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**FLOC—Field Line and Orbit Code
for the Study of Ripple Beam
Injection into Tokamaks**

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OAK RIDGE NATIONAL LABORATORY
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STUDY OF RIPPLE BEAM INJECTION INTO TOKAMAKS

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ABSTRACT

The computer code described is used to study ripple beam injection into a tokamak plasma. The collisionless guiding center equations of motion are integrated to find the orbits of single particles in realistic magnetic fields for ripple injection. In order to determine if the ripple is detrimental to the plasma, the magnetic flux surfaces are constructed by integration of the field line equations. The numerical techniques are described, and use of the code is outlined. A program listing is provided, and the results of sample cases are presented.

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1. INTRODUCTION

A major problem of neutral beam heating of reactor-size tokamak plasmas is beam penetration. Increasing the beam energy to achieve penetration is unsatisfactory because of the increasingly low neutralization efficiency of high energy ions. A viable alternative is the ripple-injection technique.¹ This method involves the creation of a ripple in the toroidal magnetic field using an appropriate arrangement of coils operating at the proper current. The fast ions resulting from the neutral beam injection are trapped in the local ripple magnetic well and drift to the center of the plasma, where they become untrapped due to the decrease in the ripple. A test of neutral beam ripple injection is planned for the ISX-B device in 1979.

The constraints on ripple injection have been described elsewhere.² The purpose of this paper is to describe a computer code which was developed to study ripple injection. Presented also are the results of calculations performed for the upcoming test on ISX-B.

The code was written so that it is usable, with only minor changes, at other installations. It has been run on a DEC PDP-10 and a CDC-7600.

2. BASIC EQUATIONS

The computer code, Field Line and Orbit Code (FLOC), has two main functions. The first is to integrate the collisionless guiding center equations of motion of single particles in a torus with realistic magnetic fields for ripple injection. Thus for a given plasma and ripple coil configuration, FLOC can be used to determine if the beam particles reach the plasma center. The second function of FLOC is to

determine if the ripple is detrimental to the plasma. This is accomplished by integration of the field line equations for the construction of the magnetic flux surfaces. The structure of the flux surfaces indicates the effect of the ripple on the plasma.

The coordinates (r, θ, ϕ) used in FLOC are defined in Fig. 1 and by the equations

$$x = R \cos \phi , \quad (2.1)$$

$$y = -R \sin \phi , \quad (2.2)$$

and

$$z = r \sin \theta , \quad (2.3)$$

where

$$R = R_0 + r \cos \theta . \quad (2.4)$$

The guiding center equations are taken from Northrop.³ We assume that the fields are time independent, i.e.,

$$\frac{\partial \vec{B}}{\partial t} = \frac{\partial \vec{E}}{\partial t} \equiv 0 , \quad (2.5)$$

and the nonelectromagnetic force is zero ($\vec{g} = 0$). Specifically, the guiding center equations in mks units are

$$\begin{aligned} \frac{d\vec{R}}{dt} = & \vec{U}_E + \frac{\hat{B}}{qB} \times \left(\mu \nabla B + mv_{||}^2 \frac{\hat{B}}{B} \cdot \nabla \vec{B} + mv_{||} \vec{U}_E \cdot \nabla \hat{B} + mv_{||} \hat{B} \cdot \nabla \vec{U}_E \right. \\ & \left. + m \vec{U}_E \cdot \nabla \vec{U}_E \right) + v_{||} \hat{B} , \end{aligned} \quad (2.6)$$

and

$$\frac{dv_{||}}{dt} = \frac{q}{m} E_{||} - \frac{\mu}{m} \hat{B} \cdot \nabla B + \vec{U}_E \cdot \left(v_{||} \frac{\hat{B}}{B} \cdot \nabla \vec{B} + \vec{U}_E \cdot \nabla \hat{B} \right) , \quad (2.7)$$

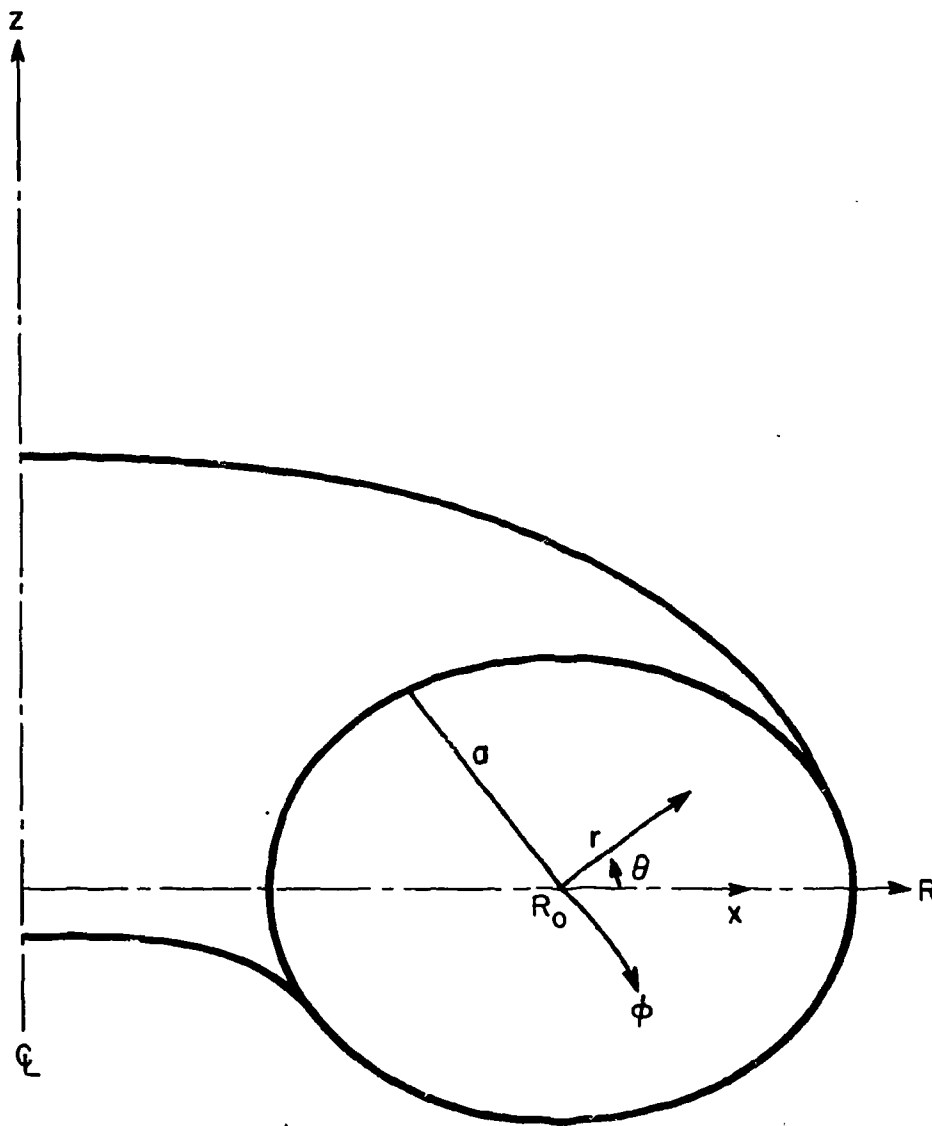


Fig. 1. Coordinate system.

where

$$\hat{\mathbf{B}} = \frac{\vec{\mathbf{B}}}{B}, \quad (2.8)$$

$$\vec{\mathbf{U}}_E = \frac{\vec{\mathbf{E}} \times \hat{\mathbf{B}}}{B}, \quad (2.9)$$

$$\mu = \frac{1}{2} \frac{mv_{\perp}^2}{B}, \quad (2.10)$$

$$E_{\parallel} = \vec{\mathbf{E}} \cdot \hat{\mathbf{B}}, \quad (2.11)$$

and

$$\mathbf{v}_{\parallel} = \frac{d\vec{\mathbf{R}}}{dt} \cdot \hat{\mathbf{B}}(\vec{\mathbf{R}}). \quad (2.12)$$

Here $\vec{\mathbf{R}}$ is the position of the guiding center. These equations are programmed in vector notation in order to easily change coordinate systems. In the coordinates of Fig. 1,

$$\frac{d\vec{\mathbf{R}}}{dt} = \begin{bmatrix} \frac{dr}{dt} \\ r \frac{d\theta}{dt} \\ R \frac{d\phi}{dt} \end{bmatrix}. \quad (2.13)$$

The magnetic field line equations are

$$\frac{dr}{d\phi} = \frac{RB_r}{B_{\phi}} \quad (2.14)$$

and

$$\frac{d\theta}{d\phi} = \frac{RB_{\theta}}{rB_{\phi}}. \quad (2.15)$$

A deferred-limit integrator written by Boris and Winsor,⁴ based upon the Bulirsch-Stoer extrapolation technique,⁵ is used to integrate the guiding center equations. A variable order, variable step formulation⁶ of the classic Adams methods is employed for the integration of the field line equations.

3. FIELD MODELS

The magnetic field is taken as a sum of the plasma magnetic field and the field produced by the ripple coils. The plasma field is usually taken from the numerical solution of the equilibrium equation as obtained by the Oak Ridge Equilibrium Code.⁷ The essential output of the equilibrium code for FLOC is the poloidal flux function $\psi(R,z)$, $F(\psi) = RB_\phi$, and $dF/d\psi$. The components of \vec{B} are

$$B_R = -\frac{1}{R} \frac{\partial \psi}{\partial z}, \quad (3.1)$$

$$B_z = \frac{1}{R} \frac{\partial \psi}{\partial R}, \quad (3.2)$$

and

$$B_\phi = \frac{F(\psi)}{R}. \quad (3.3)$$

Bicubic spline interpolation is used for the calculation of $\psi(R,z)$ and the required derivatives of ψ at arbitrary points. The function $B_\phi(R,z)$ and its derivatives are obtained by linear interpolation on F and $dF/d\psi$. Simple transformations of \vec{B} and its derivatives are made from the (R,ϕ,z) coordinates to the (r,θ,ϕ) coordinates.

As an alternative to obtaining the magnetic field numerically as described above, we have also included in FLOC the analytic model given by

$$B_r = \frac{-\delta(r/a) n e^{-\alpha\theta^2}}{R(n+2)} B_0 N r \sin N\phi, \quad (3.4)$$

$$B_{\theta} = \frac{rB_0}{R} \frac{\left\{ 1 - \left[1 - (r/a)^2 \right]^{q_{lim}/q_{axis}} \right\}}{q_{lim}(r/a)^2}, \quad (3.5)$$

and

$$B_{\phi} = B_0 \frac{R_0}{R} \left[1 - \delta \left(\frac{r}{a} \right)^n \left(1 + \frac{r}{R_0} \cos \theta \right) e^{-\alpha \theta^2} \cos N\phi \right]. \quad (3.6)$$

The plasma current representation of this model was originated by R. Goldston⁸ while the ripple part is due to N. A. Uckan, T. Uckan, and J. R. Moore.⁹ This model includes the effect of edge ripple due to the presence of N toroidal field coils. Thus, FLOC can also be used to study the effects of edge ripple created by a finite number of TF coils. The strength of the TF coil ripple is determined by the parameter δ . The decay rate away from the midplane is given by α ; q_{lim} and q_{axis} are the safety factors at the limiter and on axis, respectively, and n is the radial decay rate from the edge.

We have investigated a number of coil configurations to create a magnetic well for ripple injection, including a single straight-wire scheme, magnetic dipoles, and various combinations of straight wires. Considering the engineering and physical restrictions, we found that the optimal configuration for ISX-B is a set of eyeglass-shaped coils placed below the plasma. These coils are simulated by an arrangement of straight wires. The components of \vec{B} and its derivatives for any current-carrying straight wire are calculated in the (x,y,z) coordinates of Fig. 1 and then transformed to the (r,θ,φ) coordinates.

FLOC also includes a subroutine for the calculation of an electric field. The model used is given by

$$E_r = -\phi_0 \frac{n}{a} \left(\frac{r}{a}\right)^{n-1}, \quad (3.7)$$

$$E_\theta = 0, \quad (3.8)$$

$$E_\phi = E_0 \frac{R_0}{R}, \quad (3.9)$$

and

$$E_0 = \frac{V_0}{2\pi} R_0, \quad (3.10)$$

where

V_0 is the loop voltage around the torus,

ϕ_0 and n specify the strength and shape of the radial field, respectively.

4. PROGRAM DESCRIPTION

FLOC is a modularized code written in single precision FORTRAN IV. An attempt has been made to make it as machine independent as possible. The code was developed to run on the CDC-7600 at the National Magnetic Fusion Energy Computer Center and the PDP-10 at Oak Ridge National Laboratory's User Service Center. Comments in the program indicate changes necessary for these computers. The graphics is written using DISSPLA.¹⁰

4.1 SUBPROGRAMS

The subprograms of FLOC and those called by FLOC, excluding the DISSPLA routines, are listed below with brief summaries of their functions. This list is followed by more specific descriptions of the major subroutines in the code.

FLOC	Main program and driver for FLOC
INPUT	Reads data
ORBIT	Calculation of the guiding center orbits and the associated graphics
FLINES	Integration of the field line equations and plots of the magnetic flux surfaces
INITAL	Initialization of constants in FLOC and initial points for certain plots
LABIT	Plots one frame of data descriptive of run
SHAPES	Plots the cross-sectional shape of the torus, either rectangular or circular, and labels it
EQUAGC	Guiding center equations
EQUAFL	Field line equations
BFIELD	Calculation of the magnetic field and its derivatives
EFIELD	Calculation of the electric field and its derivatives
EYEGLA	Calculation of the coordinates of the straight wires which form the eyeglass coils
BWIRE	Computes the magnetic field vector and its derivatives due to a current-carrying straight wire of finite length
TORUS	Plots the top view of the torus, eyeglass coils, and orbit if calculated
BGRADA	Calculation of $\vec{B} \cdot \nabla \vec{A}$
PLOTIT	Plots functions of one variable
EXTINT	Used to integrate the guiding center equations by the Bulirsch-Stoer extrapolation technique
DE	Used to integrate the field line equations by a variable step, variable order formulation of the Adams methods

DERIVS	Computes derivatives for bicubic spline interpolation
COEFF	Calculation of bicubic spline coefficients
BICUBE	Evaluates the bicubic spline and derivatives through second order
FCON	Plots contours of the flux function
BOXIT	Plots flux surfaces
OUTIT	Line printer output
BLOCK DATA	Data initialization

Most of the above subprograms can be easily modified. For example, the subroutines INPUT and OUTIT would be changed according to the user's interest. Also the subroutine BFIELD would be replaced for different magnetic field models, etc.

Subroutine INPUT simply reads the input data. In the listing given at the end of this paper, the first read is made with logical unit number 30. This read uses NAMELIST /INDATA/ which is described in Table 1. Three titles are read with logical unit number IRT. These titles correspond to the fast ion orbit plots in the R-z plane and the x-y plane, and to the flux surfaces plots for four values of the angle ϕ . The final read is of data obtained from the Oak Ridge Equilibrium Code. This input is made with logical unit number IRE. This set of data includes the flux function $\psi(R,z)$, the (R,z) grid, and the parameters which describe the plasma equilibrium. Table 2 describes this data in more detail. Samples of all the input data are given with the program listing at the end of this paper.

Table 1. Namelist input

<u>FORTRAN Name</u>	<u>Meaning</u>	<u>Units</u>
RO	Major radius	m
AMINOR	Minor radius	m
ISHAPE	ISHAPE = 0 specifies a rectangular cross section, otherwise a circular cross section is used	
XWIDTH	Width of the toroidal cross section when rectangular shape is specified	m
ZWIDTH	Height of the toroidal cross section when rectangular shape is specified	m
EO	Energy of injected fast ion	keV
RS	Initial r coordinate of fast ion	m
THETA	Initial θ coordinate of fast ion	degrees
PHI	Initial ϕ coordinate of fast ion	degrees
ZETA	Initial value of $\xi = v_{ } / v$	
MASS	Mass of fast ions	m/m_p
ZN	Charge number of fast ions	
RSFL	Initial r coordinate for field line calculation	m
THETFL	Initial θ coordinate for field line calculation	degrees
PHIFL	Initial value of ϕ for starting field line tracing	degrees
IRUP	Number of flux surfaces to be generated $IRUP \leq 5$	
DELR	Distance between the initial r values for the flux surfaces	m

Table 1. (continued)

<u>FORTRAN Name</u>	<u>Meaning</u>	<u>Units</u>
NTURNS	Number of toroidal turns a given field line is followed NTURNS \leq 150	
NPARTS	Number of cross sections for flux surface plots NPARTS \leq 4	
IEYES	Number of eyeglass coils IEYES \leq 3	
R1WCOR	The major radius for the beginning point of the first wire in the eyeglass coil	m
R2WCOR	The major radius for the end point of the first wire in the eyeglass coil	m
ZW	Position above or below midplane for eyeglass coils	m
CUR	Ripple coil current	A
TIMEUP	Total time the guiding center equations are integrated	sec
BO	Magnetic field parameter B_0 (field strength)	T
DELTA	Magnetic field parameter δ (ripple at edge)	
ALPHA	Magnetic field parameter α (poloidal decay rate away from midplane)	
QLIM	Magnetic field parameter q_{lim} (safety factor at limiter)	
QAXIS	Magnetic field parameter q_{axis} (safety factor on axis)	
NS	Magnetic field parameter n (radial decay rate from edge)	
NCOILS	Number of toroidal field coils	

Table 1. (continued)

<u>FORTTRAN Name</u>	<u>Meaning</u>	<u>Units</u>
IEF	IEF = 0 specifies no electric field	
ACCURC	Accuracy of solutions, used by subroutines DE and EXTINT	
DT	Initial time step used by EXTINT	sec
IMAX	Maximum number of extrapolations made in EXTINT before the step size is halved	
IBF	If IBF \neq 0 an analytic field model is employed, otherwise plasma equilibrium data is used for the magnetic field calculations	
IPLOPT	If IPLOPT = 0 only the orbit plot is obtained, otherwise a number of plots are generated for analysis	
ICONPL	ICONPL = 0 eliminates contour plots of the flux function	
IRT	Logical unit number for reading titles	
IRE	Logical unit number for reading equilibrium data	
IOU	Logical unit number for printer output	

Table 2. Equilibrium data

<u>FORTTRAN Name</u>	<u>Meaning</u>	<u>Units</u>
BETAEQ	Ratio of the plasma pressure to the magnetic field pressure, used only for labeling	
QA	Safety factor on axis, used only for labeling	
PCUR	Plasma current, used only for labeling	A
PBO	Magnetic field strength on axis, used only for labeling	T
PSI(40,80)	The flux function $\psi(R,Z)$	T-m ²
F(41)	A table of $F(\psi) = RB_{\phi}$	T-m
FP(41)	$dF/d\psi$	m ⁻¹
PSIF(41)	The flux function at which $F(\psi)$ and $dF/d\psi$ are given.	T-m ²
R(40)	The grid of R values	m
ZZ(80)	The grid of z values	m
JMAX	Number of R values	
KMAX	Number of z values	
NPTS	Number of values in the $F(\psi)$ and $dF/d\psi$ tables	

Subroutine INITIAL initializes certain variables and prepares information for labeling a particular run. INITIAL also calls EYEGLA, which constructs the eyeglass coils for the ripple field. The positions of these coils are determined by the specification of the coordinates of the "first" wire. This is done by specifying its radial end points, R_{1w} and R_{2w} , and the wire's distance, z_w , above or below the midplane of the torus. The eyeglass coils are placed parallel to the midplane. The azimuthal coordinate of the first wire is taken to be $\phi = 0$. The other radial wires are the same length and are separated azimuthally by the angular distance between the TF coils. The number of TF coils is specified by NCOILS, which is in NAMELIST /INDATA/. The radial wires are connected appropriately to construct the eyeglasses. The magnetic field created by each of these wires and the derivatives of these fields are computed by BWIRE. Details concerning this subroutine are given in Appendix A.

It is sometimes desirable to use more than one set of ripple coils in order to reduce any ergodic behavior of the flux surfaces. If more than one set of eyeglass coils (see IEYES in Table 1) is specified, the coils are placed symmetrically around the torus.

Subroutine SHAPES plots the R-z cross section of the torus. The guiding center orbits obtained by ORBIT are plotted in this cross section. Contour plots of the flux function via the subroutine FCON are optional (see ICONPL in Table 1) when ORBIT is invoked. Subroutine ORBIT calls EXTINT, which integrates the orbit equations by the Bulirsch-Stoer extrapolation technique.⁵ The initial conditions for the guiding center equations are r_0 , θ_0 , ϕ_0 and $\xi_0 = v_{||} / v_0$ (see Table 1). Subroutine FLINES

calls the Shampine-Gordon code,⁶ DE, to integrate the field line equations. The initial conditions of the field line equations are r_{FL} and θ_{FL} , and the plane in which the integration starts is ϕ_{FL} . Subroutine BOXIT plots the flux surfaces generated by FLINES. Both ORBIT and FLINES call the subroutine TORUS to plot a top view of the torus. ORBIT also generates data for the subroutine PLOTIT, which produces graphs of variables along the fast ion orbit.

BFIELD and EFIELD calculate \vec{B} , \vec{E} , and the nine first derivatives of their components. These derivatives are stored in the two-dimensional arrays DB(I,J) and DE(I,J), where e.g., $DB_{ij} = \partial B_i / \partial R_j$. In this case $\vec{R} = (r, \theta, \phi)$. BFIELD uses the subroutines DERIVS, COEFF, and BICUBE to obtain an approximation of the function $\psi(R,z)$ and its first and second derivatives. These routines implement De Boor's method¹¹ of bicubic spline interpolation for approximating a function given its values on a rectangular grid. These routines are completely revised versions of a code published by Smith and Gaffney.¹²

Subroutine OUTIT prints out certain plasma and injection parameters. Also printed as a function of r is the total field $\vec{B} = (B_r, B_\theta, B_\phi)$, the ripple field $\vec{B}_{RC} = (B_{r_w}, B_{\theta_w}, B_{\phi_w})$, and the ripple $\delta B = B_{RC}/B$.

The information required by the FLOC subroutines called by the driver is in labeled common blocks. The calling sequence to the FLOC subroutines by the driver is as follows.

```
CALL INPUT
CALL INITAL
CALL LABIT
CALL ORBIT or CALL FLINES
CALL OUTIT
```

4.2 GRAPHICS

FLOC produces a number of graphs for analysis. Most of these graphs are self-explanatory. However, some explanations are in order. All graphics is done using DISSPLA.¹⁰ Certain graphs involve the pitch angle, which is defined as $\cos^{-1}(v_{\parallel}/v)$. Other graphs involve the angle between \hat{i}_{ϕ} and \vec{B} , which is defined as $\cos^{-1}(B_{\phi}/B)$. Finally, the angle between \hat{i}_R and \vec{B} is given by $\cos^{-1}[(\cos \theta B_r - \sin \theta B_{\theta})/B]$.

5. RESULTS

5.1 CALCULATIONS FOR ISX-B

Using computed ISX-B equilibria, we found that a sufficient magnetic well exists for a ripple current of 175 kA with $B_T = 1.2$ T. The guiding center orbits calculated using this ripple field show that fast ions reach the magnetic axis region at an injection energy of 20 keV. The ripple causes the flux surfaces near the outside of the plasma to become ergodic. This behavior can be improved by using three sets of ripple coils, but space requirements made this experimentally impractical.

The results obtained with the above parameters and for a particular equilibrium are given by Figs. 2-6. The ripple at the point of injection is 7.9% and near the plasma center is 1.8% for this case. Similar results are obtained with other reasonable equilibria.

5.2 STUDY OF RIPPLE EFFECTS OF TF COILS

Figure 7 is the guiding center orbit of a fast ion in the magnetic field given by Eqs. (3.4)-(3.6). The orbit illustrates how a particle

PLASMA CHAMBER

$E_0 = 20.0$ keV
 $I_{RC} = 175.00$ kA
 $I_P = 227.74$ kA
 $R_0 = 0.93$ m
 $a = 0.27$ m
 $B_0 = 1.2$ T
 $M = 2.0$
 $\beta = 0.006$
Chamber size
Width = 0.54 m
Height = 1.00 m

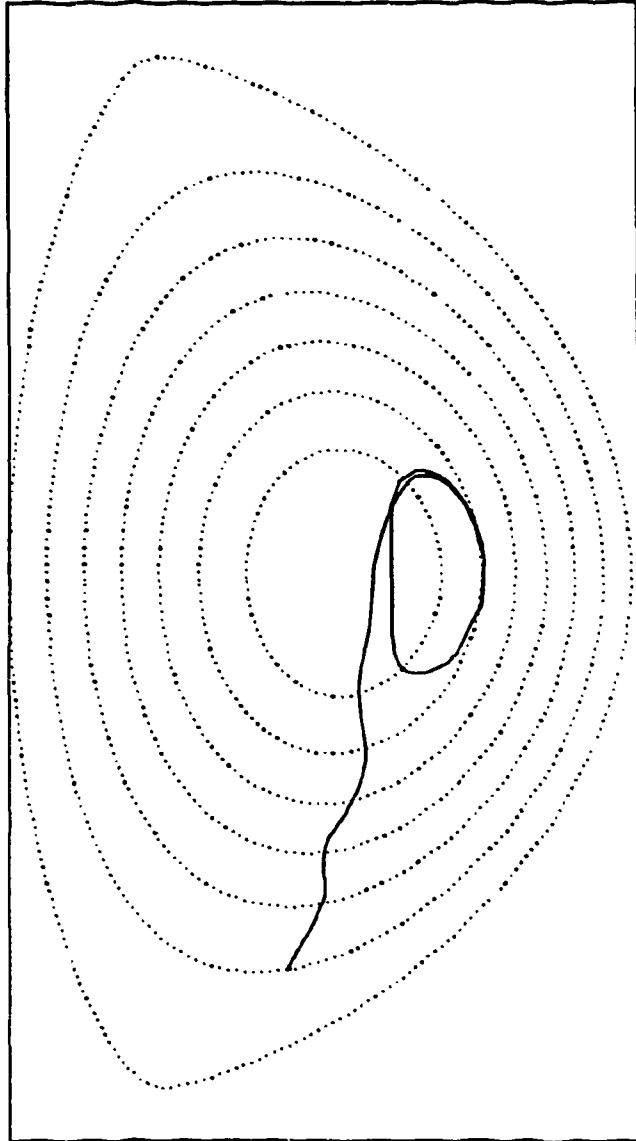


Fig. 2. Fast ion orbit and flux function contours in ISX-B.

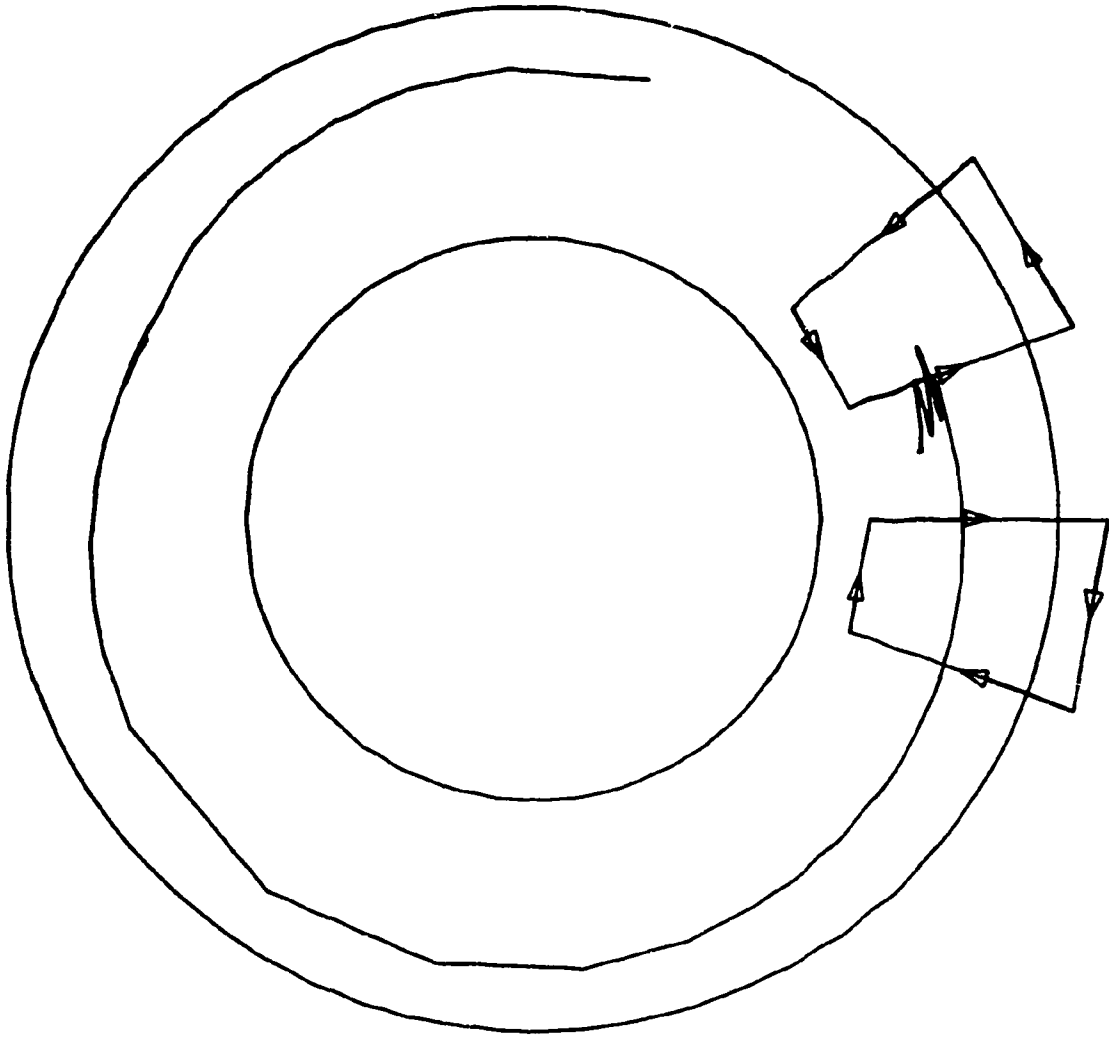


Fig. 3. Top view of fast ion orbit and ripple coils in ISX-B.

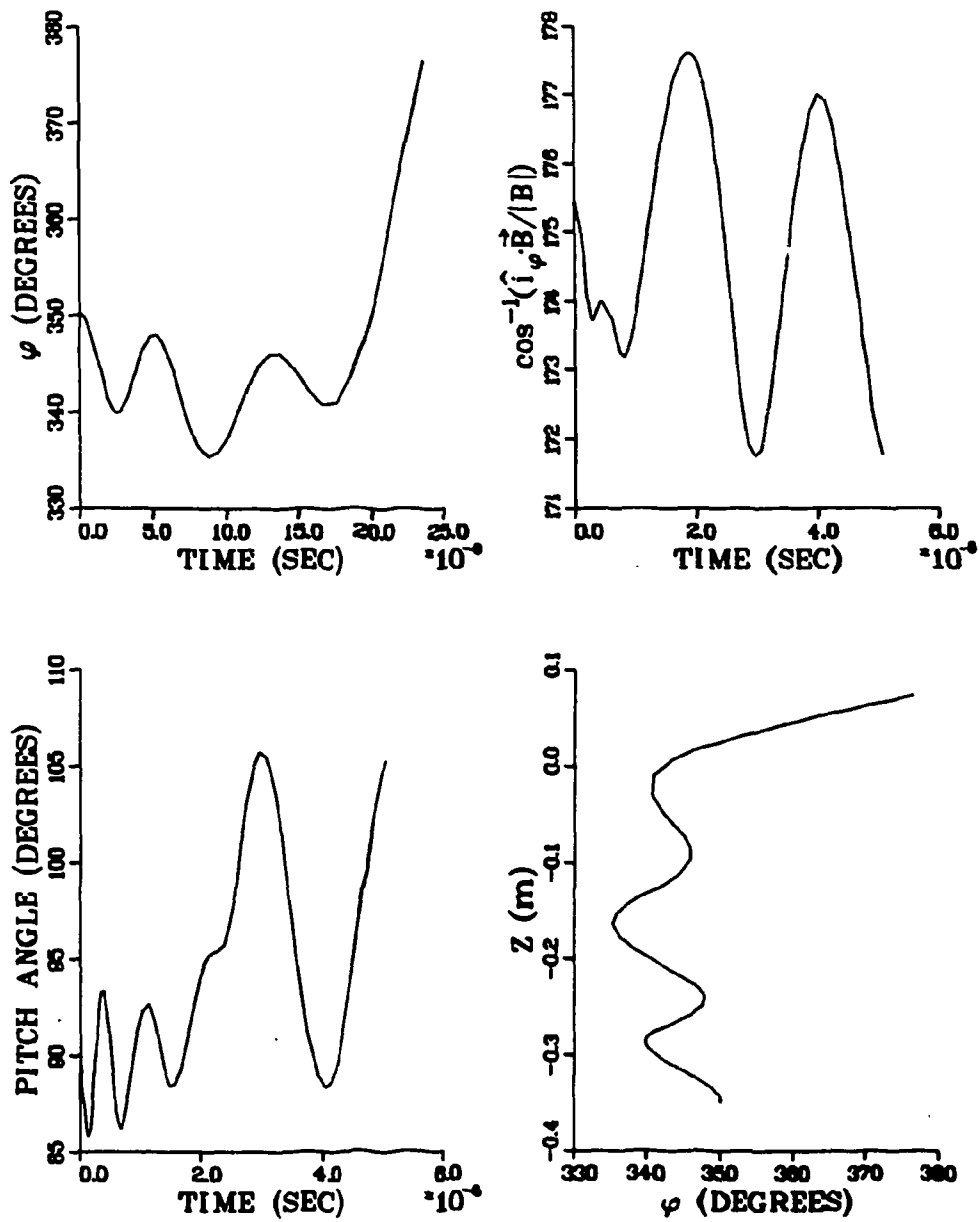


Fig. 4. The pitch angle z , ϕ , and $\cos^{-1}(\hat{i}_\phi \cdot \vec{B}/|B|)$ along the fast ion orbit.

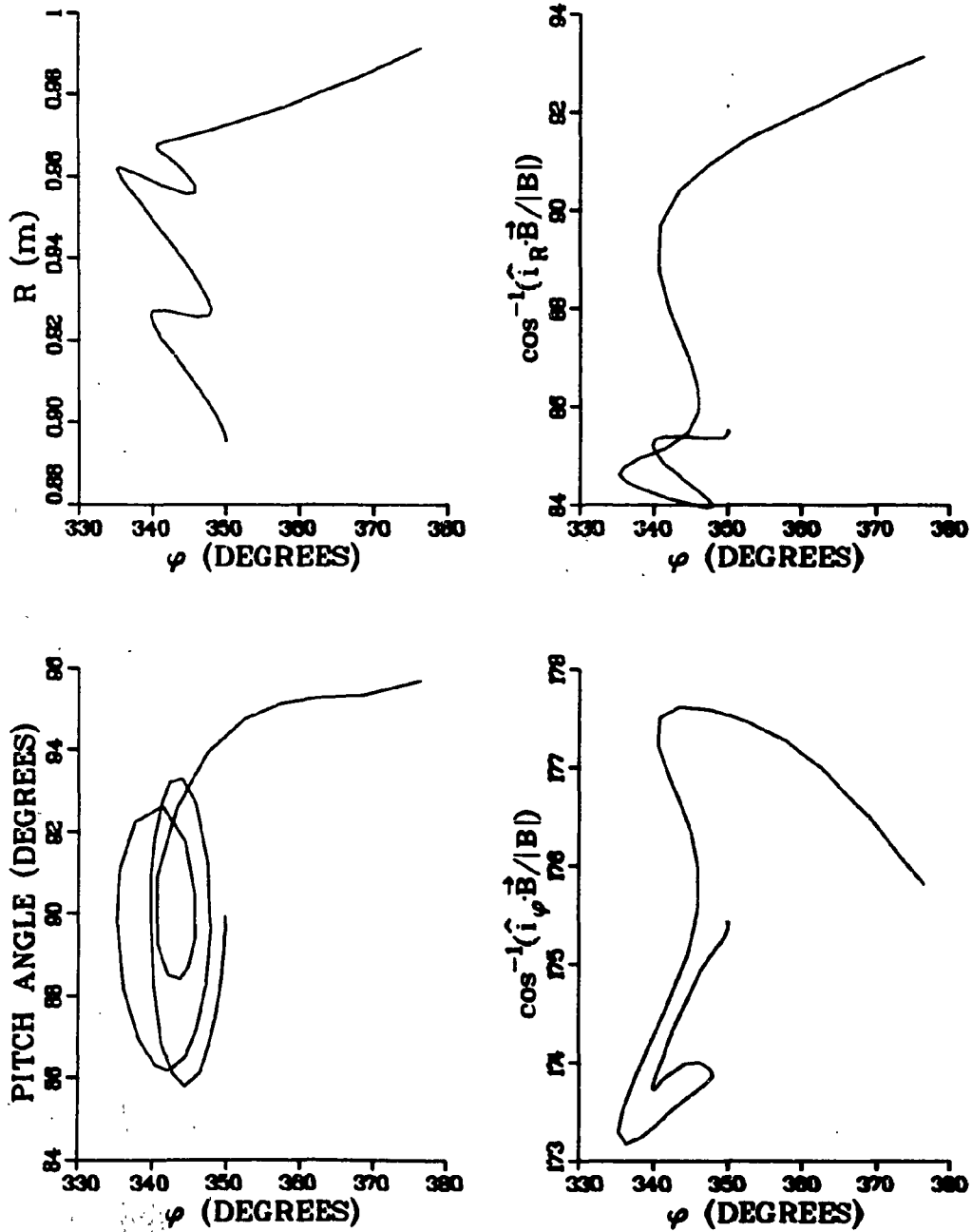


Fig. 5. The pitch angle, $\cos^{-1}(\hat{i}_\varphi \cdot \vec{B}/|\vec{B}|)$, R , and $\cos^{-1}(\hat{i}_R \cdot \vec{B}/|B|)$ along the fast ion orbit.

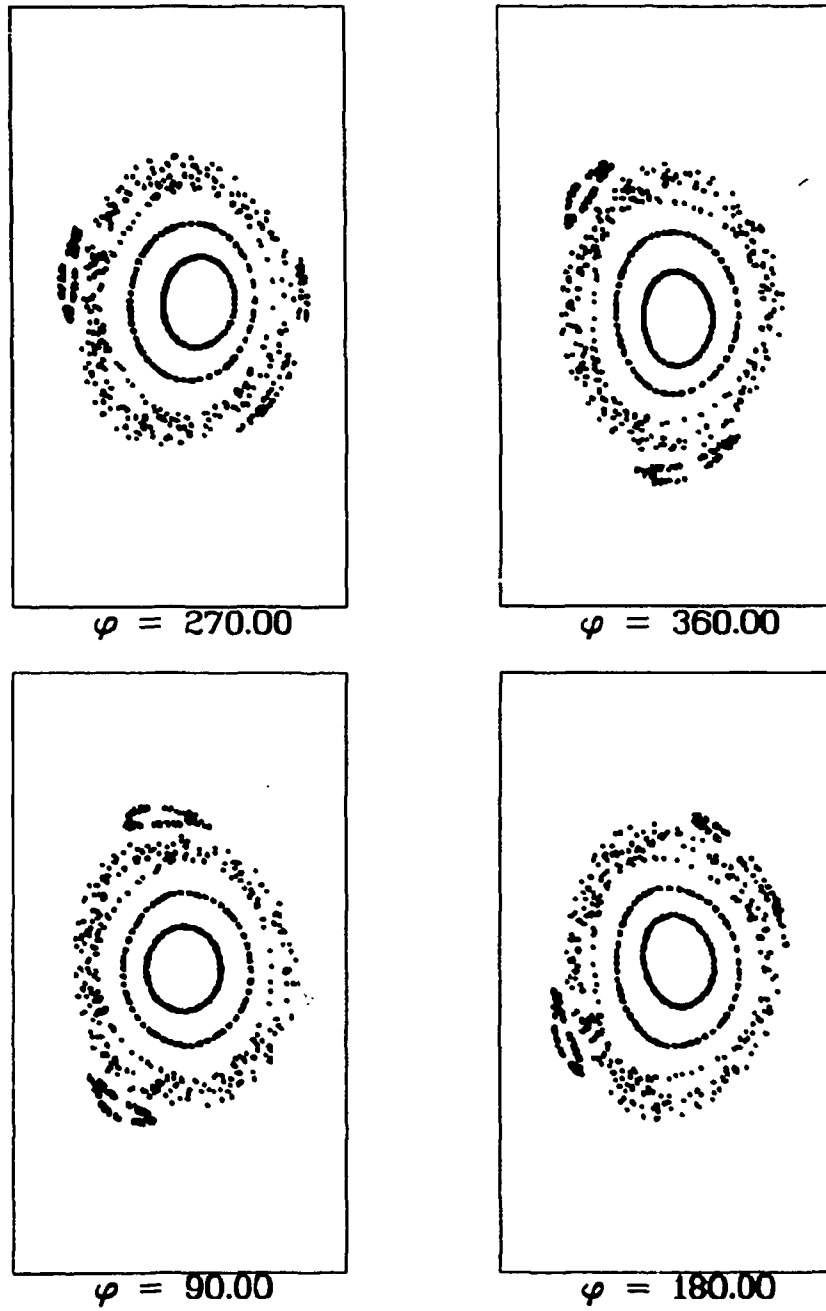


Fig. 6. ISX-B flux surfaces.

$E_0 = 45.0 \text{ keV}$
 $I_{RC} = 0.00 \text{ kA}$
 $R_0 = 3.00 \text{ m}$
 $a = 1.00 \text{ m}$
 $B_0 = 4.5 \text{ T}$
 $M = 1.0$

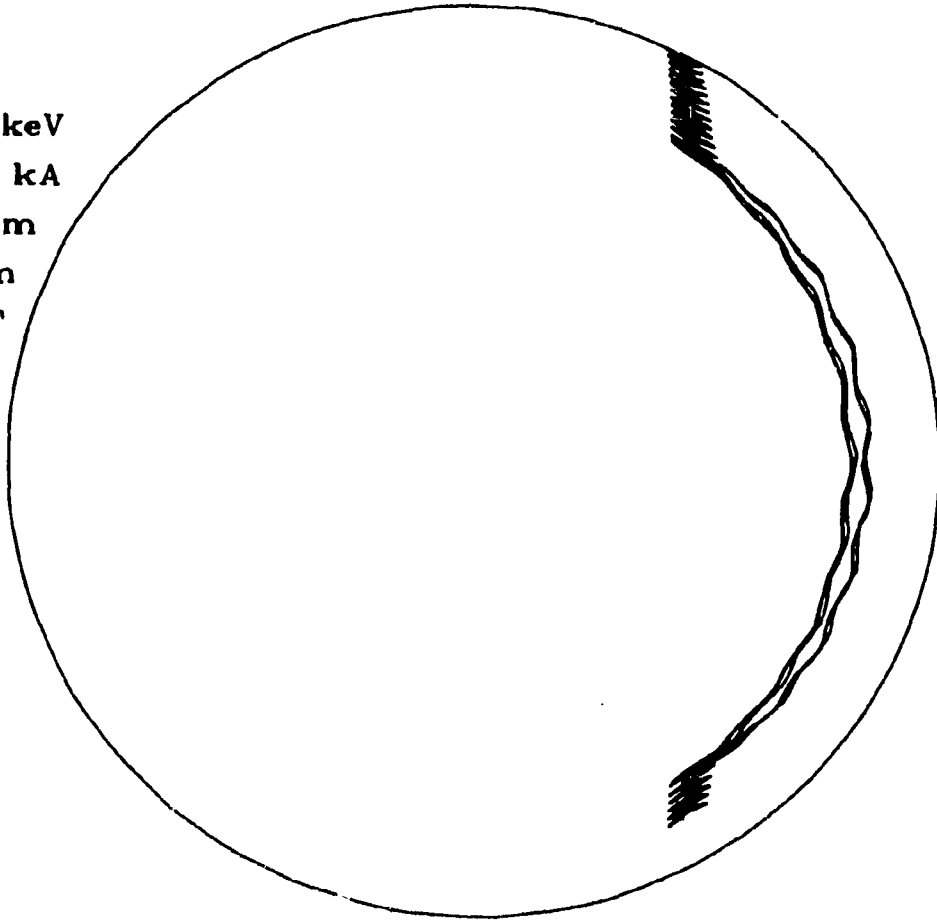


Fig. 7. Fast ion orbit in ripple field of TF coils.

can become ripple trapped due to finite spacing of the TF coils. The fast ion becomes trapped at the bottom of the torus and eventually exits at the top of the torus.

6. LIMITATIONS OF THIS MODEL

The user of FLOC must bear in mind that the magnetic field model used to describe the ripple is inconsistent because the nonrippled equilibrium flux surfaces are used to describe the field due to the plasma current. In fact, the destruction of axisymmetry due to the ripples will change the plasma equilibrium and may even invalidate the use of the Grad-Shafranov equation to describe the situation. However, so far no one has solved the self-consistent problem.

APPENDIX A
BASIC FORMULATION FOR SUBROUTINE BWIRE

We consider a problem of evaluating vectors \vec{B} , ∇B , $\nabla \times \vec{B}$, and ∇B_i , where B_i is the *i*th component of the magnetic field vector \vec{B} due to a current-carrying straight wire of finite length. The current i flows from point a to point b (see Fig. A.1), and the field point c is represented in two coordinate systems: $\vec{X} = (x_1, x_2, x_3) = (x, y, z)$ and $\vec{R} = (R_1, R_2, R_3) = (r, \theta, \phi)$. The subscripts (i, j, k) and (λ, μ, ν) are used for components in these two coordinate systems, respectively, and sometimes they represent cyclic permutations of $(1, 2, 3)$. We also use $\mu_0 i / 4\pi \equiv 1$ and $x_i^{(ab)} = (\vec{r}_{ab})_i = (\vec{r}_a - \vec{r}_b)_i$, etc.

The transition matrix for the two coordinate systems is

$$a_{\lambda i} = \frac{1}{h_\lambda} \frac{\partial x_i}{\partial R_\lambda} = \begin{pmatrix} \cos \theta & \cos \phi & -\cos \theta \sin \phi & \sin \theta \\ -\sin \theta & \cos \phi & \sin \theta \sin \phi & \cos \theta \\ -\sin \phi & & -\cos \phi & 0 \end{pmatrix}, \quad (\text{A.1})$$

where

$x_i(r, \theta, \phi)$ is given by Eqs. (2.1)-(2.4) and $(h_1, h_2, h_3) = (1, r, R)$.

The magnitude and *i*th component of the magnetic field are given, respectively, by

$$B = (r_{ac} \tan \theta_a)^{-1} + (r_{bc} \tan \theta_b)^{-1}, \quad (\text{A.2})$$

$$B_i = B G_i / (r_{ac} r_{bc} \sin \theta_c), \quad (\text{A.3})$$

where

$$G_i = (\vec{r}_{ac} \times \vec{r}_{bc})_i, \quad (\text{A.4})$$

$$\cos \theta_\alpha = \frac{1}{2} (r_{\alpha\beta}^2 + r_{\alpha\gamma}^2 - r_{\beta\gamma}^2) / r_{\alpha\beta} r_{\alpha\gamma}, \quad (\text{A.5})$$

(α, β, γ) being cyclic permutations of (a, b, c) .

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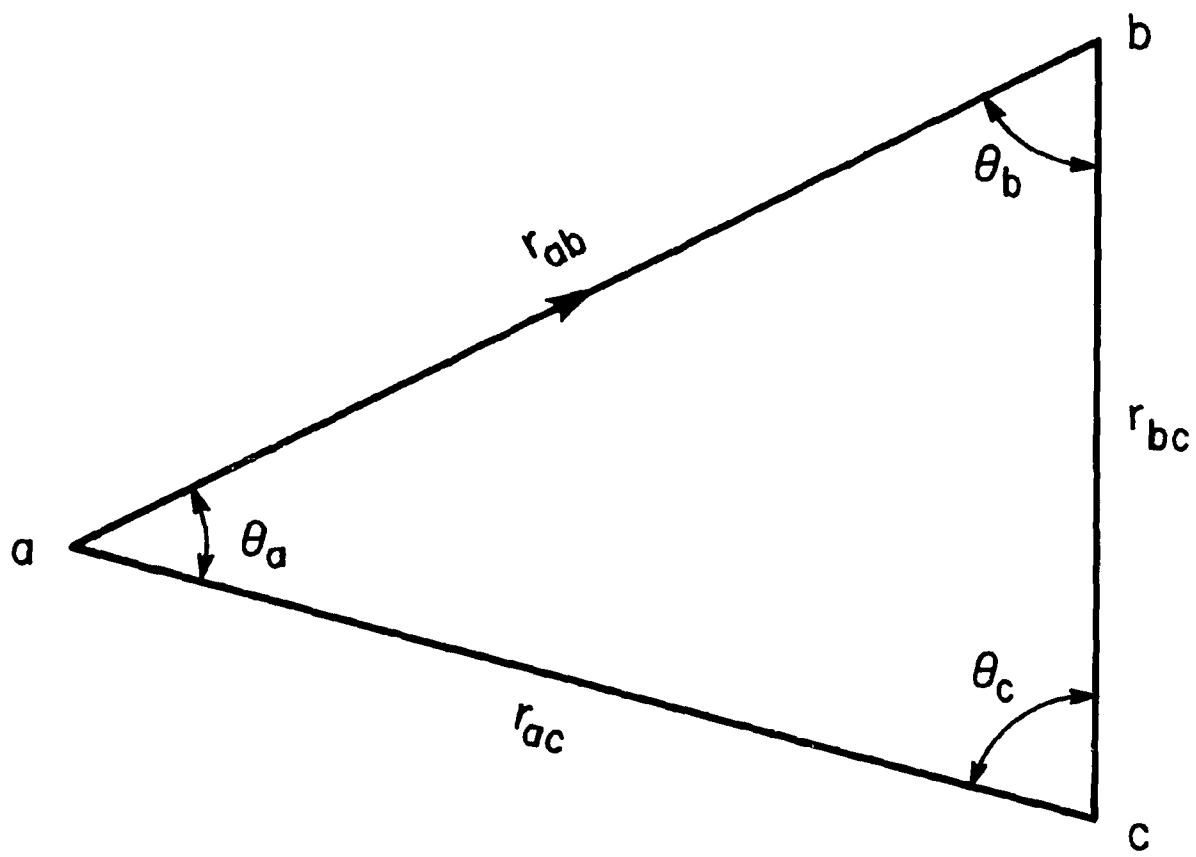


Fig. A.1. Geometry for the formulation of the subroutine BWIRE.

The following results are obtained from Eqs. (A.1)-(A.5).

$$\frac{\partial \theta_a}{\partial x_i} = \frac{x_i^{(ab)}}{r_{ab} r_{ac} \sin \theta_a} - \frac{\cot \theta_a x_i^{(ac)}}{r_{ac}^2}, \quad (\text{A.6a})$$

$$\frac{\partial \theta_b}{\partial x_i} = \frac{-x_i^{(ab)}}{r_{ab} r_{bc} \sin \theta_b} - \frac{\cot \theta_b x_i^{(bc)}}{r_{bc}^2}, \quad (\text{A.6b})$$

$$\frac{\partial \theta_c}{\partial x_i} = \frac{1}{r_{ac} r_{bc} \sin \theta_c} \left\{ x_i^{(bc)} + x_i^{(ac)} - \left[\frac{r_{ac}}{r_{bc}} x_i^{(bc)} + \frac{r_{bc}}{r_{ac}} x_i^{(ac)} \right] \cos \theta_c \right\}, \quad (\text{A.6c})$$

$$\partial G_i / \partial x_i = 0, \quad (\text{A.7a})$$

$$\partial G_i / \partial x_j = x_k^{(ab)}, \quad (\text{A.7b})$$

$$\partial G_i / \partial x_k = -x_j^{(ab)}, \quad (\text{A.7c})$$

$$\frac{\partial a_{\lambda i}}{\partial R_1} = 0, \quad (\text{A.8a})$$

$$\frac{\partial a_{\lambda i}}{\partial R_2} = \begin{pmatrix} a_{21} & a_{22} & a_{23} \\ -a_{11} & -a_{12} & -a_{13} \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{A.8b})$$

$$\frac{\partial a_{\lambda i}}{\partial R_3} = \begin{pmatrix} a_{12} & -a_{11} & 0 \\ a_{22} & -a_{21} & 0 \\ a_{32} & -a_{31} & 0 \end{pmatrix}, \quad (\text{A.8c})$$

$$\frac{\partial B}{\partial x_i} = \frac{x_i^{(ac)}}{r_{ac}^3 \tan \theta_a} - \frac{1}{r_{ac} \sin^2 \theta_a} \frac{\partial \theta_a}{\partial x_i} + \frac{x_i^{(bc)}}{r_{bc}^3 \tan \theta_b} - \frac{1}{r_{bc} \sin^2 \theta_b} \frac{\partial \theta_b}{\partial x_i}, \quad (\text{A.9})$$

$$\begin{aligned} \frac{\partial B_i}{\partial x_j} &= \frac{B_i}{B} \frac{\partial B}{\partial x_j} + \left[\frac{x_j^{(ac)}}{r_{ac}^2} + \frac{x_j^{(bc)}}{r_{bc}^2} \right] B_i - \cot \theta_c B_i \frac{\partial \theta_c}{\partial x_j} \\ &+ \frac{B}{r_{ac} r_{bc} \sin \theta_c} \frac{\partial G_i}{\partial x_j}, \end{aligned} \quad (\text{A.10})$$

$$B_\lambda = \sum_i a_{\lambda i} B_i, \quad (\text{A.11})$$

$$\frac{1}{h_\lambda} \frac{\partial B}{\partial R_\lambda} = \sum_i a_{\lambda i} \frac{\partial B}{\partial x_i}, \quad (\text{A.12})$$

$$\frac{\partial B_\lambda}{\partial R_\mu} = \sum_i \frac{\partial a_{\lambda i}}{\partial R_\mu} B_i + h_\mu \sum_{i,j} a_{\lambda i} a_{\mu j} \frac{\partial B_i}{\partial x_j}. \quad (\text{A.13})$$

The subroutine BWIRE computes Eqs. (A.11) and (A.13).

APPENDIX B
PROGRAM LISTING

(SEE INSIDE OF BACK COVER)

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