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Reconstruction of 3D Equilibria from Flux Surface Knowledge Only

H.E. Mynick, N. Pomphrey,
Princeton Plasma Physics Laboratory

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Introduction

Using the properties of the Grad-Shafranov (GS) equation, Christiansen and Taylor (CT) have shown[1] that complete MHD equilibria may be obtained for axisymmetric tokamaks with noncircular cross-sections, provided that one initially knows only the shapes of the flux surfaces. Starting from a 3D generalization of the GS equation[2], we have recently demonstrated[3] that this remarkable result can be extended to 3D systems like stellarators.

A code **Profile_Invert** to practically implement our earlier formal result is nearing completion. Here, we describe the current status of the code.

Theory

Assume we are given toroidal equilibria

$$\nabla p = \mathbf{J} \times \mathbf{B}, \quad \mu_0 \mathbf{J} = \nabla \times \mathbf{B} \qquad (1)$$

with good flux surfaces, described by flux-surface label $\rho(\mathbf{x})$, hence

$$B^\rho \equiv \nabla\rho . \mathbf{B} = 0, \quad J^\rho \equiv \nabla\rho . \mathbf{J} = 0 \ . \qquad (2)$$

We parametrize real-space position by flux coordinates $\{q^i\} \equiv \{\rho, \theta, \zeta\}$ (i=1-3). For a starting "reference" system we take $\zeta = \zeta_g$, the geometric toroidal angle.

For 2D (axisymmetric) systems, one uses the "mixed" representations

$$\mathbf{B} = \nabla\psi \times \mathbf{b} + \mathbf{b}F, \quad \mu_0 \mathbf{J} = -\mathbf{b}\Delta^*\psi + \nabla F \times \mathbf{b} \qquad (3)$$

(with $\mathbf{b}^2 \Delta^* \psi \equiv \nabla . (\mathbf{b}^2 \nabla \psi)$, $\mathbf{b} \equiv \nabla \zeta_g = \hat{\zeta} / R$, so $\mathbf{b}^2 = R^{-2}$) to obtain the GS equation:

$$\mathbf{b}^2\Delta^*\psi = -\mu_0 p'/\psi' - \mathbf{b}^2 FF'/\psi', \qquad (4)$$

where $p' \equiv dp/d\rho$.

For 3D systems, it is shown in [2] that a mixed representation may again be given, making use of 2 special coordinate systems, the "natural" & "conatural" systems $\{\rho,\theta_n,\zeta_n\}$ & $\{\rho,\theta_c,\zeta_c\}$, satisfying the similar determining equations

$$\nabla.[\nabla\rho x(\nabla\theta_n x\nabla\rho)]=0,\ \nabla.[\nabla\rho x(\nabla\zeta_n x\nabla\rho)]=0, \qquad (5)$$

$$\nabla.[\nabla\rho x(\nabla\theta_c x\nabla\rho)/|\nabla\rho|^2]=0, \nabla.[\nabla\rho x(\nabla\zeta_c x\nabla\rho)/|\nabla\rho|^2]=0$$

Then the generalized mixed rep is given by:

$$\mathbf{B} = \nabla\psi x\mathbf{b}_c+\mathbf{b}_n F,$$

$$\mu_0\mathbf{J} = \nabla x(\nabla\psi x\mathbf{b}_c)+\nabla F x\mathbf{b}_n+F\nabla x\mathbf{b}_n, \qquad (6)$$

where $\mathbf{b}_{n,c}\equiv\mathbf{e}_{n,c}/(\mathbf{e}_{n3}.\mathbf{e}_{c3})$, and $\mathbf{e}_{n,c}\equiv\partial\mathbf{x}/\partial\varsigma_{n,c}$ is the contravariant basis vector for $\varsigma_{n,c}$.

This yields the 3D-GS equation[2]:

$$\mathbf{b}_c^2\Delta_c{*}\psi = -\mu_0 p'/\psi' - \mathbf{b}_n^2 FF'/\psi' + F\mathbf{b}_c.\nabla x\mathbf{b}_n - F'\mathbf{b}_c.\mathbf{b}_n x\nabla\rho$$
$$-(F/\psi'|\nabla\rho|^2)(\mathbf{b}_n x\nabla\rho).\nabla x(\mathbf{b}_c x\nabla\psi) +$$
$$(F^2/\psi'|\nabla\rho|^2)(\mathbf{b}_n x\nabla\rho).(\nabla x\mathbf{b}_n), \qquad (7)$$

where $\mathbf{b}_c^2\Delta_c{*}\psi \equiv -\mathbf{b}_c.\nabla x(\nabla\psi x\mathbf{b}_c) = \nabla.(\mathbf{b}_c^2\nabla\psi) - \nabla\psi.\mathbf{b}_c x(\nabla x\mathbf{b}_c)$.

Following CT, we write $\psi' x(7)$ as a product of some combination of the profile functions $\{p',\psi',F\}(\rho)$ times coefs $\{A,C,D_{i=1-5}\}(\mathbf{x})$ which vary over a flux surface:

$$\psi'\psi''A+\psi'^2 C = -D_1\mu_0 p' - D_2 FF' - D_3 F^2 - D_4(F\psi')' - D_5(F\psi'), \qquad (8)$$

where $A\equiv |\nabla\rho|^2$, $C\equiv \mathbf{b}_c^2\Delta_c{*}\rho$, $D_1\equiv 1$, $D_2\equiv \mathbf{b}_n^2$,
$D_3 \equiv -(\mathbf{b}_n x\nabla\rho).(\nabla x\mathbf{b}_n)/|\nabla\rho|^2$, $D_4\equiv \mathbf{b}_c.(\mathbf{b}_n x\nabla\rho)$,
$D_5\equiv -\mathbf{b}_c.(\nabla x\mathbf{b}_n) + (\mathbf{b}_n x\nabla\rho).\nabla x(\mathbf{b}_c x\nabla\rho)/|\nabla\rho|^2$. (9)

These coefficients are all even under stellarator symmetry $\{\theta,\zeta\} \rightarrow -\{\theta,\zeta\}$. Only A, C, D_1, and D_2 are $\neq 0$ in the 2D case.

Our goal is to solve Eq.(8) for the profiles $\{p', \psi', F\}$. For this, we must

(a) compute the natural & conatural coordinates, to evaluate the coefficients $\{A, C, D_i\}$ in (8), and then

(b) solve (8) as a system of o.d.e's in ρ.

Computer Code Profile_Invert

Profile_Invert accepts, as input, a Fourier representation of flux surfaces corresponding to a 3D stellarator equilibrium. We envision the flux surface shapes being provided experimentally by, for example, soft X-ray tomographic data. The first major step of **Profile_Invert** is to obtain the natural and co-natural coordinates for the equilibrium, necessary for obtaining $\mathbf{b}_n$ and $\mathbf{b}_c$ and the coefficients that appear in Eq.(9). The second major step is the solution of Eq.(8), leading to the profiles of pressure and current.

Calculating the natural and co-natural coordinates

Following Degtyarev et al., the natural coordinates θ_n, ζ_n are related to "background" cylindrical coordinates through transformation functions η^θ and η^ζ:

$$\theta_n = \theta + \eta^\theta, \quad \zeta_n = \zeta + \eta^\zeta \ .$$

The η^θ and η^ζ are solutions of

$$\begin{bmatrix} \partial/\partial\theta\ \gamma_{33}\ \partial/\partial\theta - \partial/\partial\theta\ \gamma_{23}\ \partial/\partial\zeta \\ -\partial/\partial\zeta\ \gamma_{23}\ \partial/\partial\theta + \partial/\partial\zeta\ \gamma_{22}\ \partial/\partial\zeta \end{bmatrix} \begin{Bmatrix} \eta^\theta \\ \eta^\zeta \end{Bmatrix} = \begin{Bmatrix} -\partial/\partial\theta\ \gamma_{33} + \partial/\partial\zeta\ \gamma_{23} \\ \partial/\partial\theta\ \gamma_{23} - \partial/\partial\zeta\ \gamma_{22} \end{Bmatrix}$$

where $\gamma_{ij} = g_{ij}/\sqrt{g}$. The γ_{ij} are determined from the given plasma shape. The equation is solved by calling a MUDPACK library routine.

Having found the transformation to natural coordinates, inductances α_{ij} are calculated which relate the poloidal and toroidal fluxes to the poloidal and toroidal currents:

$$J = -\alpha_{22}\Psi' + \alpha_{23}\Phi', \quad F = -\alpha_{23}\Psi' + \alpha_{33}\Phi', \qquad (10)$$

$$\alpha_{22} = \langle \gamma_{22}\,(1+\partial\eta^{\zeta}/\partial\zeta) - \gamma_{23}\,\partial\eta^{\zeta}/\partial\theta \rangle_{\theta}$$

$$\alpha_{23} = \langle \gamma_{23}\,(1+\partial\eta^{\zeta}/\partial\zeta) - \gamma_{33}\,\partial\eta^{\zeta}/\partial\theta \rangle_{\zeta}$$

$$\alpha_{33} = \langle \gamma_{33}\,(1-\partial\eta^{\theta}/\partial\zeta) + \gamma_{33}\,\partial\eta^{\theta}/\partial\theta \rangle_{\zeta}$$

These are needed for the evaluation of the natural and co-natural **b** field expressions:

$\mathbf{b}_n = b_n^2\,\mathbf{e}_2 + b_n^3\,\mathbf{e}_3$;

$b_n^2 = -(\partial\eta^{\theta}/\partial\zeta)/(\alpha_{33}\sqrt{g})$, $b_n^{\zeta} = (1+\partial\eta^{\theta}/\partial\theta)/(\alpha_{33}\sqrt{g})$.

$\mathbf{b}_c = b_{c1}\,\mathbf{e}^1 + b_{c2}\,\mathbf{e}^2 + b_{c3}\,\mathbf{e}^3$;

$b_{c2} = (1+\partial\eta^{\theta}/\partial\theta)\,\alpha_{23}/\alpha_{33} + \partial\eta^{\zeta}/\partial\theta$,

$b_{c3} = (\partial\eta^{\theta}/\partial\theta)\,\alpha_{23}/\alpha_{33} + (1+\partial\eta^{\theta}/\partial\theta)$,

$b_{c1} = -(g^{12}/g^{11})\,b_{c2} - (g^{13}/g^{11})\,b_{c3}$.

The calculation of $\mathbf{b}_n$ and $\mathbf{b}_c$ is parallelizable.

Sol'n of radial eqn: Method-1

We generalize the method in [1], making use of the great redundancy in Eq.(8) pointed out by CT. We write (8) as

$$-A\ u_1 - C\ u_2 = D_k\ v_k, \qquad (11)$$

where $u_{j=1,2} \equiv \{\psi'\psi'', \psi'^2\}$, $v_{k=1,5} \equiv \{\mu_0 p', FF', F^2, (F\psi')', (F\psi')\}$. Taking flux-surface averages $\langle h_i(\mathbf{x})(10)\rangle$ of Eq.(11), with $h_{i=1\text{-}6}(\mathbf{x})$ 6 independent "test" functions, yields

$$-B_{ij}\ u_j = E_{ik}\ v_k\ , \qquad (12)$$

(summation over repeated indices j=1-2, k=1-5 implied), with $B_{ij} \equiv \langle h_i \{A, C\}\rangle$, $E_{ik} \equiv \langle h_i D_k\rangle$.

We 1st solve (12) for the v_k in terms of the u_j, making use of the 1st 5 equations in (12). Thus restricting i to the range 1-5 there, we solve (12) by inverting E_{ik}:

$$v_i = -F_{ij}\ u_j, \qquad (13)$$

with

$$F_{ij} \equiv E_{ik}^{-1}\ B_{kj}\ (i=1\text{-}5,\ j=1\text{-}2).$$

Putting this into the $i=6^{th}$ equation, one obtains

$$G_j\ u_j = 0, \qquad (14)$$

with

$$G_j \equiv B_{6j} - E_{6k}\ F_{kj}\ (j=1\text{-}2).$$

(14) is of the same form as CT obtain in [1], $\psi''/\psi' = u_1/u_2 = -\lambda(\rho)$, with $\lambda \equiv G_2/G_1$, solved as in [1] for $\psi'(\rho)$:

$$\psi'(\rho) = \psi_0' \exp[-I(\rho)], \text{ with } I(\rho) \equiv \int_{\rho 0}^{\rho} d\rho_1 \lambda(\rho_1). \qquad (15)$$

From this, one computes the u_j, and from (13), the v_k, which give $p'(\rho)$ and $F(\rho)$. These are then used in Eqs.(10) to get $J(\rho)$, $\Phi'(\rho)$.

-Consistency Relations (CRs):

From the $\{u_j, v_k\}(\rho)$, one notes that there is more than 1 way to compute the basic profiles $\{p', \psi', F\}(\rho)$. E.g., F is given by any of

$F=[F_0^2+2\int_{\rho 0}^{\rho} d\rho_1 v_2]^{1/2}$, $F=v_3^{1/2}$, or

$F=(F\psi')/\psi' \equiv v_5/\psi'$. (CR1)

$(F\psi')$ is given in 2 ways:

$(F\psi')= v_5$, or $(F\psi')= \int_{\rho 0}^{\rho} d\rho_1 v_4$. (CR2)

Finally, pressure balance gives 2 expressions

for $v_1 \equiv p'$: $p'=(J'\psi' -F'\Phi')/V'$, (CR3)

where $V' \equiv dV/d\rho$, $V \equiv (2\pi)^{-2} x$(volume within ρ). These CRi hold only if the coefs $\{A,C,D_i\}$ are from proper MHD equilibria.

Test Case-1: 2D Solovev equilibrium

Flux surface shape:

$$R^2(\rho,\theta) = R_m^2 + 2\rho\cos\theta,$$
$$z(\rho,\theta) = \rho\sin\theta/[\alpha(R^2-\sigma^2)]^{1/2}, \quad (16)$$

where $R_m^2 \equiv [(\Delta^2+\delta^2)/2]^{1/2}$, $\Delta \equiv R_0+a$, $\delta \equiv R_0-a$, and $\alpha > 0, 0 \le \sigma \le \delta < \Delta$.
The coefs $\{A,C,D_i\}$ can be obtained analytically:

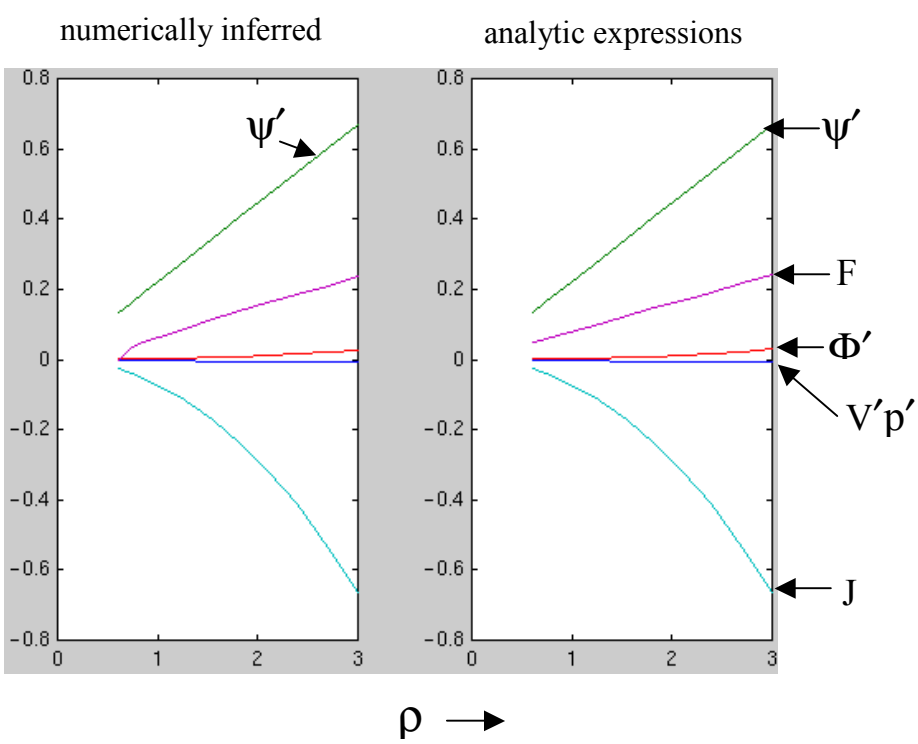
$$A^{Sol} = \cos^2\theta + \alpha^2 \sin^2\theta(R^2-\sigma^2)/R^2 + \rho\sin^2\theta[2\cos\theta + \rho\sin^2\theta/(R^2-\sigma^2)]/(R^2-\sigma^2),$$

$$C^{Sol} = \{\sin^2\theta + \alpha^2 \cos^2\theta(R^2-\sigma^2)/R^2\}/\rho - \sin^2\theta[2\cos\theta + \rho\sin^2\theta/(R^2-\sigma^2)]/(R^2-\sigma^2),$$
$$D_2^{Sol} = 1/R^2.$$

-The code computes these numerically from (16), and applies the sol'n method just discussed to obtain profiles $\{p', \psi', F\}$. These may be compared with analytic expressions for these:

$$\psi' \equiv d_\rho\psi = 2\rho/(aR_0)^2,$$
$$d_\psi p = -2(1+\alpha^2)/(aR_0)^2,$$
$$d_\psi F^2 = 4\alpha^2\sigma^2/(aR_0)^2. \qquad (17)$$

-Results:



-Method-1 has been successfully applied to 2D equilibria, including the above Solovev case, as well as to 2D numerical **VMEC** equilibria. However, it has not yet been successful on 3D equilibria, for reasons we now discuss.

Test Case-2: 3D Equilibrium

To leading order in an expansion around a circular magnetic axis, flux surfaces for an N field-period stellarator have elliptical toroidal cross sections:

$$R = R_0[1 + \varepsilon\{\cos(\theta) + \xi\cos(\theta + N\zeta)\}]$$
$$Z = \varepsilon R_0[\sin(\theta) - \xi\sin(\theta + N\zeta)\}]. \qquad (18)$$

Here, R_0 is the radius of the magnetic axis, $\rho \in [0,1]$ is a flux surface label, $\varepsilon = \rho\Gamma_0/R_0$ is the expansion parameter, $\rho\Gamma_0$ is the average minor radius of a flux surface, and $\xi \in [0,1]$ controls the ellipticity of the flux surfaces.

For a vacuum configuration (p'=0=F'), the rotational transform at the magnetic axis is $\iota_0 = N\xi/(1+\xi^2)$ (eg see Garren, Boozer [4]).

With shape Eq.(18), analytic expressions for A, C, and the D_i appearing in Eq.(8) can be found, by expansion to leading order. They are:

$A = a_1 - a_2\cos(2\theta+N\zeta)$, $C = \rho^{-1}(a_1+a_2\cos(2\theta+N\zeta))$,
$D_3 = 0$, $D_4 = \rho b_2\cos(2\theta+N\zeta)$, $D_5 = -b_1 - b_2\cos(2\theta+N\zeta)$,
where
$a_1 = (1+\xi^2)/R_0^2\Gamma_0^2(1-\xi^2)^2$, $a_2 = 2\xi/R_0^2\Gamma_0^2(1-\xi^2)^2$,
$b_1 = 2N\xi^2/R_0^3(1-\xi^2)^2$, $b_2 = N\xi/R_0^3(1-\xi^2)$. (19)
Since we <u>assume</u> a vacuum configuration ($p'=0=F'$) we can also assume $D_1=0=D_2$ in Eq.(8).

- Solution Method-1 applied to the 3D equil.

We notice that the solution procedure using Method-1, leading to Eq.(14), requires taking flux surface averages with one more independent test function than there are v_k functions to determine. In the general case, there are 5 functions $v_{k=1,5}=\{\mu_0 p', FF', F^2, (F\psi')', (F\psi')\}$. For the 3D equilibrium model discussed in this section, the radial equation analogous to Eq.(8) that has to be inverted (solved for ψ' and F) is

$$\psi'\psi''A+\psi'^2 C = -D_4(F\psi')' - D_5(F\psi'). \quad (8)$$

There are 2 v_k functions, $\{(F\psi')'$ and $(F\psi')\}$. Method-1 therefore requires 3 independent test functions $h_i(\mathbf{x})$ to obtain Eq.(14). However, the

expressions for A, C and $D_{i=4,5}$ clearly show that only 2 independent test functions exist for the 3D model, namely $h_1 = 1$ and $h_2 = \cos(2\theta + N\zeta)$.

The root of the problem appears to lie in the consistency relations: To solve Eq.(8) we should not consider F^2 to be independent of FF', or $(F\psi')'$ to be independent of $(F\psi')$.

Sol'n of radial eqn: Method-2

Noting that $2\psi'\psi'' = d(\psi'^2)/d\rho$, and $(F\psi')' = d(F\psi')/d\rho$, we define new dependent variables $X = \psi'^2$ and $Y = F\psi'$, so that Eq.(8) becomes

$$(A/2)X' + C\,X = -D_4\,Y' - D_5 Y. \qquad (20)$$

Taking 2 flux surface averages of Eq.(20) yields a matrix equation

$$\alpha \begin{bmatrix} X' \\ X \end{bmatrix} = -\beta \begin{bmatrix} Y' \\ Y \end{bmatrix} \qquad (21)$$

where α, β are 2x2 matrices. We can solve for Y', Y as functions of X' and X to obtain

$$Y' = -[(\beta^{-1}\alpha)_{11}X' + (\beta^{-1}\alpha)_{12}X],$$

$$Y = -[(\beta^{-1}\alpha)_{21}X' + (\beta^{-1}\alpha)_{22}X]. \qquad (22)$$

Equating the RHS of Eq.(22a) with $d/d\rho$ of the RHS of (22b) yields a 2nd order d.e. for $X = (\psi')^2$:

$$(\beta^{-1}\alpha)_{21}X'' + [(\beta^{-1}\alpha)_{22} + (\beta^{-1}\alpha)_{21}' - (\beta^{-1}\alpha)_{11}]X' + [(\beta^{-1}\alpha)_{22}' - (\beta^{-1}\alpha)_{12}]X = 0.$$

After solving for X Eq.(22b) is solved algebraically for Y, leading to $F=Y/\psi'$.

For the 3D equilibrium model coefficients, Eq.(19),

$(\beta^{-1}\alpha)_{11}=-(a_1/b_1+a_2/b_2)/2\rho$, $(\beta^{-1}\alpha)_{12}=-(a_1/b_1-a_2/b_2)/\rho^2$,

$(\beta^{-1}\alpha)_{21}=-a_1/2b_1$, $(\beta^{-1}\alpha)_{22}=-a_1/b_1\rho$.

This leads to the solution $X \propto \rho^2 \Longrightarrow \psi'=\psi'_{\rho=1}\,\rho$.

Substituting for X in Eq.(22b) gives $F = 2\psi'_{\rho=1}\, a_1/b_1 =$ Const, as required for a vacuum solution.

Using the inversion derived expressions for F and ψ', expressions a_1 and b_1 from Eq.(19), and using $\sqrt{g} = \rho\Gamma_0^2 R_0(1-\xi^2)$ from Eq.(16), we obtain an expression for the rotational transform at the magnetic axis, $\iota_0=(\psi'/\sqrt{g})/(F/R_0^2)$:

We find $\iota_0 = N\xi^2/(1+\xi^2)$, in agreement with the known value of ι_0 for the model equilibrium[4].

The Method-2 formulation is easily generalized to the case where $p', F' \neq 0$: Variables X and Y are supplemented with a 3rd variable $Z \equiv F^2$.

$\langle h_1(\mathbf{x})\,\mathrm{Eq.8}\rangle$ is used to eliminate the p′ term, and an additional 4 independent averages lead to a second order d.e. for $X=\psi'^2$. After solving for $X=\psi'^2$, algebraic substitution again obtains F.

Although Method-2 incorporates several consistency relations, the <u>nonlinear</u> CR that relates variables ψ'^2, $F\psi'$ and F^2, namely $(F\psi')^2 = F^2 \times \psi'^2$, has not been incorporated. While Method-2 has successfully demonstrated inversion of the model 3D equilibrium, it remains to be seen whether it can successfully invert a full current, full beta NCSX equilibrium. To test this, **Profile_Invert** will take plasma shapes from the output of VMEC equilibria. Predicted profiles from **Profile_invert** will then be compared with the profiles originally input to VMEC.

Sol'n of radial eqn: Method-3

-An alternate sol'n method to Method-2 writes Eq.(8), after the p′ term has been removed, as

$$\boldsymbol{\alpha}\,.\,\mathbf{X}' = -\boldsymbol{\beta}.\mathbf{X}\ , \qquad (23)$$

where $\mathbf{X} \equiv [X,Y,Z] \equiv [\psi'^2, (F\psi'), F^2]$, and $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are 3x3 matrices of the coefficients already displayed.

This is a system of 3 1st-order o.d.e.'s, which may be simply integrated in ρ. It does not require taking higher derivatives of the coefs. The merits & weaknesses of Methods 2 & 3 are under study.

Summary & Discussion:

-We have built a code **Profile_Invert** which implements a method described earlier[3] for inferring the radial profiles of 3D equilibria from only knowledge of the flux surface shapes.

-The 1st method of solving the radial equations called for by the is successful on 2D equilibria, but thus far not on 3D equilibria, probably because of difficulties satisfying consistency rel'ns in the equations. 2 additional methods are now under study which should help to remedy this problem.

-Applying Method-2 to a model analytic 3D equilibrium, we have analytically established that 3D profiles can in fact be inferred from the basic equation (8) of the method.

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