A MULTI-GRID SOLVER FOR UP-DOWN ASYMMETRIC TOKAMAK EQUILIBRIA*

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The computer code TOQ produces tokamak equilibria in a coordinate system which uses the poloidal flux surfaces as coordinate surfaces. It is well-suited for providing accurate equilibria to stability analyses. It has been extremely useful for beta-optimization in modeling Advanced Tokamak scenarios and the study of bootstrap current driven Spherical Torus. To solve the Grad-Shafranov equation, TOQ uses a mult-grid (MG) package\(^1\), which has been shown to be very robust in solving elliptic problems. The MG algorithm as implemented has to be modified in order to deal with up-down asymmetric equilibria. In this work we discuss an implementation of the new MG algorithm and give examples of up-down asymmetric high-beta equilibria using DIII-D geometry and the ITER geometry. We also explore the stability of such equilibria vis a vis the up-down symmetric ones.

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OBJECTIVES

Extend the MHD equilibrium code (TOQ) to

- solve for fixed-boundary equilibria with boundary flux surfaces which can be up-down asymmetric

- employ multi-grid method for 2-D elliptic equations with periodic boundary condition in one dimension for numerical efficiency
BACKGROUND

- For up-down symmetric equilibria, DeLucia, Jardin and Todd\textsuperscript{1} obtained solutions of finite-difference Grad-Shafranov equation in flux coordinates via iterative change of coordinates

- A modified approach at GA (Miller and Lin-Liu) was implemented in TOQ

- Recent use of a multi-grid method package\textsuperscript{2} in TOQ improved speed of convergence by a large measure, allowing exploration of new equilibrium regimes\textsuperscript{3}

- Need for up-down asymmetric equilibria exists both for DIII-D and future tokamak reactors such as devices similar to ITER

- Periodic boundary conditions are required for general equilibria

- Neither TOQ nor the multigrid package are equipped to handle periodic boundary conditions

DEVELOPMENTAL TASKS

1. Create iterative 2-D elliptic equation solver with periodic boundary condition in one dimension

2. Implement multi-grid approach for the above problem

3. Modify TOQ to accommodate periodic boundary conditions and incorporate multi-grid solver

4. Validate against existing TOQ
THE 2-D ELLIPTIC PROBLEM

\[ A \frac{\partial^2 f}{\partial \rho^2} + B \frac{\partial^2 f}{\partial \rho \partial \theta} + C \frac{\partial^2 f}{\partial \theta^2} + D \frac{\partial f}{\partial \rho} + E \frac{\partial f}{\partial \theta} + F f = g \]

in the domain \( a \leq \rho \leq b \) \( 0 \leq \theta \leq 2\pi \) with Dirichlet boundary conditions for \( \rho \) and periodic conditions for \( \theta \). Coefficients depend on \( \rho, \theta \)

Finite-differencing leads to alternate representations:

**FORM 1: NINE-POINT STENCIL**

\[ a_7 f_{i-1,j+1} + a_8 f_{i,j+1} + a_9 f_{i+1,j+1} \\
    a_4 f_{i-1,j} + a_5 f_{i,j} + a_6 f_{i+1,j} = g_{i,j} \\
    a_1 f_{i-1,j-1} + a_2 f_{i,j-1} + a_3 f_{i+1,j-1} \\
\]

**FORM 2: BLOCK TRIDIAGONAL** \( Lf = g \)

\[
L = \begin{pmatrix}
D_1 & P_1 \\
M_2 & D_2 & P_2 \\
& & \ddots \\
& & & M_n & D_n
\end{pmatrix}
\]

coupling \( \rho \) grid lines.

\[
D, P, M = \begin{pmatrix}
\times & \times & \ldots & \times \\
\times & \times & \times \\
& \ddots \\
\times & \times & \times & \times
\end{pmatrix}
\]

coupling \( \theta \) values (cyclic tridiagonal)
SOLUTION BY ILLU DECOMPOSITION

The matrix equation is iteratively solved by a modified Thomas algorithm which involves the calculation of \( \overline{D}_j \) by

\[
\begin{align*}
\overline{D}_1 &= D \\
\overline{D}_j &= D_j - \text{tridiagonal part of } M_j \overline{D}_{j-1}, \quad j = 2, \ldots, n
\end{align*}
\]

which enter into the approximate LU decomposition

\[
L \approx \begin{pmatrix}
I & & & \\
M_2 \overline{D}_1^{-1} & I & & \\
& M_3 \overline{D}_2^{-1} & & \\
& & \ddots & \\
& & & M_n \overline{D}_{n-1}^{-1}
\end{pmatrix} \begin{pmatrix}
\overline{D}_1 & P_1 \\
\overline{D}_2 & P_2 \\
& & \ddots \\
& & & \overline{D}_n
\end{pmatrix}
\]

The solution of linear equations with cyclic tridiagonal matrix \( C \) employs a decomposition

\[
C = T + u \tilde{v}
\]

where \( T \) is a tridiagonal matrix and \( u, v \) are column vectors, followed by Sherman-Morrison's formula

\[
C^{-1} = T^{-1} - \frac{(T^{-1}u)(\tilde{v}T^{-1})}{1 + \lambda} \quad \lambda = \tilde{v}T^{-1}u
\]

Thomas algorithm is used for solving tridiagonal systems.
CONVERGENCE IS ACCELERATED USING MULTIGRID METHOD

WHICH REPEATEDLY USES MGCS CYCLES

1. Initial guess for \( f \)

2. form residue

\[
  r_1 = g - Lf
\]

3. restrict \( r_1 \) to successively coarser grids

\[
  r_1 \rightarrow r_2 \rightarrow \cdots \rightarrow r_{l_{\text{max}}}
\]

4. solve residue equation on coarsest grid:

\[
  L_{l_{\text{max}}} \delta f_{l_{\text{max}}} = r_{l_{\text{max}}}
\]

5. for \( i = l_{\text{max}} \) to 2

   prolongate \( \delta f_i \) to finer grid: \( \delta f_i \rightarrow \delta f_{i-1} \)

   smooth \( \delta f_{i-1} \) by relaxation on \( L_{i-1} \delta f_{i-1} = r_{i-1} \)

6. obtain corrected solution

\[
  f \rightarrow f + \delta f_1
\]

7. smooth solution \( f \) by relaxation on \( Lf = g \)
COMPONENTS IN MULTI-GRID METHOD

GRID LAYOUT

\[ m = 2^m \quad n = 2^n + 1 \quad \Delta \theta = \frac{2\pi}{m} \quad \Delta \rho = \frac{b-a}{n-1} \]

\[ m_c = m/2 \quad n_c = (n+1)/2 \quad \Delta \theta_c = \Delta \theta / 2 \quad \Delta \rho_c = \Delta \rho / 2 \]

PROLONGATION \( P_\ell \): 

\[
\begin{array}{c}
1 \\
1/2 \\
1/4 \\
\end{array}
\]

RESTRICTION \( R_\ell \):

\[
\begin{array}{c}
+ \\
+ \\
1/4 \\
1/8 \\
1/16 \\
\end{array}
\]

RESTRICTION OF LINEAR OPERATOR: \( L_\ell = R_{\ell+1} L_{\ell+1} P_\ell \)

SMOOTHING: iterate once with ILLU

SOLVING: iterate 8 times with ILLU
TREATMENT OF CO-ORDINATE ORIGIN

When one boundary is the co-ordinate origin \( \rho = 0 \) at \( j = 1 \), the equations there become

\[
f_{i1} = f_0 \quad i = 1, \ldots, m \quad f_0 = \frac{1}{m} \sum_{i=1}^{m} f_{i2}
\]

which do not conform to forms 1 or 2. The problem can be solved by the following method (Lin-Liu and Miller):

1. Obtain solution to “homogeneous” problem:

\[
Lf^{(0)} = 0 \quad f^{(0)} = \begin{cases} 
1 & j = 1 \\
0 & j = n
\end{cases}
\]

2. Obtain solution to “inhomogeneous” problem

\[
Lf^{(1)} = g \quad f^{(1)} = \begin{cases} 
0 & j = 1 \\
given\ values & j = n
\end{cases}
\]

3. The required solution is

\[
f = f^{(1)} + \lambda f^{(0)}
\]

where \( \lambda \) is determined by the requirement

\[
f_0 = \frac{1}{m} \sum_{i=1}^{m} f_{i2}
\]
VALIDATION OF ELLIPTIC EQUATION SOLVER

Soloviev equilibrium with magnetic axis at $(R_a, Z_a)$ is solved in toroidal co-ordinate system centered at $(R_o, Z_o)$. The boundary is a circle on which the poloidal flux $\psi$ assumes values given by the analytic equilibrium.

On a 64x64 grid, with the convergence criterion that L-2 norm of successive correction be less than $10^{-6}$, the solution is obtained with point-wise accuracy of order $10^{-3}$.

![The $\rho - \theta$ grid and $\psi$ contour]

COMPUTATIONAL EFFICIENCY: The CPU times in seconds on the K machine for various algorithms are as follows.

<table>
<thead>
<tr>
<th>grid</th>
<th>SOR</th>
<th>ILLU</th>
<th>Multi-grid</th>
<th>4 levels</th>
<th>5 levels</th>
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</thead>
<tbody>
<tr>
<td>32x33</td>
<td>9.3</td>
<td>1.86</td>
<td>0.70</td>
<td>0.70</td>
<td></td>
</tr>
<tr>
<td>64x65</td>
<td>----</td>
<td>17.34</td>
<td>3.23</td>
<td>3.10</td>
<td></td>
</tr>
<tr>
<td>128x129</td>
<td>----</td>
<td>468.50</td>
<td>15.61</td>
<td>17.56</td>
<td></td>
</tr>
</tbody>
</table>
THE PROBLEM SOLVED BY TOQ

- Solve Grad-Shafranov equation in general coordinate system $\rho, \theta$

$$\frac{R^2}{J} \left[ \frac{\partial}{\partial \rho} \left( h_{\rho \rho} \frac{\partial \chi}{\partial \rho} + h_{\rho \theta} \frac{\partial \chi}{\partial \theta} \right) + \frac{\partial}{\partial \theta} \left( h_{\theta \rho} \frac{\partial \chi}{\partial \rho} + h_{\theta \theta} \frac{\partial \chi}{\partial \theta} \right) \right] = -(\psi_b - \psi_a)(4\pi p' + f'')$$

where $\chi = \frac{\psi - \psi_a}{\psi_b - \psi_a}$, $\psi_b$ and $\psi_a$ are poloidal fluxes at the boundary and the magnetic axis respectively.

The metric tensor components are

$$h_{\rho \rho} = \left( J/R^2 \right) (R^2_{\rho} + Z^2_{\rho}) \quad h_{\theta \theta} = \left( J/R^2 \right) (R^2_{\theta} + Z^2_{\theta}) \quad h_{\rho \theta} = -\left( J/R^2 \right) (R_{\rho} R_{\theta} + Z_{\rho} Z_{\theta})$$

and $R(\theta, \rho), Z(\theta, \rho)$ are cylindrical coordinates. The Jacobian is

$$J = (R_{\rho} Z_{\theta} - R_{\theta} Z_{\rho})$$. The shape functions $p'(\chi)$ and $f''(\chi)$ are given. The domain in the general coordinates is defined by $0 \leq \rho \leq 1 \quad 0 \leq \theta \leq 2\pi$. The boundary curve is prescribed, as is also the boundary value $\psi_b$.

- Determine $\chi, R, Z$ so that

  1. $\chi = G(\rho)$, a prescribed function

  2. $\theta$ grid points divide poloidal flux contours into segments of equal-arc length
GRID ITERATION SCHEMES

DeLucia, Jardin and Todd:

Step 1: Construct initial grid \( R(\theta, \rho_j) Z(\theta, \rho_j) \)

Step 2: Solve finite-difference modified G-S equation which assumes poloidal flux \( \chi \) to depend only on \( \rho \):

\[
\overline{\Delta} \chi \equiv \frac{R^2}{J} \left[ \frac{\partial}{\partial \rho} \left( h_{\rho \theta} \frac{\partial \chi}{\partial \rho} \right) + \frac{\partial}{\partial \theta} \left( h_{\theta \theta} \frac{\partial \chi}{\partial \rho} \right) \right] = -(\psi_b - \psi_a)(4\pi p' + ff')
\]

Step 3: Construct new grid \( R'(\theta, \rho_j) Z'(\theta, \rho_j) \) so that constant \( \rho \) surfaces are \( \chi \) contours satisfying \( \chi = G(\rho) \), a prescribed function.

Step 4: Repeat Steps 2 and 3 until convergence.

Modified approach in TOQ

Step 2: Solve finite-difference G-S equation

\[
\Delta^* \chi = -(\psi_b - \psi_a)(4\pi p' + ff')
\]

Differences:

DeLucia et al: Solution of G-S equation is obtained only at the end of iteration together with the requisite grid

TOQ: Solution of G-S equation is obtained in every iteration. Purpose of iteration is to provide accurate input to stability codes.
INITIAL CHOICE OF GRID FOR TOQ

A uniform grid is chosen for \((\theta, \rho)\):

The grid points \(P_{ij}\) in physical space is chosen as follows:

1. Uniformly spaced points \(P_{in}\) are chosen on the boundary curve
2. The coordinate origin \(O\) is chosen arbitrarily
3. Grid points \(P_{ij}, j = 2, \ldots, n - 1\) are laid on the line \(OP_{in}\) proportionately according to the grid function \(G(\rho)\):

\[
\frac{OP_{ij}}{OP_{in}} = G(\rho)
\]
HOW NEW GRIDS ARE FORMED

1. Start with solution \( \chi \) on old grid

2. Retain grid points on boundary: \( P_{in}' = P_{in} \quad i = 1, \ldots, m \)

3. Move co-ordinate origin to location of minimum \( \chi : O \rightarrow O' \)

4. Points \( P_{ij}' \) for \( j \) such that \( G(\rho_j) \leq \chi_0 \) where \( \chi_0 \) is the value at the origin are laid out similarly as the initial grid:

5. Other points \( P_{ij}' \) are chosen on constant \( \theta \) lines \( OP_{in} \) so that Evaluation of Interpolated \( \chi \) along \( OP_{in} \) at \( P_{ij}' = G(\rho_j) \)

6. Points on each constant \( \rho \) surface are rearranged so they are equally spaced.
WHERE TOQ USES THE 2-D
ELLIPTIC EQUATION SOLVER

NONLINEAR ITERATION

The nonlinear G-S equation is iteratively solved:

\[ \Delta^* \chi^{(n+1)} = - (\psi_b - \psi_a^{(n)}) (4 \pi \rho'(\chi^{(n)}) + f f'(\chi^{(n)}) ) \]

until convergence.
TOQ UP-DOWN SYMMETRIC EQUILIBRIUM IS REPRODUCED

NEW CODE
EXISTING CODE

The $\rho - \theta$ grid

$\psi$ contours
GOOD AGREEMENTS WITH EXISTING CODE

INTEGRATED QUANTITIES

<table>
<thead>
<tr>
<th></th>
<th>NEW CODE</th>
<th>EXISTING CODE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_a$</td>
<td>262.493</td>
<td>262.474</td>
</tr>
<tr>
<td>$Z_a$</td>
<td>3.0\times10^{-5}</td>
<td>0</td>
</tr>
<tr>
<td>$\langle \beta \rangle$</td>
<td>0.02313</td>
<td>0.02312</td>
</tr>
<tr>
<td>$\beta_p$</td>
<td>0.185</td>
<td>0.184</td>
</tr>
<tr>
<td>$I_i$</td>
<td>0.03309</td>
<td>0.03280</td>
</tr>
<tr>
<td>$q_a$</td>
<td>3.015</td>
<td>2.930</td>
</tr>
<tr>
<td>$\psi_b^{-1}\psi_a$</td>
<td>3.432\times10^7</td>
<td>3.426\times10^7</td>
</tr>
</tbody>
</table>

SELECTED FLUX FUNCTION PROFILES
(EXISTING CODE: DASHED; NEW CODE: SOLID)
AN UP-DOWN SYMMETRIC EQUILIBRIUM
SHIFTED UPWARD

When an up-down symmetric boundary is shifted upward relative to the mid-plane of the R-Z coordinates, the code is able to reproduce the intrinsically symmetric equilibrium:
EXAMPLES OF UP-DOWN ASYMMETRIC EQUILIBRIUM

A sequence of up-down asymmetric equilibria is generated with boundary flux surfaces consisting of the upper half of an ellipse joined on to the lower part of a dee:

\[ R = R_0 + R_{\text{max}} \cos(\theta + \Delta \sin \theta) \]
\[ \Delta = \begin{cases} 
0 & 0 \leq \theta \leq \pi \\
\sin^{-1} \delta & \pi \leq \theta \leq 2\pi
\end{cases} \]

\[ Z = e R_{\text{max}} \sin \theta \]

TRENDS OF SELECTED QUANTITIES
AN UP-DOWN ASYMMETRIC EQUILIBRIUM

GRIDS AND POLOIDAL FLUX CONTOURS ($\delta=0.8, \epsilon=2.0$)
CONCLUDING REMARKS

- A multigrid solver of 2-D elliptic equations with periodic boundary condition in one dimension is developed

- TOQ is generalized to also produce up-down asymmetric equilibria

- Convergence of coordinate iteration scheme is demonstrated in TOQ for up-down asymmetric equilibria

- Computation of equilibrium quantities near magnetic axis needs refinement

- Coupling to the stability code GATO is to be performed