chosen. The discrete equations are then uniquely determined by minimizing the finite sum with respect to the nodal values of the unknowns. This facilitated nonlinear stability studies, but the resolution at the magnetic axis was never completely satisfactory. Spectral codes have more freedom in how the axis is treated, and several

approaches have been tried.

NSTAB contains a new residue condition for the axis location, developed from the variational principle and the concept of a weak solution. Other aspects of the code are based largely on BETAS. The new axis condition involves an integral over an arbitrarily small flux tube containing the magnetic axis. We call this a residue condition because the integral is zero when there is no singularity at the axis. In practice, the residue calculation is performed on the innermost flux surface provided by the computational mesh. The resultant axis equations are substantially different from those used by BETAS and VMEC, which are based on linear extrapolation and impose constraints on the innermost flux surface. The residue condition requires no such constraints, so for complicated geometries it allows for more realistic shapes at standard meshes and may provide a more accurate value for the energy.

NSTAB, like BETAS, has been optimized to run on the vector architecture of CRAY supercomputers. NSTAB is limited to configurations with nested flux surfaces, so a factor of two in speed has been gained over BETAS by eliminating an extra flux function used to study the effects of magnetic islands. However, NSTAB sometimes converges at a slower rate than BETAS due to the higher resolution near the magnetic axis. Another factor of two in speed might be gained by exploiting odd and even symmetry properties of the variables.

1.3 Nonlinear Stability

Several codes have been developed to study stability properties of MHD equilibria. Linearized theories can be used to determine growth rates of small perturbations from a previously calculated equilibrium solution [1, 17]. Equilibrium codes have also been used for stability calculations. After performing a first energy minimization to arrive at an equilibrium solution, the BETA code can test for nonlinear instabilities by performing a second constrained energy minimization and looking for regions in function space with lower energy levels [3]. This method requires very accurate estimates of the energy that involve making several runs and extrapolating to zero mesh size.

Both NSTAB and BETAS have the resolution to perform a more direct kind of stability test. Due to the coordinate system, the arrangement of the unknowns, and the radial differencing scheme, these codes can capture weak solutions with current sheets near rational surfaces and other less localized modes that are important in the applications. This allows one to test for nonlinear instability by looking for bifurcated solutions that demonstrate strong nonuniqueness. Results along these lines will be presented for several configurations of interest.

Energy level comparisons by the spectral method turn out to be difficult. The bifurcated solutions may have lower energy levels when compared to a more standard equilibrium solution on the same mesh, but the difference is very small. A true convergence study, with extrapolation to zero mesh size, would have to be performed before the energy comparisons can be considered meaningful. Configurations like the axisymmetric tokamak or one field period of the LHD stellarator do not have complicated structure and accurate solutions can be computed quickly at crude meshes. In contrast, the weak solutions characterizing unstable modes tend to have much higher harmonics and represent a true challenge to the

code. Much work has gone into tuning NSTAB so that the iterative scheme will converge in these cases, but the convergence may be very slow. It is thus impractical to perform the extrapolation to zero mesh size required for true energy level comparisons in all these cases, but the existence of the bifurcated solutions themselves can be determined by relatively short runs, and this forms the basis of our nonlinear stability test.

1.4 Summary of Results

In Chapter 2 we give a description of the mathematical model implemented in the NSTAB code for three-dimensional MHD equilibria. An improved flux coordinate formulation of the variational principle is outlined that clarifies the role of weak solutions and the nested surface hypothesis. In Chapter 3 we describe the spectral method and derive the weak form of the Euler-Lagrange equations in flux coordinates. Through the choice of unknowns, the Jacobian in this coordinate system factors into the product of an angular term and a single radial derivative. When differenced carefully, this method provides the resolution to capture weak solutions with clearly visible current sheets. Chapter 4 describes problems with the coordinate system at the magnetic axis and the derivation and implementation of a new axis residue condition. Chapter 5 outlines the second order Richardson iterative scheme used to solve the equilibrium equations. Chapter 6 contains the details of the numerical implementation of these ideas and the mechanism used to trigger unstable modes.

Numerical results from the NSTAB code are presented in Chapter 7. The new equations for the magnetic axis are validated through comparisons with other codes, and their advantage is demonstrated for a high β equilibrium of the LHID stellarator with severely deformed flux surfaces. Despite the increased resolution of the spectral method, several studies are presented that show the convergence of the energy and other major quantities

is only of first order in the radial mesh size. The high accuracy of the method is indicated by its ability to capture current sheets at relatively crude radial meshes in a bifurcated equilibrium solution for the proposed International Thermonuclear Experimental Reactor [7]. This case has a well developed $m = 1, n = 1$ mode which appears as a current sheet at the rational surface where the rotational transform crosses unity.

Nonlinear stability can be easily tested with relatively few radial mesh points because of the flux variable formulation of the problem. However, it is important to use many poloidal and toroidal harmonics in the calculations to resolve accurately the high mode structure of the most dangerous instabilities. This is demonstrated by calculating bifurcated equilibria for the LHD stellarator being built at the National Institute for Fusion Science in Japan. We present an equilibrium solution over one field period, but show the existence of an unstable mode over two field periods when very small sidebands are included in the wall shape. This mode has a complicated structure which is not localized like the current sheet in the ITER tokamak.

Satisfactory convergence properties of NSTAB when many harmonics occur are established in more extreme cases where other codes seem to experience difficulty. Two such cases are the H1 Helic at the Australian National University and an advanced stellarator similar to the Helias designed in Germany [18]. For the H1 Helic we include a fully converged fine mesh equilibrium run, and for an unstable version of the advanced stellarator we present two bifurcated equilibria, establishing that the solution of the problem is not unique.

CHAPTER 2

Mathematical Model

2.1 MHD Equations

To determine the structure of the magnetic field in the plasma we use the equations of magnetohydrodynamics. We introduce time-averaged equilibrium equations in which the plasma fluid velocity has been set to zero. The equations are

$$\nabla \cdot \mathbf{B} = 0, \tag{1}$$

$$\mathbf{J} \times \mathbf{B} = \nabla p, \tag{2}$$

where $\mathbf{B}$ is the magnetic field, p is the scalar pressure, and $\mathbf{J}$ is the current density defined by $\mathbf{J} = \nabla \times \mathbf{B}$. Thus (1) and (2) represent four equations in four unknowns. Equation (1) comes from Maxwell's equations and (2) shows that the Lorentz force $\mathbf{J} \times \mathbf{B}$ on a fluid element balances the pressure gradient. An important dimensionless constant is the beta parameter

$$\beta = \frac{2 \iiint p \, dV}{\iiint B^2 \, dV},$$

which measures how much plasma energy can be confined by a given amount of energy in the magnetic field. The value of β must be at least several percent for a cost-effective reactor.

These equations are to be solved in three-dimensional toroidal domains. Following earlier work [2], several assumptions are imposed to make the problem computationally tractable. For good confinement of the plasma it is desirable that the magnetic field lines, which are the integral curves of the vector field $\mathbf{B}$, remain in a torus. We assume that they

form a nested family of toroidal flux surfaces, labeled by s (see Fig. 2). We take $s = 1$ to represent the plasma boundary and $s = 0$ to represent the innermost degenerate flux surface, which is a simple closed curve called the magnetic axis. On each torus $s = \text{const.}$ we introduce periodic coordinates u and v , representing the poloidal and toroidal angles respectively.

We define the net toroidal flux in a solid torus $s < s_0$ to be the flux of $\mathbf{B}$ through a cross section $v = \text{const.}$ This is independent of which cross section is used because $\nabla \cdot \mathbf{B} = 0$. In most cases of interest $\mathbf{B}$ will have a strong toroidal component that does not reverse direction, so we further assume that we can choose s itself to be the toroidal flux.

We can now integrate the equation $\nabla \cdot \mathbf{B} = 0$ by setting

$$\mathbf{B} = \nabla s \times \nabla \psi,$$

where the level sets $\psi = \text{const.}$ define another set of flux surfaces. Locally, every divergence free vector field has such a representation, but in general s and ψ will not have single-valued global extensions. Under the nested surface hypothesis s is single valued, but ψ is not. However, since $\mathbf{B}$ itself is single-valued, it can be shown that

$$\psi = u - \iota(s)v + \tilde{\psi}(s, u, v),$$

where $\tilde{\psi}$ is periodic in u and v . Here the rotational transform $\iota(s)$ is the derivative of the poloidal flux with respect to the toroidal flux s . It measures, in an average sense, how much a field line turns in the poloidal direction u as it traverses the torus in the toroidal direction v . On surfaces s where $\iota(s)$ is irrational, each field line will be dense, but on a rational surface the field line closes on itself after a finite number of toroidal circuits.

Returning to the force balance equation (2) and taking a dot product with $\mathbf{B}$, we see

that

$$\mathbf{B} \cdot \nabla p = 0,$$

which means that p is constant on magnetic field lines. In our formulation of the variational principle this magnetic differential equation has been integrated by putting $p = p(s)$. We are thus left with two equations in two unknowns, s and ψ . There are no boundary conditions on ψ other than the periodicity requirements mentioned above, but ψ is only determined up to an arbitrary function of s .

There are two arbitrary functions $p(s)$ and $\iota(s)$ in our model. The pressure $p(s)$ will be prescribed, although physically it would be more natural to give the mass within each flux tube $s = \text{const.}$ and to compute $p(s)$ from the equation of state. This simplification seems to produce more or less equivalent results about equilibrium and stability. The treatment of the rotational transform depends on the type of experiment we are modeling. In a tokamak, $\iota(s)$ is prescribed, which fixes the net poloidal flux as a function of the net toroidal flux. For stellarators this constraint is dropped and $\iota(s)$ is treated as one of the unknowns. Its value is determined by minimizing the energy, which is achieved at zero net toroidal current.

2.2 Variational Principle

The considerations we have just described are contained in the standard variational principle of magnetohydrodynamics. The energy of the plasma, defined by

$$\mathbf{E} = \iiint \left(\frac{1}{2} B^2 - p(s) \right) dV,$$

is minimized subject to the following constraints:

1. There is a nested family of toroidal flux surfaces. Each surface is labeled by s , the net toroidal flux that it encloses.
2. In a tokamak, $\iota(s)$ is prescribed. For stellarators, this constraint is dropped and $\iota(s)$ is chosen to minimize the energy, which is achieved at zero net toroidal current.
3. The pressure $p(s)$ is prescribed.
4. The location of the plasma boundary $s = 1$ is given.

The Euler-Lagrange equations in the calculus of variations, which come from formally minimizing the energy for all possible functions s and ψ subject to these constraints, are equivalent to the MHD equilibrium equation (2). Equation (1) is imposed as a flux constraint by the use of s and ψ in the representation of $\mathbf{B}$.

For several important reasons our computations will be performed with s , u and v as the independent variables. This gives a convenient rectangular computational domain and allows us to implement the flux constraints $p = p(s)$ and $\iota = \iota(s)$. It also permits us to define ψ uniquely.

2.3 Weak Solutions

The restriction to nested flux surface configurations greatly simplifies the model, but there are theoretical issues concerning the validity of this assumption. There are axisymmetric solutions in special cases which do satisfy the nested surface hypothesis, but the KAM theorem has been used to demonstrate the nonexistence of smooth equilibria in three dimensions. Line tracing codes which track magnetic field lines in a vacuum show that islands can appear at rational surfaces. The islands consist of smaller tori which can themselves be nested. Even in axisymmetric cases where solutions with nested surfaces do exist, there are resonances at rational surfaces where significant instabilities can be found by introducing three-dimensional perturbations.

The NSTAB code handles these problems within the framework of the nested flux surface topology by calculating weak solutions [4]. The weak solutions can include current sheets which develop at rational surfaces and serve to model magnetic islands. Numerical examples of these weak solutions are presented in Chapter 7. A current sheet represents a jump in the tangential components of $\mathbf{B}$ resulting in a surface current and is analogous to the widely accepted vortex sheet model of fluid dynamics. In our calculations it appears as an intersection of two or more flux surfaces. In Section 3.3 the variational principle is used to define the concept of a weak solution and suggests how to capture such solutions numerically by giving a natural conservation form of the MHD equations.

A combination of finite differences and the spectral method is ideal for computing these weak solutions. The solutions are continuous and periodic in the two angles u and v , making them well suited for a spectral representation. The discontinuities appear in s , the radial direction. In Section 3.1 we show how the flux coordinate system and arrangement of the unknowns isolate a critical radial derivative in the Jacobian. The second order accurate

radial differencing scheme described in Section 6.1 provides minimal coupling between the flux surfaces in the radial direction and thus reduces artificial viscosity tending to smear discontinuities. We believe it is the combination of these two features of the model that allows current sheets of the weak solutions to be captured effectively.

CHAPTER 3

Computational Domain

3.1 Mixed Euler-Lagrange Coordinate System

Let x_1, x_2 and x_3 be the usual Cartesian coordinates. We introduce cylindrical coordinates $A + r, z$ and v (see Fig. 1), where A is the major radius of the confinement device, and

$$x_1 = (A + r) \cos(2\pi v), \quad x_2 = (A + r) \sin(2\pi v), \quad x_3 = z.$$

The independent variables in the computation will be s, u and v , where the Lagrangian variable s labels a nested family of toroidal flux surfaces and the Eulerian variable v is the true toroidal angle. The choice of the poloidal angle u is arbitrary and will be determined by how the shape of the outer plasma wall is parametrized. We take $r_1 = r_1(u, v)$ and $z_1 = z_1(u, v)$ to be a given parametrization of the outer wall $s = 1$, and we let $r_0(v)$ and $z_0(v)$ represent the location of the magnetic axis $s = 0$, which must be computed.

Imposing a star-like condition on the shape of the flux surfaces, we write

$$r = r_0(v) + R(s, u, v) [r_1(u, v) - r_0(v)],$$

$$z = z_0(v) + R(s, u, v) [z_1(u, v) - z_0(v)],$$

where R is a generalized radius that is zero at $s = 0$ and 1 at $s = 1$. Computations will be carried out to solve for the unknowns ψ, R, r_0 , and z_0 as functions of s, u , and v . To derive equations for these quantities, the energy integral E is written in our new coordinate system and the Euler-Lagrange equations are calculated.

The Jacobian of the transformation $(s, u, v) \rightarrow (x_1, x_2, x_3)$ has the remarkable factorization

$$\frac{\partial(x_1, x_2, x_3)}{\partial(s, v, u)} = K \frac{\partial(r, z)}{\partial(s, u)} = K H R R_s, \quad (3)$$

where

$$H = \frac{\partial z_1}{\partial u}(r_1 - r_0) - \frac{\partial r_1}{\partial u}(z_1 - z_0)$$

depends only on u and v and $K = 2\pi(A + r)$ is the Jacobian from Cartesian to cylindrical coordinates. The evaluation of the Jacobian is crucial if the numerical method is to capture weak solutions where it becomes singular. Separation of the Jacobian into an angle factor H independent of s and the radial factor RR_s , involving just one derivative, seems to account for the high accuracy in the computations. In the radial direction where discontinuities occur, the s derivative is isolated to the term RR_s and is computed with very little truncation error by the differencing scheme given in Chapter 6.

To write $\mathbf{B}$ in this coordinate system, we exploit the invariance of Jacobians to observe that

$$\mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{X} = (\nabla s \times \nabla \psi) \cdot \nabla \mathbf{X} = \frac{\partial(s, \psi, \mathbf{X})}{\partial(x_1, x_2, x_3)} = \frac{\psi_u \mathbf{X}_v - \psi_v \mathbf{X}_u}{K H R R_s},$$

where $\mathbf{X}$ is the position vector. Now the energy integral defined in Chapter 2 can be written in the elegant form

$$E = \iiint \left(\frac{(\psi_u \mathbf{X}_v - \psi_v \mathbf{X}_u)^2}{2K H R R_s} - p(s) K H R R_s \right) ds du dv.$$

We derive equations for the unknowns R and ψ by calculating the first variation of the energy with respect to perturbations δR and $\delta \psi$, so that

$$\delta E = - \iiint \left[L_2(R) \delta R + L_1(\psi) \delta \psi \right] ds du dv \quad (4)$$

after integrating by parts. Since δE must be zero for all choices of the test functions δR and $\delta \psi$, we arrive at the two Euler-Lagrange equations

$$L_1(\psi) = 0, \quad L_2(R) = 0.$$

These equations, along with the pressure constraint $p = p(s)$ and the representation $\mathbf{B} = \nabla s \times \nabla \psi$, are equivalent to the magnetostatic equations (1) and (2) in Section 2.1. The expressions for L_1 and L_2 will be given in Section 3.3. Further equations for the remaining unknowns r_0 and z_0 , which determining the location of the magnetic axis, will be given in Chapter 4.

3.2 The Spectral Method

The NSTAB code uses the pseudospectral or collocation method [12] in the two angles on the torus. The unknowns R and ψ and the differential operators $L_1(\psi)$ and $L_2(R)$ are expanded in truncated Fourier series in u and v . To solve the Euler-Lagrange equations $L_1 = L_2 = 0$, the Fourier coefficients of the unknowns are iterated to drive the corresponding Fourier coefficients of L_1 and L_2 to zero. Because of the nonlinear form of L_1 and L_2 , it is not practical to compute their Fourier coefficients directly from the Fourier coefficients of the unknowns. Instead, the pseudospectral method involves first computing L_1 and L_2 at equally spaced collocation points in u and v and then applying the Fourier transform. To evaluate L_1 and L_2 at these points, R , ψ , and their u and v derivatives are computed at the collocation points from their Fourier coefficients. Finite differences are used to compute derivatives with respect to s .

The variational principle shows there is a simple correlation between the Fourier coefficients of the unknowns and the Fourier coefficients of the differential operators. To see this, we expand these quantities in Fourier series

$$\begin{aligned} R(s, u, v) &\sim \sum_{m,n} R^{m,n}(s) e^{i(mu+nv)} \\ \psi(s, u, v) &\sim u - \iota(s)v + \sum_{m,n} \psi^{m,n}(s) e^{i(mu+nv)} \\ L_1(\psi) &\sim \sum_{m,n} L_1^{m,n}(s) e^{i(mu+nv)} \\ L_2(R) &\sim \sum_{m,n} L_2^{m,n}(s) e^{i(mu+nv)}. \end{aligned}$$

If we make a perturbation

$$\begin{aligned} \delta\psi &= \delta\psi^{m,n}(s) e^{-i(mu+nv)}, \\ \delta R &= \delta R^{m,n}(s) e^{-i(mu+nv)}, \end{aligned}$$

equation (4) becomes

$$\begin{aligned}\delta E &= - \iiint \left[L_2(R) \delta R^{m,n} + L_1(\psi) \delta \psi^{m,n} \right] e^{-i(mu+nv)} ds du dv \\ &= - \int \left[L_2^{m,n} \delta R^{m,n} + L_1^{m,n} \delta \psi^{m,n} \right] ds\end{aligned}$$

and the Euler-Lagrange equations are

$$L_1^{m,n} = 0, \quad L_2^{m,n} = 0.$$

Thus the m, n Fourier coefficient of an unknown is determined by the equation for the same Fourier coefficient of the corresponding differential operator. To solve this system of equations, we use an iterative scheme discussed in Chapter 5.

Problems can develop if nonuniqueness in the unknowns is not handled correctly [16]. The flux function ψ is only defined up to an arbitrary function of s , but the spectral method gives us a unique representation if we set the coefficient $\psi^{0,0} = 0$.

3.3 Weak Form of the Magnetostatic Equations

We proceed to derive a weak form of the Euler-Lagrange equations and to show how the spectral method allows us to implement them. Consider the general expression,

$$\delta E = \iiint \left[\mathbf{B} \cdot \delta(\psi_u \mathbf{X}_v - \psi_v \mathbf{X}_u) - \left(\frac{1}{2} B^2 + p \right) \delta(K H R R_s) \right] ds du dv, \quad (5)$$

for the first variation of the energy with respect to an arbitrary displacement in the unknowns. To compute the first variation with respect to $\delta\psi$, we put $\delta(\psi_u \mathbf{X}_v - \psi_v \mathbf{X}_u) = \mathbf{X}_v \delta\psi_u - \mathbf{X}_u \delta\psi_v$ and note that $K H R R_s$ does not depend on ψ . Using equation (5) we get

$$\delta E_1 = \iiint \left[(\mathbf{B} \cdot \mathbf{X}_v) \delta\psi_u - (\mathbf{B} \cdot \mathbf{X}_u) \delta\psi_v \right] ds du dv. \quad (6)$$

To derive the first variation with respect to R , we use the identity $\delta(K H R R_s) = (K H R \delta R)_s$ and find

$$\delta E_2 = \iiint \left[\psi_u \mathbf{B} \cdot (\mathbf{X}_R \delta R)_v - \psi_v \mathbf{B} \cdot (\mathbf{X}_R \delta R)_u - \left(\frac{1}{2} B^2 + p \right) (K H R \delta R)_s \right] ds du dv. \quad (7)$$

Since no second order derivatives appear in equations (6) and (7), we need only assume that the unknowns R and ψ have first derivatives. A weak solution is thus defined as a pair of functions R and ψ that satisfy the integral equations $\delta E_1 = 0$ and $\delta E_2 = 0$ for all continuously differentiable test functions $\delta \psi$ and δR .

Returning to (6), we integrate twice by parts and obtain the Euler-Lagrange equation

$$L_1(\psi) = (\mathbf{B} \cdot \mathbf{X}_v)_u - (\mathbf{B} \cdot \mathbf{X}_u)_v.$$

This equation is left in the conservation form that results from the variational principle, so that the equations $L_1^{m,n} = 0$ used by the spectral method give exactly the condition for a weak solution defined above. From equation (7), we can similarly derive the pseudo-conservation form (undifferentiated terms also appear) of the Euler-Lagrange equation $L_2(R) = 0$. However, a slight rearrangement of the terms leads to the computationally more efficient formula

$$L_2(R) = \frac{1}{R_s} \left\{ \psi_v \left[(\mathbf{B} \cdot \mathbf{X}_u)_s - (\mathbf{B} \cdot \mathbf{X}_s)_u \right] + \psi_u \left[(\mathbf{B} \cdot \mathbf{X}_s)_v - (\mathbf{B} \cdot \mathbf{X}_v)_s \right] - p'(s) K H R R_s \right\}.$$

In the case of a stellarator, where the rotational transform $\iota(s)$ is not held fixed, it must be determined by minimizing the energy. The first variation of the energy with respect to ι is

$$\delta E = \iiint (\mathbf{B} \cdot \mathbf{X}_u) \delta \iota(s) ds du dv = \int I(s) \delta \iota(s) ds,$$

where

$$I(s_0) = \iiint \mathbf{B} \cdot \mathbf{X}_u du dv$$

is the net toroidal current through the region enclosed by the flux surface $s = s_0$. Thus the Euler-Lagrange equation which determines $\iota(s)$ is the zero net current condition $I(s) = 0$

CHAPTER 4

Axis Residue Condition

4.1 Magnetic Axis Equations

Let us determine next the equations for the location of the magnetic axis. As noted in the previous chapter, the two Euler-Lagrange equations $L_1 = 0$ and $L_2 = 0$ for the unknowns ψ and R are equivalent to the MHD equations. However, because of our use of a polar coordinate system, there is a singularity at the magnetic axis $s = 0$, and we need equations to guarantee that the solution will remain continuous there. By allowing for this singularity, we have developed a new regularity condition that comes from a more careful consideration of weak solutions defined by the variational method.

If we repeat the procedure used to derive the equations $L_1 = 0$ and $L_2 = 0$, two additional Euler Lagrange equations can be found by calculating the first variation of the energy with respect to the axis location r_0 and z_0 . These equations have been implemented in previous codes with mixed success. Apparently numerical errors involved in many of the terms can become larger than the more critical quantities.

The VMEC and BETAS spectral codes have relied on the Taylor series expansion of s near the magnetic axis to generate equations and constraints on the innermost flux surfaces. This expansion suggests that when the flux surfaces contract down to the magnetic axis, the limiting shape has an elliptical cross section. In BETAS, the innermost surface is required to have elliptical cross sections. The equations for the axis location and the parameters describing the ellipses are derived from the variational principle. In VMEC the axis location is computed by linear extrapolation from the location of the first and second flux surfaces.

Higher Fourier coefficients which describe non-elliptical shapes of the innermost flux surface are determined from their values on the second flux surface in a way consistent with the Taylor expansion of s .

The regularity condition implemented by NSTAB comes instead directly from the variational principle and requires no constraints on the innermost flux surface. We use the fact that there is a singularity at the axis to isolate the most critical quantities. Since the unknowns r_0 and z_0 are functions of v alone, we are free to integrate the terms in the first variation of the energy by parts with respect to s and u . When this is done in a natural way the resulting equations turn out to involve simple combinations of $L_1(\psi)$ and $L_2(R)$. However, there is a residue at $s = 0$, so integration by parts in s can only be carried out away from the magnetic axis. When this integration by parts is performed outside a small flux tube $s = s_0$ containing the axis, a residual surface integral at $s = s_0$ remains, forming the basis of our new axis condition. Details of the derivation showing how the condition eliminates a singularity at $s = 0$ will be presented in the next two sections.

4.2 Derivation of the Residue Condition

We return to the general form of the first variation of the energy in Section 3.3 and write

$$\delta(\psi_u \mathbf{X}_v - \psi_v \mathbf{X}_u) = \psi_u \delta \mathbf{X}_v - \psi_v \delta \mathbf{X}_u,$$

$$\delta(K H R R_s) = 2\pi H R R_s \delta r + K \delta(r_s z_u - r_u z_s),$$

where the position vector $\delta \mathbf{X} = \delta r \hat{\mathbf{r}}(v) + \delta z \hat{\mathbf{z}}$ is defined in terms of unit vectors $\hat{\mathbf{r}}(v)$ and $\hat{\mathbf{z}}$. Here we have used equation (3) from Section 3.1 to write $H R R_s = \partial(r, z)/\partial(s, u)$. The first variation of the energy with respect to r and z is given by

$$\begin{aligned} \delta E = \iiint \left[\psi_u \mathbf{B} \cdot \delta \mathbf{X}_v - \psi_v \mathbf{B} \cdot \delta \mathbf{X}_u - \left(\frac{1}{2} B^2 + p \right) 2\pi H R R_s \delta r \right. \\ \left. - \left(\frac{1}{2} B^2 + p \right) K \delta(r_s z_u - r_u z_s) \right] ds du dv = \iiint T ds du dv, \end{aligned}$$

where the symbol T is used to denote the integrand. To compute the first variation with respect to the axis location r_0 and z_0 , we first integrate by parts to remove all derivatives from δr and δz . We then use $r = r_0 + R(r_1 - r_0)$ and the similar relation for z to obtain

$$\delta r = (1 - R) \delta r_0, \quad \delta z = (1 - R) \delta z_0.$$

Since integration by parts with respect to s can only be done outside an inner flux tube $s = s_0$ containing the magnetic axis, we obtain both a volume term and surface integrals at $s = s_0$ and $s = 1$. The surface integral at $s = 1$ disappears because there $R = 1$.

After performing these steps, the first variation of the energy can be written in the form

$$\begin{aligned} \delta E = - \iiint_{s > s_0} [L'_3(r) \delta r + L'_4(z) \delta z] ds du dv + \iiint_{s < s_0} T ds du dv \\ - \iint_{s = s_0} \left(\frac{1}{2} B^2 + p \right) K (r_u \delta z - z_u \delta r) du dv. \end{aligned}$$

It is easy to verify that

$$r_u L'_3(r) + z_u L'_4(z) = -\psi_u L_1(\psi) = 0,$$

$$(r_1 - r_0) L'_3(r) + (z_1 - z_0) L'_4(z) = L_2(R) = 0,$$

and by combining these two relations we see that $L'_3(r) = L'_4(z) = 0$ is a consequence of the Euler-Lagrange equations $L_1 = L_2 = 0$. We are therefore left with the residue

$$\delta E = - \iiint_{s=s_0} \left(\frac{1}{2} B^2 + p \right) K(1-R) [r_u \delta z_0(v) - z_u \delta r_0(v)] du dv + \iiint_{s < s_0} T ds du dv. \quad (8)$$

4.3 A Numerical Approximation

There are several problems with implementing equation (8) numerically. Large terms in the integrand which do not depend on u contribute nothing to the residue, but have numerical errors that dominate the more critical terms. There are also errors arising from quantities in the expression for B^2 which are poorly computed near the magnetic axis. To handle these difficulties we make several simplifications in the integrand.

The first simplification is to keep only the surface integral from equation (8) and to neglect the lower order volume term over the region $s < s_0$. The Euler-Lagrange equations then reduce to contour integrals around a closed curve circling the magnetic axis and lying on an arbitrarily small inner tube $s = s_0$. Numerically we evaluate this integral over the innermost surface provided by the computational mesh. We may remove terms which do not depend on u , such as $p(s)$, since they will integrate to zero on the closed contour and contribute nothing to the residue. We also divide out the terms $1 - R$ and K because near the magnetic axis they are constant in u to lowest order in s .

The only quantity left is B^2 , which can be written in the form

$$B^2 = \frac{(\mathbf{B} \cdot \mathbf{X}_v)^2}{\mathbf{X}_v^2} + \frac{\psi_v^2 |\mathbf{X}_u \times \mathbf{X}_v|^2}{\mathbf{X}_v^2 (K H R R_s)^2}.$$

The first term is the norm of the toroidal component of $\mathbf{B}$ and the second term is the norm of the poloidal component. For tokamaks and stellarators, the toroidal magnetic field is much stronger than the poloidal field and the equation $L_1(\psi) = 0$ can be used to show that it is independent of u at the magnetic axis. On the infinitesimal surface $s = s_0$ the toroidal part of B^2 will be nearly constant in u and contribute little to the residue. It is thus preferable to neglect this term, since numerical errors in its calculation may suppress the remaining poloidal part of B^2 .

We make a final simplification by replacing $\psi_v^2/\mathbf{X}_v^2$ by a constant. In the axisymmetric case $\psi_v = -\iota(s)$, so this assumption can be justified for configurations close to having such symmetry near the magnetic axis. A similar argument can be made for configurations close to helical symmetry due to the invariance of the representation of the integrand.

Combining these considerations, the simplified Euler-Lagrange equations are

$$L_3(\tau_0) = - \int_{s=s_0} \frac{|\mathbf{X}_u \times \mathbf{X}_v|^2}{(K H R R_s)^2} z_u du = 0,$$

$$L_4(z_0) = \int_{s=s_0} \frac{|\mathbf{X}_u \times \mathbf{X}_v|^2}{(K H R R_s)^2} r_u du = 0.$$

The most important feature of the equations is the fact that the Jacobian $K H R R_s$ appears in the denominator. This keeps the magnetic axis roughly centered inside the innermost flux surface and results in a continuous solution at the axis. For if the axis gets too close to the flux surface $s = s_0$, the Jacobian will become very small and the residue will differ from zero. Another important feature of the equations is that their implementation requires no constraints on the innermost flux surface $s = s_0$.

To further justify the simplified axis equations we use the identity

$$(\nabla s)^2 = \frac{|\mathbf{X}_u \times \mathbf{X}_v|^2}{(K H R R_s)^2} = \frac{(K r_u)^2 + (K z_u)^2 + (r_u z_v - r_v z_u)^2}{(K H R R_s)^2}$$

to write them in the purely geometrical form

$$L_3(r_0) = - \oint_{s=s_0} (\nabla s)^2 dz, \quad L_4(z_0) = \oint_{s=s_0} (\nabla s)^2 dr.$$

If we now assume that the innermost flux surface $s = s_0$ has elliptical cross sections $r = a_1 \cos(u)$, $z = a_2 \sin(u)$ with the axis at the center, then the two equations $L_3 = L_4 = 0$ follow to lowest order by Fourier analysis, since $(\nabla s)^2$ behaves like a combination of 1, $\cos(2u)$ and $\sin(2u)$. In this sense, our axis condition is equivalent to the more geometrical considerations used in BETAS. Indeed, in Chapter 7 very good agreement between the NSTAB and BETAS codes will be shown in two special cases.

CHAPTER 5

Iterative Scheme

5.1 The Second Order Richardson Iterative Scheme

We use a preconditioned iterative scheme to solve the Euler-Lagrange equations for the plasma problem. The scheme is based on the second order Richardson method invented by Frankel [8], with a preconditioner and an adaptive algorithm used for determining the acceleration parameters due to Betancourt [6]. In this chapter we describe how the iterative scheme accelerates the convergence of the slow modes while maintaining numerical stability. The preconditioner plays an equally important part in providing fast convergence of the method by removing the CFL restriction on the acceleration parameters and making the convergence rate independent of mesh size. It is described in Section 5.3.

Let U denote the vector of unknowns and let $L(U) = 0$ denote Euler-Lagrange equations associated with the first variation of the energy

$$\delta E = - \iiint L(U) \cdot \delta U \, ds \, du \, dv.$$

The simplest iterative scheme is the steepest descent method, which amounts to solving the equation

$$U_t = L(U), \tag{9}$$

where t is an artificial time parameter. The iteration process is defined by

$$\frac{U^{j+1} - U^j}{\Delta t} = L(U^j),$$

where U^j is the value of U at the j th iteration. The standard calculation

$$E_t = - \iiint L(U) \cdot U_t \, ds \, du \, dv = - \iiint U_t \cdot U_t \, ds \, du \, dv \leq 0 \tag{10}$$

shows that the energy decreases at each iteration.

The NSTAB code uses the pseudospectral method, where the iteration is applied to the Fourier coefficients of U rather than to U itself. Taking the Fourier transform of (9), we see that

$$U_t^{m,n} = L^{m,n}(U),$$

and the iterative scheme is unchanged except we use the m, n Fourier coefficient of $L(U)$ to iterate the m, n Fourier coefficient of U . For the remainder of this chapter, we will drop the m, n superscripts and treat U as the vector obtained after discretizing in the variable s .

For many problems, the steepest descent algorithm may be slow. NSTAB uses the faster second order Richardson method, which solves the discretized second order equation

$$aU_{tt} + eU_t = L(U). \quad (11)$$

By scaling a and e , we can always take $\Delta t = 1$, and thus there are two free parameters in the scheme. In the linear case, where the discretized equation $L(U) = 0$ requires solving a system of linear equations for a sparse positive definite matrix, it is the eigenvalues of this matrix which control the rate of convergence. Using the steepest decent algorithm, the time step Δt is bounded by the largest eigenvalue from stability considerations. The fast modes, which are the terms in the eigenfunction expansion of the error associated with these large eigenvalues, decay very quickly. The slow modes, associated with the smaller eigenvalues, decay at proportionally slower rates and lead to most of the computational effort. This is particularly true for the plasma problem when we are looking for physical modes associated with instabilities. One can accelerate the convergence of these slow modes by increasing Δt , but then the high modes become numerically unstable and reappear in the error. The remarkable feature of the second order Richardson method is that a can be chosen so that

all the modes are stable for all choices of e . This allows the slow modes to be accelerated by lowering e after the fast modes have converged without leading to instabilities for the fast modes.

To show why this is true, let us consider the model scalar equation

$$a(U^{j+1} - 2U^j + U^{j-1}) + e(U^{j+1} - U^j) = -\lambda U^j \quad (12)$$

for an eigenvalue λ satisfying $0 < \lambda \leq \lambda_{\max}$. This equation is obtained from (11) by applying the von Neumann test and discretizing in time. We will restrict a and e to be positive.

The solutions of the recurrence relation (12) are of the form

$$U^j = c_1 e^{-\omega_1 j} + c_2 e^{-\omega_2 j},$$

where the constants c_1 and c_2 are determined by the initial data. For this scheme to be numerically stable, the amplification factors $e^{-\omega_1}$ and $e^{-\omega_2}$ must both have norm less than one. They are given by the two roots of the quadratic equation

$$(a + e)e^{-2\omega} + (\lambda - e - 2a)e^{-\omega} + a = 0. \quad (13)$$

If the roots are complex, then they must be complex conjugates of each other and will have the same absolute value, so that the relation $e^{-\omega_1} e^{-\omega_2} = a/(a + e) < 1$ shows that the scheme is unconditionally stable. On the other hand, suppose that the roots are real. If we then take $a > \lambda/2$, both roots are positive and the largest is

$$\begin{aligned} e^{-\omega} &= \frac{2a + e - \lambda + \sqrt{(2a + e - \lambda)^2 - 4a(a + e)}}{2(a + e)} \\ &< \frac{2a + e + \sqrt{(2a + e)^2 - 4a(a + e)}}{2(a + e)} = 1. \end{aligned}$$

The choice $a > \lambda_{\max}/2$ thus guarantees stability of the iterative scheme for all λ and for all choices of e . After the initial quick convergence of the fast modes, we are then free to lower e to accelerate the convergence of the remaining slow modes.

To obtain the optimal convergence rate for a given λ , we choose e to minimize both amplification factors. For small ω , this leads to the condition

$$e/a = 2\omega. \quad (14)$$

For these choices of a and e , we can also estimate the convergence rate by solving for ω in terms of λ/a . For small λ , we obtain $\omega \approx \sqrt{\lambda/a} = \sqrt{2\lambda/\lambda_{\max}}$. The steepest descent algorithm converges at the substantially slower rate of $\omega \approx 2\lambda/\lambda_{\max}$.

The stability conditions discussed above for the steepest descent and second order Richardson methods can be shown to be equivalent to the usual CFL conditions resulting from treating (9) and (11) as parabolic and hyperbolic equations, respectively [2]. We thus refer to the restriction $a > \lambda_{\max}/2$ as a CFL condition.

5.2 Betancourt's Acceleration Scheme

Generalizing the above considerations for the nonlinear equation (11) leads to a very robust iterative scheme, which is ideal for many nonlinear problems. In practice, a fixed value of a is chosen empirically so that the iterative scheme remains numerically stable. When the iterative scheme is combined with the preconditioner described in the next section, a is constant over a wide range of mesh sizes. To achieve the maximum convergence rate during the iteration, we need only monitor the decay rate of the error ω and choose e at each time step according to the relation (14).

To estimate ω at time t in the iteration, we set

$$F(t) = \iiint U_t^2 dV.$$

Assuming exponential decay of the error $F(t) \approx F_0 e^{-2\omega t}$, we obtain ω by

$$\omega = -F_t/2F.$$

Performing a calculation similar to (10), it can be shown that $e/a > -F_t/2F = \omega$ is required to maintain descent of the energy. Our choice for e/a given in (14) satisfies this requirement.

The NSTAB code uses a more sophisticated, empirically verified formula given in [3] to determine ω at each iteration. In practice, we average this value over the previous N time steps so that

$$e/a = 2 \left(\frac{1}{N} \sum_k \omega_{j-k}^2 \right)^{1/2},$$

where $N \approx 50$. We have found that the value for e determined in this way represents too much acceleration when computing bifurcated solutions with complicated structure. We have thus added a lower bound for e which must be determined experimentally.

We note here that in the linear case there are many other second order methods, such as conjugate gradient, SOR, and Chebyshev semi-iterative, which can be used to solve $L(U) = 0$. All of these iterative schemes can be written in the form of equation (11). They only differ in how a and e are chosen at each time step [11]. Methods such as conjugate gradient rely closely on the matrix structure of the problem to determine optimal values of a and e .

5.3 Preconditioner

Preconditioning can improve the convergence of iterative schemes for a wide class of linear and nonlinear problems. It has become a standard technique and is even used in modern proofs of the implicit function theorem. Instead of solving the system $L(U) = 0$ we may solve $M^{-1}L(U) = 0$ for some linear operator M . The general principle is to choose the preconditioner M to bring the eigenvalues associated with the new system $M^{-1}L$ closer to unity. Such a choice for M also bounds the eigenvalues independently of the mesh size, removing the CFL restriction on Δt . We use a preconditioner which succeeds in both these respects. Furthermore, the number of iterations needed to achieve a given level of convergence is observed to be independent of the mesh size [6, 13].

We would like M to be as good an approximation of L as possible, while still being easily inverted. The preconditioner must also be positive definite so that the standard argument showing descent of the energy is still valid. Such a choice for M is obtained by taking the principal part of a linearized version of L and averaging its coefficients over the poloidal and toroidal angles u and v . These approximations of $L_1(\psi)$ and $L_2(R)$ are given by

$$M_1(\psi) = b_1 \psi_{uu} + b_2 \psi_{vv},$$

$$M_2(R) = \frac{c_1}{\sqrt{s}} (\sqrt{s} R)_{ss} + c_2 R_{uu} + c_3 R_{vv},$$

where

$$c_1(s) = \left\langle \frac{K H R B^2}{R_s} \right\rangle, \quad c_2(s) = \left\langle \frac{\psi_v^2 \mathbf{X}_R^2}{K H R R_s} \right\rangle, \quad c_3(s) = \left\langle \frac{\psi_u^2 \mathbf{X}_R^2}{K H R R_s} \right\rangle.$$

Here $\langle \cdot \rangle$ represents averaging over both u and v and the formulas for b_1 and b_2 are similar to those for c_1 , c_2 , and c_3 . With respect to u and v , the two preconditioners M_1 and M_2

are constant coefficient differential operators which can be explicitly inverted by the Fourier transform.

The preconditioned iterative scheme for the Fourier coefficients of the unknowns is written

$$\hat{M}_1(a\psi_{tt}^{m,n} + e\psi_t^{m,n}) = \hat{L}_1(\psi),$$

$$\hat{M}_2(aR_{tt}^{m,n} + eR_t^{m,n}) = \hat{L}_2(R).$$

After discretizing the variable s , the operator $\hat{M}_1$ is a diagonal matrix and $\hat{M}_2$ is tridiagonal. Thus both of these operators are easily inverted. The combination of the Fourier transform and a tridiagonal solver allows us to incorporate efficiently the preconditioners into the iterative scheme (c.f. [5]).

The remarkable performance of this simple preconditioner is due primarily to the fact that the equations $L_1 = 0$ and $L_2 = 0$ are derived from a variational principle. It is the variational principle that permits us to use only the m, n Fourier coefficient of L to iterate the m, n Fourier coefficient of the corresponding unknown (see Section 3.2). The preconditioner for $L_1(\psi)$ simply scales $L_1^{m,n}$ by $b_1 m^2 + b_2 n^2$. It is this scaling by $m^2 + n^2$ which removes the CFL restriction on the artificial time step, and any reasonable approximation for b_1 and b_2 would work almost as well. The preconditioner $\hat{M}_2$ for $L_2(R)$ combines this scaling with the inversion of a tridiagonal system in s .

CHAPTER 6

The NSTAB Computer Code

6.1 Discrete Equations

In this chapter we describe the discrete version of the Euler-Lagrange equations implemented in the NSTAB code. The use of the second order Richardson method to solve these equations requires the evaluation of the Fourier coefficients of the operators $L_1(\psi)$, $L_2(R)$, $L_3(r_0)$ and $L_4(z_0)$ at each iteration. The operators are computed from the unknowns by a combination of the spectral method in the angles on the torus and a finite difference scheme in the radial direction.

The unknowns are the Fourier coefficients $R^{m,n}$, $\psi^{m,n}$, r_0^n and z_0^n . Let N_u and N_v represent the maximum degree in u and v of the trigonometric polynomials that occur, and let N_r be the number of radial mesh points. At each step in the iteration cycle, R , ψ , r_0 , z_0 , and their u and v derivatives are evaluated directly from the Fourier coefficients at equally spaced collocation points in u and v . To avoid aliasing errors when calculating the Fourier coefficients of the nonlinear terms which appear in the differential operators, we might expect to use $4N_u$ and $4N_v$ collocation points, but in practice it is found that the errors become negligible when only $3N_u$ and $3N_v$ points are used. The double Fourier transforms involved in these calculations are performed via optimized matrix multiply routines.

Finite differences are used to compute the s derivatives by means of a scheme which provides very high resolution and minimal coupling between flux surfaces when combined with our simple representation for the Jacobian $KHRR_s$. These properties are desirable if current sheets and other localized modes are to be captured accurately. Codes bases on

similar and more elaborate differencing schemes [15], but with a different arrangement of the unknowns, do not seem to have the resolution to calculate solutions with current sheets and other types of modes as accurately as NSTAB and BETAS.

The radial differencing scheme evaluates R and $L_2(R)$ at the nodes s_i of the mesh intervals, but ψ and $L_1(\psi)$ are evaluated at centers $s_{i+1/2}$, where

$$s_i = \frac{i}{N_s}, \quad s_{i+1/2} = \frac{i + 1/2}{N_s}.$$

This scheme is conveniently implemented because R has boundary conditions at $s = 0$ and $s = 1$ and because ψ has no boundary conditions and need not be evaluated at the boundary. It allows second order differences to be used that produce minimal coupling between the surfaces.

The difference formulas used to evaluate the s derivatives and the averaging formulas that are used to evaluate a quantity at a center from its values on two adjacent nodes are taken from [3, 4]. They are chosen to be second order accurate and to give the exact answer in the example of a one-dimensional screw pinch. The Jacobian is evaluated as $K H R R_s = .5 K H (R^2)_s$, and the derivatives of quantities like R^2 which behave linearly in s are computed with the usual centered difference approximation. To evaluate terms in the operators like $(\mathbf{B} \cdot \mathbf{X}_s)_v$, first $\mathbf{B} \cdot \mathbf{X}_s$ is computed at collocation points from the above considerations and then its v derivative is computed at collocation points via back to back Fourier transforms.

The NSTAB code has the option of adding artificial viscosity in u and v to the Euler-Lagrangic equations. For a second order operator such as $L_1(\psi)$ we add a biharmonic term of the form $\Delta \Delta \psi$. This is easily implemented in our iterative scheme for the Fourier

coefficients by putting

$$a\psi_{tt}^{m,n} + e\psi_t^{m,n} = L_1^{m,n}(\psi) - \nu \frac{(m^2 + n^2)^2}{N_u^2 + N_v^2} \psi^{m,n}.$$

Similar terms are used for $L_2(R)$ and the axis equations. However, our experience is that artificial viscosity is not needed to assure convergence of the method.

6.2 Zoning of the Plasma Boundary

The NSTAB code takes as input the parametrization in u and v of the separatrix which defines the outer plasma wall. The coordinate v has been defined as the toroidal angle, but the definition of u is arbitrary. The actual location on a flux surface of the equally spaced mesh points in u will depend on how the outer wall is parametrized and on the location of the magnetic axis.

Let θ represent the polar angle in the coordinate system centered at the magnetic axis. The coordinate system puts the mesh points at the intersection of the rays $\theta = \text{const}$ and the flux surfaces $s = \text{const}$. If the outer wall is far from circular, or the magnetic axis is substantially shifted from the center of the plasma, points equally spaced in arc length along the boundary will not necessary be equally spaced in θ , and that results in poor spacing on the flux surfaces near the magnetic axis. In practice, we rezone the parametrization of the outer wall to get a compromise between equally spaced points in arc length on the boundary versus equally spaced points in θ . This simple method works well but does require some care. A more sophisticated procedure where the zoning is chosen to maximize the convergence of the Fourier series of the other unknowns is described in [16]. However, that method is questionable because it introduces an additional unknown.

The coordinates of the outer wall r_1 and z_1 are defined by

$$r_1 + iz_1 = e^{iu} \sum_{m,n} \Delta_{m,n} e^{-i(mu-nv)}.$$

We have used this formula because it provides a natural association between the coefficients $\Delta_{m,n}$ and the corresponding harmonics in the winding law used to determine the separatrix. Zoning is handled by making the change of variable

$$u = u' + \sum_{m,n} Z_{m,n} \sin(mu' - nv),$$

with collocation points chosen to be equally spaced in u' . In the simplest cases only $Z_{1,0}$ is nonzero to account for an outward shift in the position of the magnetic axis. In harder examples such as the H1 Heliac, where the outer wall is far from circular, proper zoning is critical for good convergence. It is found that large coefficients $\Delta_{m,n}$ may require rezoning by the corresponding coefficient $Z_{m,n}$, as can be seen from the calculation of the H1 Heliac in Section 7.4. Another feature of the code introduces the change of variable $u' = u - kv'$ so that helically symmetric cases can be computed with $N_v = 1$ and only 3 toroidal mesh points, exploiting the two-dimensional geometry. Axisymmetric solutions can be similarly computed with NSTAB by setting $N_v = 0$ and using only one toroidal mesh point.

We also rezone in s by specifying radial points according to the rule

$$s_i = \left(\frac{i}{N_s} \right)^\alpha.$$

The choice $\alpha = 1$ gives radial points equally spaced in the toroidal flux s , whereas $\alpha = 2$ produces equally spaced points in radius and provides more resolution near the magnetic axis. Best convergence of the code is achieved with the flux zoning $\alpha = 1$.

6.3 Inhomogeneous Term for Stability Test

The NSTAB code determines the stability properties of a configuration by looking for bifurcated solutions with current sheets or other less localized modes. In cases like the ITER tokamak and the LIID stellarator discussed in Sections 7.2 and 7.3, there are simple equilibria which are calculated by restricting the solution to be axisymmetric or by restricting the calculations to only one field period. When these restrictions are lifted, the solutions are shown to be nonlinearly unstable by establishing the existence of a family of deformed equilibria in some neighborhood of the original solution.

To obtain these bifurcated solutions, NSTAB allows for the temporary addition of an inhomogeneous term ξ to the Euler-Lagrange equations. As will be demonstrated in Sections 7.2, bifurcated equilibria can sometimes be found by simply performing a long run of NSTAB and letting truncation error and noise trigger any unstable modes, but the use of an inhomogeneous term is more efficient. The perturbation ξ is added to the equations for only one or two hundred iterations to bring some familiar mode to a reasonable level in the solution. It is then it is removed so that a new equilibrium solution can be calculated. In a stable cases, the mode should quickly decay and the calculation will converge to the original equilibrium. In mildly unstable cases the mode may produce a bifurcated equilibrium different from the usual one. However, in very unstable cases the mode continues to grow and the calculations may break down with a Jacobian approaching zero.

The inhomogeneous term ξ is chosen to approximate the type of unstable mode that is expected. These unstable modes are associated with resonances in the m, n Fourier coefficients near rational surfaces where $\iota = n/m$. We use a term for ξ similar to that given in the references about a second energy minimization [3, 4]. The inhomogeneous terms

added to the equations $L_1(\psi) = 0$ and $L_2(R) = 0$ are respectively

$$\xi_R = \xi_0 s^2 (1 - s) \cos(mu - nv),$$

$$\xi_\psi = -\xi_0 s (1 - 2s) \sin(mu - nv),$$

where ξ_0 is a fixed constant used to adjust the amplitude. The actual form of the inhomogeneous term can easily be changed, but it does not appear to be critical as long as the correct mode numbers m and n are chosen. If $m = 1$, then an inhomogeneous term is also added to the axis equations that has the form

$$\xi_r = \xi_0 \cos(nv), \quad \xi_z = \xi_0 \sin(nv).$$

CHAPTER 7

Numerical Results

7.1 Convergence Studies

In this section several studies are presented to demonstrate the convergence properties of the computational method and validate our simplified axis equations. The equilibria used in this study are an axisymmetric tokamak, a straight helical stellarator, and the LHD stellarator being built at the National Institute for Fusion Science in Japan. These cases show the convergence of the method is only first order with respect to the radial mesh size. In spite of this, the method is still very accurate so that stability tests can be performed with as few as 15 radial points. The well known high order convergence of the spectral method in the poloidal and toroidal directions is established, and there is very little improvement once one increases the number of harmonics above a certain value. However, even in relatively simple cases this threshold is surprisingly high. In terms of the degrees N_u and N_v of the trigonometric polynomials used to represent the solution in the poloidal and toroidal angles, $N_u = N_v = 8$ is adequate for equilibrium, while $N_u = N_v = 16$ may be required for stability.

The axisymmetric tokamak and straight helical equilibria are presented primarily to establish the validity of the new axis condition. For these cases we compare NSTAB to BETAS, which has been shown elsewhere to converge to exact solutions [6]. The first such comparison is shown in Fig. 3, where the location of the magnetic axis in a tokamak is plotted as a function of the radial mesh size. Satisfactory agreement is seen between the two codes. Fig. 3 shows the axis location is accurate to 1% of the plasma radius when only 12 radial points are used, but the convergence is only first order. Satisfactory agreement

is also obtained for the energy levels, since extrapolated values agree to seven figures. A $\beta = 0$ tokamak was used for this example with an aspect ratio of 3.33, a circular outer wall and a rotational transform $\iota(s) = 1.1 - .75s$. The computations were performed with 12, 24 and 48 radial points and with all poloidal modes in the Fourier series included up to degree $N_u = 12$.

A comparison of the two codes in the case of a straight helical stellarator is shown in Fig. 4, where the energy is plotted with respect to the radial mesh size. It is clear from the graph that the computational method is only first order accurate even in such a simple case as this. The energy levels from the two codes agree to seven figures at every mesh, so their data points are indistinguishable. The same agreement is achieved for the location of the magnetic axis, thus validating our simplified representation of the axis equations in the presence of large helical effects. The plasma boundary for this vacuum case was an infinite column with a period 2π , a radius $\Delta_{0,0} = 1$, and helical excursion $\Delta_{1,1} = .75$. The computations were performed with 12, 24, 48 and 96 radial points, and $N_u = N_v = 12$.

The convergence of the energy and axis location with regard to the degrees of the poloidal and toroidal harmonics N_u and N_v are displayed for the LHD stellarator in Figs. 5 and 6. Clearly $N_u = N_v = 4$ is inadequate, even in this simple case where the plasma column has elliptical cross sections. However, the spectral method has converged quite well as soon as $N_u = N_v = 8$. The figures show the convergence of the energy and the shift in the magnetic axis is again only first order with respect to the radial mesh size, but the method is still very accurate. Even at the crudest radial mesh of 15 points, the error in the axis position is only 2% of the plasma radius, which should not affect stability results. For this study we used an aspect ratio of 6.23 and a pressure profile of $p(s) = .04(1 - s)$, which gives $\beta = 3\%$. In each of the ten field periods, the plasma column forms a rotating

ellipse given by $\Delta_{0,0} = 1$ and $\Delta_{2,1} = -.325$. The equilibrium calculations were performed over just one field period of the device with 15, 22, 29 and 57 radial points.

To show the advantages of the new axis condition we compare NSTAB and BETAS in the case of the LHID stellarator with $\beta = 6\%$. At this value of β , the axis has a noticeable helical excursion and a large outward shift which substantially deforms the inner flux surfaces. The results from NSTAB are displayed in Fig. 8. The new axis condition imposes no constraints on the inner flux surfaces, and the calculations show that even at a fine radial mesh these surfaces have a pronounced tear-drop shape. The magnetic axis has an outward shift of .48, or half the plasma radius. The BETAS code requires that the innermost flux surface be an ellipse. This in turn forces other surfaces to have less of a tear drop shape and introduces errors over a significant volume of the plasma. The overall effect is that all the flux surfaces become less deformed and the magnetic axis has an outward shift of only .36. Errors in the axis location of this size can affect stability results. At $\beta = 9\%$, NSTAB places the axis at .60 and the flux surfaces become incompatible with the elliptical outer wall, so perhaps free boundary calculations might show that a true equilibrium does not exist.

For all the runs presented here, the discrete Fourier transforms of degree N_u and N_v were performed with $3N_u$ and $3N_v$ collocation points in the poloidal and toroidal angles. This confirms the assertion made in Section 6.1 that a ratio of 3 between mesh size and degree of the Fourier coefficients is sufficient to control any aliasing errors. We also note that the observed computation time for these runs scales like the product $N_s N_u N_v$ because of the preconditioned iterative scheme.

7.2 Capturing Current Sheets

In this section we demonstrate the high accuracy of the flux coordinate method and its ability to calculate weak solutions with well resolved current sheets. The success of the method suggests that it could also be used to capture vortex sheets in fluid dynamics. In Fig. 7 a bifurcated equilibrium, calculated with only 12 radial points, is shown for the ITER tokamak [7]. A current sheet has developed so that several flux surfaces intersect at $\iota = 1$. A whole family of such solutions can be found by rotating the mode in the toroidal direction.

The existence of bifurcated equilibria form the basis of our stability test. They confirm the well known result that a tokamak equilibrium becomes unstable when the rotational transform crosses unity in the plasma. At the meshes we use to make these runs, it is not always practical to rely on the energy landscape to determine stability. The bifurcated solutions do indeed have lower energy than the axisymmetric solution, but the difference is small, and convergence studies become difficult in harder cases with more complicated geometry.

The bifurcated equilibria are produced by the procedure described in Chapter 6. At $\iota = 1$ we look for the internal kink mode which has an $m = 1, n = 1$ mode structure. To trigger this mode, we add an $m = 1, n = 1$ inhomogeneous term to the partial differential equations for a few hundred iterations. After the term has been removed the run converges to the bifurcated equilibrium shown in Fig 7. The convergence rate for the bifurcated solution is substantially slower than the convergence rate of the axisymmetric solution. The axisymmetric case completely converges in 1,000 iterations. While it only takes 3,000 iterations to establish the existence of a bifurcated solution, 50,000 iterations are required to converge the run to 14 significant figures in the energy, which takes 15 minutes on the

CRAY Y-MP computer.

A similar bifurcated solution can be computed without using an inhomogeneous term by simply using more iterations and allowing noise to trigger the unstable mode. When such a run is made, it at first converges to the axisymmetric solution. The energy decreases monotonically to the axisymmetric value, where it remains until the mode finally emerges. Then the energy starts to decrease further and the run converges to a bifurcated solution that is like the one shown in Fig. 7 except that the mode may be rotated in the toroidal direction. The level of convergence is not as good as in the previous example if the mode has a phase angle clashing with the toroidal mesh.

To model the ITER tokamak in these computations, we used an aspect ratio of 3.33, a D-shaped plasma boundary given by $\Delta_{0,0} = 1$, $\Delta_{2,0} = -.2$, and $\Delta_{-1,0} = .2$, and the rotational transform $\iota(s) = 1.2 - .75s$. The pressure profile was taken to be $p(s) = .04(1 - s)$ with $\beta = 4.4\%$, but the instability is current driven and can be seen even at zero β . The computations were performed with 12 radial, poloidal and toroidal points with degrees $N_u = N_v = 4$.

7.3 Stability Test

In addition to the localized current sheet modes in the previous example, our computational method also has the resolution to test for nonlinear instability by looking for bifurcated solutions with broader perturbations. Such computations require many poloidal and toroidal harmonics because the instabilities are associated with high mode numbers. The bifurcated solutions presented here demonstrate that NSTAB can handle these difficult cases.

One example is the LHD stellarator described in Section 7.1. In the standard configuration it is known to be marginally stable [17]. However, we analyze a family of nearby configurations that can be made unstable by reducing the outward shift of the magnetic axis. This is achieved by adding small harmonics to the shape of the outer wall that model the effect of increasing the vertical magnetic field. For moderate shifts, bifurcated solutions appear over two field periods of the device. The existence of these additional solutions prove that the equilibrium over just one field period is unstable.

A ballooning instability is shown in the bifurcated equilibrium presented in Fig. 9. This calculation was performed in two field periods, with an average β of 3%. Small values $\Delta_{1,1} = .03$ and $\Delta_{3,1} = .01$ were added to the shape of the outer wall, but they are barely visible in the figure. They have the effect of reducing the outward shift of the magnetic axis from 28% to 22% of the plasma radius. The mode appears in the middle third of the plasma volume where the rotational transform crosses $5/6$ and $5/5$, so it has a combined $m = 6, n = 5$ and $m = 5, n = 5$ structure over the full 10 field periods of the LHD.

This bifurcated solution is computed in a similar manner as the current sheet mode in the tokamak. The calculations are performed in two field periods, where the mode has an $m = 6, n = 1$ and $m = 5, n = 1$ structure. The mode is triggered by the temporary addition of an $m = 6, n = 1$ inhomogeneous term to the equilibrium equations. The effect

of this term on the $m = 6, n = 1$ component of the mode and on the convergence of the run is shown in Fig. 10. The spike that appears in the error and mode plots occurs when the inhomogeneous term was added. After this term is released the mode decays quickly, but it eventually levels off to a value which produced the bifurcated solution shown in Fig. 9. The computation required 3,000 iterations and used 30 minutes of CPU time on the CRAY Y-MP to converge to 7 significant figures in the energy. It was performed with 22 radial points and a trigonometric polynomial of degree $N_u = 16$ in the poloidal angle and $N_v = 24$ in the toroidal angle.

It is important to choose a fine enough mesh if instabilities are to be resolved. For the mode described above, meshes with as few as 15 radial points are adequate. However, in the poloidal direction harmonics must be allowed up to $N_u = 16$. If less are used, the mode is not seen because one must resolve adequately its $m = 7$ sideband and $m = 12$ overtone. The method seems well adapted to modes with moderate m and n values which occur in one or two field periods. Lower modes, such as the $m = 2, n = 1$, occur in the full 10 field periods of the LHD where the calculations become more difficult due to the different length scales involved.

It is only in special cases that we can compute completely converged bifurcated equilibria. For example, in stable configurations of the LHD with smaller values of the sidebands in the outer wall, the mode decays after the inhomogeneous term is removed, eventually becoming negligible. On the other hand, if the value of $\Delta_{3,1}$ is increased to .02 moving the axis in another 5%, the equilibrium becomes highly unstable. After the inhomogeneous term is removed the mode grows so large that the computations eventually break down. In such cases the energy decreases indefinitely and is clearly lower than the energy of the regular equilibrium. The difference of the energy levels in this case is in the seventh figure.

Stellarators may also have very poor plasma confinement for reasons not associated with MHD instabilities. Using Monte Carlo methods to track individual particles in an LHD equilibrium provides a good estimate of transport [9, 10]. In the LHD, calculations based on a plasma radius of 60 cm, a magnetic field of $B = 4$ tesla, an average temperature of 3 keV, and a plasma density of 10^{14} cm^{-3} predict an energy confinement time of only 5 ms.

7.4 Advanced Stellarators

Compared to the tokamak and the LHD, many of the recently designed stellarators have a quite complicated shape. More harmonics are needed to represent the outer wall, and the solutions have a much fuller Fourier series. The fine structure of these devices and the large poloidal and toroidal meshes required to model them have caused difficulties with the equilibrium codes. We have developed a very robust, general tuning of the input parameters for NSTAB that works well in a variety of these harder cases.

Two advanced stellarators are presented here. The first is similar to the Helias designed in Germany [18], but has been modified to provide an unstable test case for the NSTAB code. We have calculated two different, fully converged bifurcated solutions over one field period of the device. The two dramatically deformed equilibria, shown in Figs. 11 and 12, were calculated by triggering the $m = 7, n = 6$ mode with opposite signs of the inhomogeneous term. The existence of these two minima leads us to conjecture that there is a third, less deformed but linearly unstable solution lying between these two bifurcated solutions. This is plausible because of the mountain pass theorem.

To capture this high order instability, the computations were performed with $N_u = 16$ and $N_v = 12$ which required 42 collocation points in the toroidal direction and 36 in the

poloidal direction. The mode is not seen if less harmonics are used, but just 19 radial points were sufficient. One of these cases has been run for 40,000 iterations, taking 200 minutes on the CRAY Y-MP and convergence of the bifurcated solutions to 9 significant figures in the energy was observed. The computed rotational transform varies between 6/7 and 6/8 with very little shear, and the stellarator has an aspect ratio of 10 with 6 field periods and a pressure profile $p(s) = .03(1 - s)$ at $\beta = 3\%$.

Our second case is the H1 Heliac at the Australian National University. This experiment has a large helical excursion of the magnetic axis and pronounced triangularity of the wall shape, so many harmonics are required to describe the solution. A fully converged equilibrium computed by the NSTAB code is shown in Fig. 13. For this run we used 15 radial points and degree $N_u = N_v = 12$ for the trigonometric polynomials. Rezoning of the outer wall to distribute the collocation points well on the inner flux surfaces proved important in achieving good convergence. In a series of runs at the Australian National University it was not possible to get the VMEC code to converge on such a fine mesh. We have also been unable to get BETAS to converge in this case, although the performance of both codes could probably be improved with additional tuning.

The H1 equilibrium computed by NSTAB required two hours on a CRAY 2 and 40,000 iterations to achieve 11 significant figures in the energy. The energy E reached a minimum when only 9 of the 11 figures had stabilized, and then E was increasing as it converged to its final value. In using the spectral method, this type of behavior is not unexpected, since the discrete quadrature formula for the energy is not directly related to the equilibrium equations. The decay of the error for this run is shown in Fig. 14, and there is no reason to believe that NSTAB would not converge to more figures if the run were continued.

To model the H1, we used an aspect ratio $A = 5$, 3 field periods and a pressure profile

$p(s) = .055(1 - s)^2$ which gives $\beta = 2\%$. The plasma wall is defined by $\Delta_{1,1} = 1.25$, $\Delta_{-1,-1} = 0.30$, $\Delta_{2,1} = -.10$, $\Delta_{2,2} = -.36$, and $\Delta_{3,3} = 0.10$. It was rezoned to give a more even distribution of the mesh points in u by putting $Z_{-1,-1} = 0.30$, $Z_{2,1} = -.10$, $Z_{2,2} = -.15$, $Z_{3,3} = 0.10$, and making the change of variable $u' = u - v$. The computations were performed with 15 radial points and $N_u = N_v = 12$. The computed rotational transform increases from 1.08 on axis to 1.14 at the outer wall.

CHAPTER 8

Conclusions

We have developed the new three-dimensional MHD equilibrium code NSTAB. The code uses the spectral method and a flux coordinate formulation of the variational principle associated with the MHD equations. It has the resolution to compute bifurcated equilibria with well resolved current sheets at rational surfaces and other, broader perturbations. A configuration is considered to be nonlinearly unstable when several bifurcated solutions can be shown to exist. It is less practical to use the energy landscape to determine stability properties, although in cases where comparisons are possible the energy levels of the bifurcated solutions are less than those of the more standard equilibria, verifying that they represent true physical instabilities.

The method has low order convergence with respect to the radial mesh size, but is still highly accurate. Conclusive stability tests can be performed with as few as 15 radial mesh points. The method is well adapted to the moderate mode numbers of the instabilities that develop in one or two field periods of typical stellarators. To capture bifurcated solutions with these modes, many poloidal and toroidal harmonics must be used, but NSTAB does converge in these hard cases.

We have given a new residue condition to determine the location of the magnetic axis. It is derived from the weak form of the equations resulting from the variational principle and imposes no constraints on the shape of the flux surfaces. Several simplifications are made to implement the condition numerically, but it has held up well in practice. In cases with elliptical flux surfaces at the axis the resulting condition is related to the geometrical condition used by BETAS and there is good agreement between NSTAB and BETAS. In

harder cases, the lack of constraints allows for more realistic flux surfaces. The shape of these surfaces can have a significant effect on the axis location, which is critical for accurate stability results.

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Fig. 1. A model of the LIID stellarator plasma showing the cylindrical coordinate system used by NSTAB. The cross sections are elliptical and there are ten field periods.

Fig. 2. Cutaway view of a section of the ITER tokamak showing the flux coordinate system. The magnetic axis $s = 0$, an intermediate flux surface, and the plasma boundary $s = 1$ are shown.

Fig. 3. First order convergence of the shift in the magnetic axis with respect to mesh size for a $\beta = 0$ tokamak is shown for both the NSTAB and BETAS codes. The axis shift is measured in units of the plasma radius. This convergence study is part of a series of runs using the BETAS code to debug and validate the NSTAB code.

Fig. 4. First order convergence of the energy E with respect to mesh size for a $\beta = 0$ straight helical stellarator with $\Delta_1 = .75$ is shown. In this case, NSTAB and BETAS give almost identical values for E and the location of the the magnetic axis.

Fig. 5. First order convergence of the energy E with respect to radial mesh size is shown for the $\beta = 3\%$ LHID stellarator at three degrees of the trigonometric polynomials specifying the spectral truncation. The limited accuracy of the spectral method when $N = 4$ is perhaps surprising for this simple problem where the outer wall is defined by a rotating ellipse. In this case only 6 figures in the energy are significant and this is too few to resolve stability issues from the energy landscape.

Fig. 6. First order convergence of the shift in the magnetic axis with radial mesh size is shown for the $\beta = 3\%$ LHID stellarator at different degrees of the trigonometric polynomials specifying the spectral truncation. For a degree N truncation, $4N^2$ terms are used in the spectral representation of the solution and the mesh sizes in the poloidal and toroidal directions are $1/(3N)$.

Fig. 7. An $m = 1, n = 1$ mode in the ITER tokamak with $\beta = 4.4\%$. A current sheet has developed where ι crosses unity, and it becomes clearly visible in this calculation on a $12 \times 12 \times 12$ mesh of radial, toroidal and poloidal points and Fourier terms up to degree 4×4 . This plot is evidence of the contention that the NSTAB code captures weak solutions of the equilibrium problem characterized by nested KAM surfaces.

Fig. 8. Flux surfaces in four cross sections of one field period of the LHD stellarator showing the deformed structure of the inner surfaces with an average $\beta = 6\%$. This calculation was performed with 31 radial points and degree 8 trigonometric polynomials. At larger β , the surfaces become more incompatible with the elliptical outer wall and free boundary calculations may show that a true equilibrium does not exist.

Fig. 9. Four cross sections of two field periods of a bifurcated LHID stellarator equilibrium with $\beta = 3\%$ are shown. A mode which breaks the one field period symmetry is visible. In two field periods, the mode has an $m = 6, n = 1$ and $m = 5, n = 1$ structure. Small sidebands $\Delta_{1,1} = .03$ and $\Delta_{3,1} = .01$ in the shape of the separatrix have reduced the usual outward shift of the magnetic axis, destabilizing what is otherwise considered to be a standard configuration. Nonuniqueness of the solution is made evident by the asymmetry.

Fig. 10. Decay of the error and convergence of the $m = 6$, $n = 1$ mode in two field periods are shown for the bifurcated LHD equilibrium pictured in Fig. 9. Fast convergence followed by slower convergence after the unstable mode has been triggered can be seen for the residuals as a function of the iteration. The graph of the norm of the $m = 6$, $n = 1$ mode shows the effect of the inhomogeneous term triggering convergence to a level visible in the equilibrium.

Fig. 11. Four cross sections of one field period of a bifurcated equilibrium solution for an advanced stellarator configuration with $\beta = 3\%$. In one field period, ι is roughly $1/7$ throughout the plasma, and the mode clearly shows an $m = 7, n = 1$ structure. The run has exemplary convergence, establishing that the NSTAB code can handle equilibria with complicated harmonics on a fine mesh with $22 \times 48 \times 36$ points and Fourier terms up to degree 16×12 .

Fig. 12. A bifurcated equilibrium for the advanced stellarator similar to that shown in Fig. 11 but with the opposite sign of the displacement, which establishes the existence of two different solutions.

Fig. 13. Four cross sections of one field period of the $\beta = 2\%$ H1 Helic at ANU. The complicated triangularity and crescent structure of this case were resolved on a mesh with $15 \times 36 \times 36$ points and Fourier terms up to degree 12×12 . The run has converged to 11 significant figures in the energy.

Fig. 14. Steady decay of the residuals as a function of the iteration is shown for the fine mesh run of the H1 Helic in Fig. 13. The run has converged to 11 significant figures in the energy E , but E reached its minimum when only 9 figures were accurate.

```

ns      nu      nv      nuf      nvf      nvfAX      irot      alpha
15      36      36      12      12      6          1          1.00

A      zlen      Q      Qext
5.00   0.00      3      1

m      n      DELmn      Zmn
-1     -1      0.300      0.300
1      1      1.250      0.000
2      1      -0.100     -0.100
2      2      -0.360     -0.150
3      3      0.100      0.100

p0      xpr      ypr      zpr      iota0      iota1      stell      eiota
0.055   2.00     1.00     1.00     0.400     0.010     T          20.0

aR      aPSI     emin      nav      safi      aAX      eAX      axisw
4.0     4.0      0.20     50      2.00     4.00     0.20      1.00

numit   numext   ic      nprint   rays      lthick   bndj      fixAX
40000   0          4000    1        F          2.00    200.00    0.00

starth   stoph     mh      nh      mode      artvR    artvPSI   artvAX
0         0          3       1      0.0050    0.0010   0.0010    5.0000

iter      energy      Jac      ratio      mode      max R err      PSI err      Axis err      iota err
1  40.844946628171    0.104E+02    -0.786E-04    0.495E+00    0.574E+00    0.145E+01    0.411E+01
4000 30.542984649598    0.212E+02    0.232E-01    0.529E-04    0.304E-05    0.151E-03    0.339E-05
8000 30.542994385833    0.205E+02    0.232E-01    0.762E-05    0.393E-06    0.296E-04    0.206E-06
12000 30.542993630741    0.205E+02    0.232E-01    0.115E-05    0.714E-07    0.408E-05    0.244E-07
16000 30.542993523674    0.205E+02    0.231E-01    0.384E-06    0.144E-07    0.125E-05    0.561E-08
20000 30.542993537099    0.205E+02    0.231E-01    0.196E-06    0.738E-08    0.659E-06    0.275E-08
24000 30.542993550399    0.205E+02    0.231E-01    0.101E-06    0.385E-08    0.367E-06    0.158E-08
28000 30.542993557001    0.205E+02    0.231E-01    0.519E-07    0.198E-08    0.200E-06    0.830E-09
32000 30.542993559972    0.205E+02    0.231E-01    0.265E-07    0.102E-08    0.107E-06    0.430E-09
36000 30.542993561273    0.205E+02    0.231E-01    0.135E-07    0.518E-09    0.572E-07    0.221E-09
40000 30.542993561828    0.205E+02    0.231E-01    0.687E-08    0.263E-09    0.303E-07    0.114E-09

CPU time: 132.88 minutes.

```

Fig. 15. A sample run for the H1 Helic from Fig. 13. The output shows the convergence of the energy and the universal settings of the input parameters.

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