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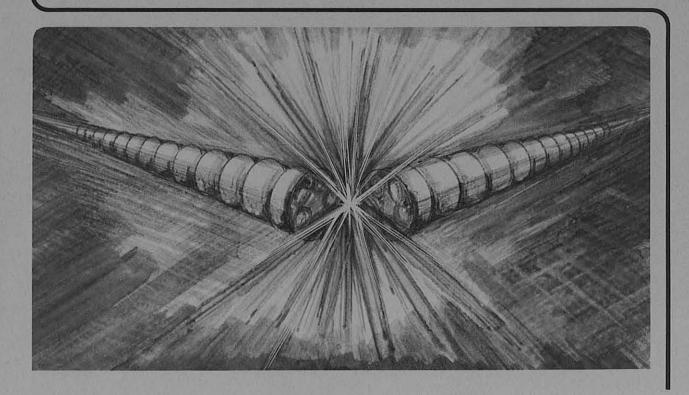
# Accelerator & Fusion Research Division

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## The Use of Toroidal Boundary Conditions in the Program POISSON

S. Caspi, M. Helm, and L.J. Laslett

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#### THE USE OF TOROIDAL BOUNDARY CONDITIONS IN THE PROGRAM POISSON\*

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#### Abstract

In circular particle accelerators of moderate size, one cannot entirely neglect the <u>curvature</u> of the structure and of the guide field. In practice, one may wish to restrict the region of analysis to that near the working aperture, while excluding a very substantial area closer to (and including) the axis of rotational symmetry. In this way, a more efficient mesh can be generated for a program such as POISSON. In restricting the solution to the region of interest, there must be concern regarding a suitable termination of the problem at the boundary of the mesh. For these reasons, we have employed <u>toroidal coödinates</u> in constructing the boundary to a relaxation mesh, and in formulating the boundary conditions that then would be imposed at such boundaries.

#### Introduction

This paper is an extension of a series of papers and reports on the use of boundary conditions associated with application of relaxation methods in the solution of partical differential equations. The current paper is a summary of one such report on the use of such boundary conditions in problems with axial symmetry.

Magnetostatic problems with circular symmetry are soluble by relaxation programs such as POISSON in  $\rho$ , Z cylindrical coördinates. As is the case with other applications of relaxation methods, however, there must be concern regarding a suitable termination of the problem at the boundary of the mesh. (The condition that normally is required is one consistent with the absence of any "sources" in the region exterior to such a boundary.) In analyzing the magnetic fields of circular particle accelerators, one may wish to restrict the region of examination to that near the working aperture and surrounding magnet structure, while excluding a very substantial area closer to (and including) the axis of rotational symmetry for the entire structure.

For the reason just indicated, one accordingly is led to consider the use of toroidal coördinates in constructing the boundary to a relaxation mesh for use in analyzing the magnetic fields of circular devices (such as accelerators and spectrometers), and in formulating the boundary conditions that then may be usefully imposed at such boundaries. The procedure adopted makes use internally of the characteristic form of the vector-potential function, in a source-free region, when expressed in toroidal coördinates. The relevant properties of associated Legendre functions of half-integral degree are used in this connection and their introduction into the program POISSON is outlined. Results of some test cases are included, to illustrate the application of this technique for configurations with median-plane symmetry. We pursue such issues in the following Sections, commencing with a review of the characteristics of toroidal coördinates and continuing with an examination of related magnetostatic issues that will permit formulation of a boundary condition analogous in spirit to those devised previously at this Laboratory for application to other configurations.1-9

#### The Differential Equation for the Potential

Through use of the appropriate metric coefficients, one can write explicitly in toroidal coördinates Laplace's differential equation for a scalar potential function. As has been shown in some detail by MacRobert, 12 solutions then may be found in which this potential function has the form of a factor (Cosh  $\eta$  - cos  $\xi$ ) 1/2 times the product of separate functions of the coördinates  $\eta$ ,  $\xi$ , and  $\varphi$  (Fig. 1). For such solutions, the functions of  $\xi$  and of  $\varphi$  are each just circular functions of their respective arguments, and the functions of  $\eta$  are Legendre functions (or associated Legendre functions) of half-integral degree and argument z = Cosh  $\eta$ .

In the present work, however, we are specifically interested in POISSON computations of <u>magnetic</u> field for cases with <u>axial</u> <u>symmetry</u>, and wish to make use of a <u>vector-potential</u> <u>component</u>  $A_{\varphi}$  (or  $A^* = \rho A_{\varphi}$ ) to characterize this field. The homogeneous equation  $\nabla \times [\nabla \times A] = 0$  for  $A = A_{\varphi} 2_{\varphi}$  then may be written

$$\frac{\partial}{\partial \eta} \begin{bmatrix} \frac{\cosh \eta - \cos \xi}{\sinh \eta} & \frac{\partial}{\partial \eta} \left( \frac{\sinh \eta}{\cosh \eta - \cos \xi} A_{\varphi} \right) \end{bmatrix} + \frac{\partial}{\partial \xi} \begin{bmatrix} \frac{\cosh \eta - \cos \xi}{\sinh \eta} & \frac{\partial}{\partial \xi} \left( \frac{\sinh \eta}{\cosh \eta - \cos \xi} A_{\varphi} \right) \end{bmatrix} = 0$$

- - wherein the dependent variable  $A_{\varphi}$  is to be regarded as a function of  $\eta$  and  $\xi$  , but independent of  $\varphi$  .

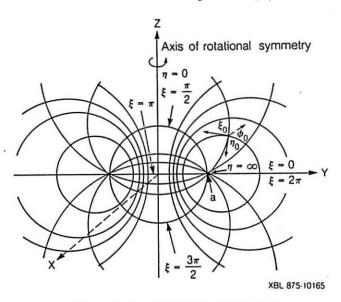


Figure 1. Toroidal Coördinates (ξ, η, φ)

Guided by the form known to be appropriate for the scalar-potential solutions to Laplace's equation in toroidal coördinates, we may proceed heuristically to achieve a separation of variables in the present case, once  $A_{\Phi}$  is divided by the factor (Cosh  $\eta$  - cos  $\xi$ ). We accordingly write the vector-potential component  $A_{\Phi}$  in the form

$$A_{\Phi} = (\cosh \eta - \cos \xi)^{1/2} \cos \eta G(\eta).*$$

<sup>\*</sup>This work was supported by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, High Energy Physics Division, U.S. Dept. of Energy, under Contract No. DE-AC03-76SF00098.

With this substitution, the differential equation assumes the

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\left(z^{2}-1\right)\frac{\mathrm{d}G}{\mathrm{d}z}\right]-\left[\frac{1}{z^{2}-1}+\nu(\nu+1)\right]G=0,$$

(following some intermediate algebraic work), the  $\xi$  dependence then is found to disappear (as hoped), and there remains only the ordinary differential equation for the factor G(z) itself with z=Cosh  $\eta$  serving as the independent variable (and v=n-1/2). Solutions to the differential equation for G can be written as directly proportional to associated (m=1) Legendre functions of degree v=n-1/2 and argument z=Cosh  $\eta$ . We shall employ in the work to follow only the functions of the first kind,  $P_{v=n-1/2}^1(z)$  or quantities proportional thereto, in order to avoid singularities developing at remote locations (as the argument z approaches unity from above). With the index n confined to integer values (to insure a single-valued dependence upon the coördinate  $\xi$ ), we thus are confined to terms of the form

For 
$$A_{\Phi}$$
:  $(\cosh \eta - \cos \xi)^{1/2} P_{\nu=n-1/2}^{1}(z) \cos n\xi$  or 
$$\frac{\sinh \eta}{(\cosh \eta - \cos \xi)^{1/2}} P_{\nu=n-1/2}^{1}(z) \cos n\xi$$
 (1)

that contain as factors Legendre functions of half-integral degree (v = -1/2, 1/2, 3/2, ...) and which we choose to be even about the mid-plane  $\xi = 0$ .

#### Application

The proposed boundary condition is illustrated by a boundary so located that no external sources are present. The vector potential function external to that boundary is therefore expressible as a summation of terms of the form of Eq. l. If the boundary is conveniently placed on a curve (surface) on which the toroidal coördinate  $\eta$  has a constant value  $\eta=\eta_{in}$ , the Legendre functions represent a series of harmonic coefficients. If, in practice, values of the potential are known at only a finite number of points on the "inner boundary" then, of course, only a finite number of harmonic coefficients could be evaluated. Such a series may, however, be adapted to provide adequate estimates of the corresponding values of the potential at various points on a nearby surrounding "outer boundary" curve, with  $\eta=\eta_{OUt}$ .

In performing a relaxation computation on a mesh bounded by such a pair of curves (external to all "sources"), any full relaxation pass through the mesh may be followed by a step wherein the values of potential at points on the outer boundary are revised (updated) on the basis of a harmonic description of the potential function on the inner curve. Such revised values would then be employed, as boundary values, in proceeding with the next relaxation pass through the mesh.

In application, we shall use the forms for  $A^* = \rho A$  to guide the means of extending this function from an "inher" boundary curve,  $\eta = \eta_{in}$ , to points on a surrounding "outer" boundary curve. This "outer", or surrounding, boundary curve may conveniently be taken also to be a curve (surface) on which the toroidal coördinate  $\eta$  has a constant value ( $\eta = \eta_{out}$ ).

It appears computationally desirable, however, to regard the function  $A^{*}$  as represented not in the form of a series that contains as explicit factors the Legendre

functions  $P_{v=n^{-1}/2}^{1}(z)$ , but that introduces in their place factors  $ASP_{0}(z)$  that represent such functions renormalized through division by the asymptotic form for  $P_{0}^{1}$ , to provide the working functions for computational use.

To specify in toroidal coördinates a suitable inner boundary, for POISSON computation of a magnetostatic problem with rotational symmetry, we first select a suitable region of interest in  $\rho$ , Z space such that one is assured that there are no "sources" exterior to this region.

We may imagine the values of the provisional vector potential on the boundary curve  $\eta_{in}$  to be developed in the form of a Fourier series for the working variable  $A^* = \rho A_{\Phi}$ 

$$A^{*}(\eta_{in},\xi) = \frac{\sinh \eta_{in}}{\sqrt{\cosh \eta_{in} - \cos \xi}} \sum_{k=1}^{\Sigma} C_k \cos(k-1)\xi$$

(for situations of even symmetry, with respect to  $\xi$ , about z = 0).

Given values of the function  $A^*(\eta_{in}, \xi_i)$  for points  $\xi_i$  on the boundary  $\eta_{in}$ , we wish to make a weighted least-squares fit (with weights  $w_i$ ) so as to minimize

$$\frac{1}{2}\sum_{i}^{L} \left\{ w_{i} \begin{bmatrix} \sum_{k=1}^{L} C_{k} \cos(k-1)\xi_{i} - \frac{A(\eta_{in},\xi_{i})}{\sinh \eta_{in}} \\ \sqrt{\cosh \eta_{in} - \cos \xi_{i}} \end{bmatrix}^{2} \right\}$$

[Regarding suggested forms for the weight factors  $w_i$ , see the section included on p.5 of Ref. 5 pertaining to weights used in connection with <u>circular</u> functions F(v).]

This minimization objective leads to the set of algebraic equations that can be written, in matrix notation,  $\sum_{k} M_{k,k} C_{k} = V_{k}$ , where M is the symmetric matrix with k, k elements

$$M_{k,\ell} = \sum_{i} w_{i} \cos(k-1) \xi_{i} \cos(\ell-1) \xi_{i}$$
and
$$V_{k} = \sum_{i} w_{i} \cos(k-1) \xi_{i} \cdot \frac{A^{*}(\eta_{in}, \xi_{i})}{\frac{\sinh \eta_{in}}{\sqrt{\cosh \eta_{in} - \cos \xi_{i}}}}$$

Accordingly, the solution may be written in terms of the elements of the <u>inverse matrix</u>, as  $C_{\ell} = \sum_{k} (M^{-1})_{\ell,k} V_k$ .

With substitution of the expression for  $C_{\ell}$ , there results the working equation (for use in updating values of A  $^*$  on the outer boundary):

$$\mathsf{A}^{*}(\mathsf{n}_{\mathsf{out}},\,\boldsymbol{\xi}_{\mathsf{j}}) = \sum\limits_{\mathsf{i}} \mathsf{E}_{\mathsf{j},\mathsf{i}}\,\mathsf{A}^{*}(\mathsf{n}_{\mathsf{in}},\,\boldsymbol{\xi}_{\mathsf{i}})\,,$$

where the "working matrix" (a rectangular matrix) is composed of the elements

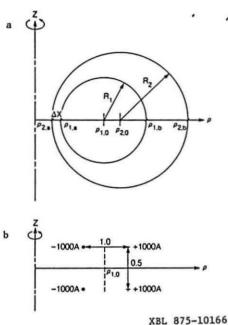
$$\begin{split} E_{j,i} &= \frac{\sinh \eta_{out}}{\sqrt{\cosh \eta_{out} - \cos \xi_{j}}} \bullet \frac{\sqrt{\cosh \eta_{in} - \cos \xi_{i}}}{\sinh \eta_{in}} \\ &\bullet w_{i} \left\{ \sum_{\mathfrak{L}=1}^{\Delta SP_{\mathfrak{L}}(\eta_{out})} \frac{ASP_{\mathfrak{L}}(\eta_{out})}{ASP_{\mathfrak{L}}(\eta_{in})} \cdot \left( \frac{Cosh \eta_{out}}{Cosh \eta_{in}} \right)^{\alpha \mathfrak{L}} \\ &\bullet \cos(\mathfrak{L}-1)\xi_{j} \left[ \sum_{k=1}^{\Sigma} (M^{-1})_{\mathfrak{L},k} \cos(k-1)\xi_{i} \right] \right\} , \end{split}$$

Only the use of a factor cos n $\xi$  (in preference to a factor sin n $\xi$ ) is indicated here, since we shall ultimately wish to specialize to cases with median-plane symmetry such that the function  $A_{\Phi}$  is even with respect to the variable  $\xi$ .

and where 
$$\alpha_{\ell} = \begin{cases} O \text{ for } \ell = 1 \\ \ell - 3/2 \text{ for } \ell \ge 2 \end{cases}$$
.

#### Introducing The Boundaries Into POISSON'S Mesh Generator

The use of the toroidal coordinate system in solving problems with axial symmetry requires an eccentric pair of circular arcs at the boundary of such a problem (i.e., no external sources are permitted). The specification for the center and radius of one of the arcs is a matter of choice: these values are then used to compute the center and radius of the other arc, using the procedure described below (Fig. 2a).



(a) The inner and outer boundary used with the toroidal coördinate system. (b) Location of the 4 current loops used in the example.

We have chosen to assign values for  $\rho_{1,0}$  and R<sub>1</sub> (center and radius) of the inner boundary and compute the corresponding values,  $\rho_{2,0}$  and R<sub>2</sub> of the outer boundary. (The values of  $\rho_{1,0}$  and R<sub>1</sub> are arbitrary as long as there are no sources outside R,.)

Once  $R_1$  and  $\rho_{1,0}$  are known, we calculate the focal length a;  $a^2 = \rho_{1,0}^2 - R_1^2$ .

The minor intersection point between a circular boundary and the abscissa is a • Tanh( $\frac{\pi}{2}$ ). The distance  $\Delta x$ (Fig. 2a) between two such boundaries on the abscissa is:

$$\Delta x = \rho_{1,o} - R_1 - a \cdot Tanh(\frac{n_{out}}{2}).$$

Assuming that 
$$\Delta x$$
 is assigned, we calculate  $\eta_{out}$ :
$$\eta_{out} = 2 \text{ Tanh}^{-1} \left[ \frac{\rho_{1,o} - (R_1 + \Delta x)}{a} \right]$$

$$= 2n \left[ \frac{a + \rho_{1,o} - (R_1 + \Delta x)}{a - \rho_{1,o} + (R_1 + \Delta x)} \right]$$

We can now calculate the center and radius of the outer boundary:

$$\rho_{2,o} = \frac{a}{\text{Tanh } \eta_{\text{out}}}$$
;  $R_2 = \frac{a}{\text{Sinh } \eta_{\text{out}}}$ .

When the mesh generator to the program POISSON is used to generate such boundaries,  $\Delta x$  can be set to the nominal grid spacing. This will assure the existence of a finite distance between the boundaries and prevent them from collapsing into each other. It is, however, advisable to increase the mesh density at this point, which can be easily done by choosing a  $\Delta x$  that is larger by an integer multiple of the nominal grid spacing.

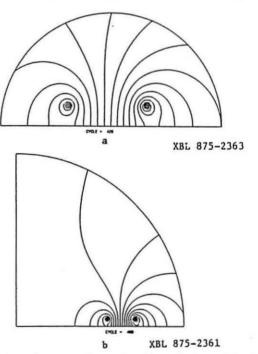
Example

To demonstrate the use of the toroidal boundary condition, we have used a set of coils in a configuration shown in Fig. 2b. We have placed 1000 A in each coil in the indicated directions and computed  $A^* = \rho A$  vs.  $\rho$  at z = 0. We further computed Bz along that same path and Br vs. z at the mid radius between the two coils. In addition, the same functions have been computed analytically for both conventional axisymmetric and cartesian geometries. The above computations were done at an increasing focal dimension (parameter a); however, the relative position of the coils, with respect to each other and to the mesh boundaries, remained unchanged. (In all problems a midplane symmetry is assured by specification of a Neumann boundary condition for A\* at z = 0, and the relaxation computations were then performed only in the region z ≥ 0.)

#### Case A - Coils Close to the Axis

The coils were placed at  $\rho$  = 3.25 cm ( -1000 A),  $\rho_{\rm b}$  = 4.25 cm ( +1000 A), with each at z = 0.25 cm. The inner boundary was centered midway between the coils at  $\rho_{1,0}$  = 3.75, with a radius of R<sub>1</sub> = 1.25. We assumed  $\Delta x = 0.1$  and computed  $\eta_{\rm out} = 1.65385404$  rad., so that  $\rho_{\rm 2,0} = 3.8042$  and R<sub>2</sub> = 1.4042.

The close proximity of the coils to the axis of symmetry in this example permitted a solution that includes the axis of symmetry and a circular type boundary condition. Flux plots for a toroidal b.c. and a circular b.c. are shown in Fig. 3. Variations in A\* are compared



Flux plot around a pair of conductors; (a) axial symmetry with toroidal boundary, (b) axial symmetry with circular boundary (drawn to a reduced scale so as to include the axis of rotational symmetry).

in Fig. 4. These variations include a comparison between two solutions that differ in the number of mesh points that have been used. (The cartesian case is a poor approximation and is therefore omitted from Fig. 4.) Good agreement (<0.5%) in A\* is obtained between theory, circular b.c., and toroidal b.c.. The values for B<sub>r</sub> are compared in Fig. 5.

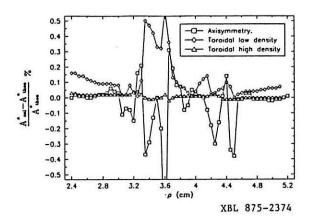


Fig. 4. Comparison between the calculated vector potential  $A^*$  (=  $\rho A$ ) and theoretical values along the midplane of symmetry (z=0). The axisymmetric case includes the axis of symmetry and employs a circular boundary, whereas the toroidal case employs a circular boundary around the sources. The need for a high mesh density is evident. It is noted that numerical difficulties will arise when  $A^*$  approaches zero, causing fractional errors to be large. Such difficulties are present near  $\rho_{1,0}$  for the toroidal case and exactly at  $\rho_{1,0}$  for the cartesian case. In the data presented here, no attempt was made to overcome such difficulties and large fractional errors near  $\rho_{1,0}$  accordingly do not reflect a real difference between the computated and expected values.

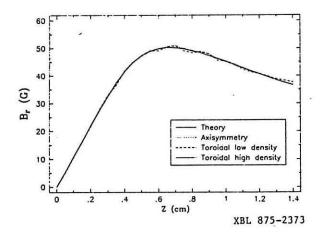


Fig. 5. The magnetic flux density in the  $\rho$  direction along  $\rho = 3.75$  (note that  $B_{\Gamma}$  for the Cartesian case is 0).

#### Case B - Coils Far From Axis

The coils are now moved to  $\rho_{1,0} = 225$  cm away from the axis of symmetry (Fig. 6). Good agreement between the toroidal case and theory is maintained (A\* < 0.5%).

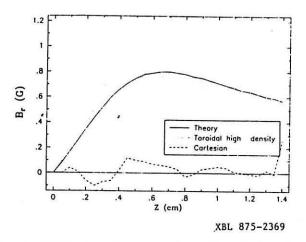


Fig. 6. Field values for a case where the coils have been extended to  $\rho_{1.0} = 225$  cm.

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