LA-8113-MS

Informal Report

2

Calculation of Cell Volumes and Surface Areas in MCNP

LOS ALAMOS SCIENTIFIC LABORATORY
Post Office Box 1663 Los Alamos, New Mexico 87545

This report was not edited by the Technical Information staff.

UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

LA-8113-MS
Informal Report

UC-32
Issued: January 1980

Calculation of Cell Volumes and Surface Areas in MCNP

John S. Hendricks

CALCULATION OF CELL VOLUMES AND SURFACE AREAS IN MCNP

by

John S. Hendricks

ABSTRACT

MCNP is a general Monte Carlo neutron-photon particle transport code which treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces, and some special fourth degree surfaces. It is necessary to calculate cell volumes and surface areas so that cell masses, fluxes, and other important information can be determined. The volume/area calculation in MCNP computes cell volumes and surface areas for cells and surfaces rotationally symmetric about any arbitrary axis.

I. INTRODUCTION

The particle flux in Monte Carlo transport problems is often estimated as the track length per unit volume or is related to the current per unit area. Therefore, knowledge of the volumes and surface areas of various geometric regions in a Monte Carlo problem is very important. Knowledge of volumes is also useful in calculating the masses and densities of problem cells and thus in calculating volumetric or mass heating.

Unfortunately, the calculation of volumes and surface areas in modern Monte Carlo transport codes is non-trivial. This is because the description of geometric regions, or cells, in sophisticated Monte Carlo codes is becoming more general and hence, much more complicated. In particular the general-purpose, continuous-energy Monte Carlo Neutron-Photon code MCNP[1] now allows for cells to be constructed from the union and/or intersections of any regions defined by an arbitrary combination of second degree surfaces and/or toroidal fourth degree surfaces. These surfaces may have different orientations, they may be segmented for tallying purposes, or the cell they compose may even consist of several disjoint subcells. Although such generality greatly increases the flexibility of a three-dimensional Monte Carlo code like MCNP, computing cell volumes and surface areas understandably requires increasingly elaborate computational methods.

The algorithm for computing cell volumes and surface areas in MCNP is capable of treating the complicated geometry just described provided that the individual cells and surfaces have a unique axis of rotational symmetry. This is not a serious restriction because most cells and surfaces used in MCNP are in practice rotationally symmetric. The procedure for the volume and surface area calculation may be summarized as:

1. All surfaces bounding a given cell are identified. Second-degree surfaces in the MCNP (x,y,z) Cartesian coordinate system are put into the generalized form

$$Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fxz + Gx + Hy + Jz + K = 0 \quad . \qquad (1)$$

For toroidal surfaces this step is a special case.

2. The (x',y',z') coordinate system in which the cell is rotationally symmetric is identified if it exists. This procedure is not straight-forward when the bounding surfaces of the cell are not symmetric about a single axis parallel to a major axis. In the case of a skew axis, Eq. 1 must be rewritten in matrix form and then diagonalized.[2] A special translation method has been developed for parabolic cases in which the resulting singular matrices cause the standard procedure to fail.

3. All surfaces bounding a cell are rotated and translated into the (x', y',z') coordinate system so that Eq. (1) is of the two-dimensional cylindrical form, or "Q-form,"

$$ar^2 + br + cs^2 + ds + e = 0 \;\; (r^2 = x'^2 + z'^2;\; s = y') \quad , \qquad (2)$$

or

$$r = f(s) \quad .$$

4. The intersections of all bounding surfaces with each other are found, but only those intersections which are corners of the cell are kept. Identifica-

tion of which intersections are corners is done by Boolean algebra and a complicated procedure which will be described later.

5. The surfaces are integrated (using standard integration formulas) between corners as

$$V_i = \pi \int r^2 \, ds \text{ for volumes,}$$

$$A_i = 2\pi \int r \sqrt{1 + \frac{\partial r}{\partial s}^2} \, ds \text{ for areas;}$$

(Only for toroidal surfaces must A_i be computed by numerical integration.)

6. The integrals are appropriately added and subtracted to determine the total volume of each cell and the total active area of each surface. The area integrals are actually computed twice; once for each side of the surface. In this way rotationally symmetric surfaces bounding some nonsymmetric cells may still be considered.

The details of the above steps will now be described.

II. CONVERSION OF SURFACES TO Q-FORM

The MCNP volume and surface area calculator only works for cells and surfaces which are rotationally symmetric. A surface is rotationally symmetric if it can be written in the two-dimensional cylindrical Q-form of Eq. (2). A cell is rotationally symmetric if all its bounding surfaces are rotationally symmetric about a common axis - that is, if a single rotation and translation applied to each bounding surface will convert these surfaces into Q-form. Therefore, the conversion of surface parameters to Q-form is essential to the MCNP volume and surface area calculation.

A. Step 1: Identification of Surfaces

The first step in converting surfaces to Q-form is to identify the bounding surfaces of a given cell and to put these surfaces into the generalized form of Eq. (1). Identification of bounding surfaces is trivial because this information is required user input in MCNP. Converting second degree surfaces into the form of Eq. (1) is also trivial since the permissible MCNP surfaces are mostly in this form. This is shown in TABLE I which is a list of permissible MCNP input surfaces. Only one-sheet cones and tori cannot be put into the form of Eq. (1). Hence one-sheet cones are treated as two sheet cones at this point and tori are treated as a special case which will be described later. Note that Eq. (1) may be written in matrix (capitol letters in italics represent matrices) form as

$$\vec{x}^t A \vec{x} + \vec{b}^t \vec{x} + c = 0 \quad , \tag{3}$$

where

$\vec{x}$ = the column vector (x,y,z),

$\vec{b}$ = the column vector (G,H,J),

c = K, a scalar, and

$$A = \begin{bmatrix} A & D/2 & F/2 \\ D/2 & B & E/2 \\ F/2 & E/2 & C \end{bmatrix} .$$

Note also that A is symmetric.

B. Step 2: Identification of Coordinate System

The second step in converting surfaces to Q-form is to identify the (x',y',z') coordinate system in which the cell is rotationally symmetric. Any two Cartesian coordinate systems, (x,y,z) and (x',y',z'), may be related by

$$\vec{x} = B\vec{y} + \vec{x}_o \quad . \tag{4}$$

where

$\vec{x}$ = (x,y,z),

$\vec{y}$ = (x',y',z'),

$\vec{x}_o$ = translation vector = (x,y,z) system coordinates of the (x',y',z') system origin, and

B = 3 x 3 rotation matrix.

If the result of substituting Eq. (4) into Eq. (3) is an equation in Q-form (Eq. (2)), then $\vec{x}_o$ and B define the $\vec{y}$ = (x',y',z') coordinate system of rotational symmetry.

The appropriate choice for B is the orthonormal modal matrix of A.[2] That is, the columns of B are the eigenvectors of A and

TABLE I

MCNP SURFACE CARDS

Mnemonic	Type	Description	Equation	Card Entries
P	Plane	General	$Ax + By + Cz - D = 0$	A,B,C,D
PX		Normal to X-axis	$x - D = 0$	D
PY		Normal to Y-axis	$y - D = 0$	D
PZ		Normal to Z-axis	$z - D = 0$	D
SO	Sphere	Centered at Origin	$x^2 + y^2 + z^2 - R^2 = 0$	R
S		General	$(x - \bar{x})^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{x},\bar{y},\bar{z}$,R
SX		Centered on X-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	$\bar{x}$,R
SY		Centered on Y-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	$\bar{y}$,R
SZ		Centered on Z-axis	$x^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{z}$,R
C/X	Cylinder	Parallel to X-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{y},\bar{z}$,R
C/Y		Parallel to Y-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{y},\bar{z}$,R
C/Z		Parallel to Z-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	$\bar{x},\bar{y}$,R
CX		On X-axis	$y^2 + z^2 - R^2 = 0$	R
CY		On Y-axis	$x^2 + z^2 - R^2 = 0$	R
CZ		On Z-axis	$x^2 + y^2 - R^2 = 0$	R
K/X	Cone	Parallel to X-axis	$\sqrt{(y - \bar{y})^2 + (z - \bar{z})^2} - t(x - \bar{x}) = 0$	$x,y,z,t^2, \pm 1$
K/Y		Parallel to Y-axis	$\sqrt{(x - \bar{x})^2 + (z - \bar{z})^2} - t(y - \bar{y}) = 0$	$x,y,z,t^2, \pm 1$
K/Z		Parallel to Z-axis	$\sqrt{(x - \bar{x})^2 + (y - \bar{y})^2} - t(z - \bar{z}) = 0$	$x,y,z,t^2, \pm 1$
KX		On X-axis	$\sqrt{y^2 + z^2} - t(x - \bar{x}) = 0$	$\bar{x},t^2, \pm 1$
KY		On Y-axis	$\sqrt{x^2 + z^2} - t(y - \bar{y}) = 0$	$\bar{y},t^2, \pm 1$
KZ		On Z-axis	$\sqrt{x^2 + y^2} - t(z - \bar{z}) = 0$	$z,t^2, \pm 1$
				± 1 used only for 1 sheet cone
SQ	Ellipsoid Hyperboloid Paraboloid	Major axis parallel to X,Y, or Z-axis	$A(x - \bar{x})^2 + B(y - \bar{y})^2 + C(z - \bar{z})^2 + 2D(x - \bar{x}) + 2E(y - \bar{y}) + 2F(z - \bar{z}) + G = 0$	A,B,C,D,E, F,G,$\bar{x},\bar{y},\bar{z}$
GQ	Cylinder Cone Ellipsoid Hyperboloid Paraboloid	Major axis is not parallel to X,Y, or Z-axis	$Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fzx + Gx + Hy + Jz + K = 0$	A,B,C,D,E, F,G,H,J,K
TX	Eliptical or Circular Tori	Major axis parallel to X-axis	$\frac{(x - \bar{x})^2}{B^2} + \frac{(\sqrt{(y - \bar{y})^2 + (z - \bar{z})^2} - A)^2}{C^2} = 1$	$\bar{x},\bar{y},\bar{z}$,A,B,C
TY		Major axis parallel to Y-axis	$\frac{(y - \bar{y})^2}{B^2} + \frac{(\sqrt{(x - \bar{x})^2 + (z - \bar{z})^2} - A)^2}{C^2} = 1$	$\bar{x},\bar{y},\bar{z}$,A,B,C
TZ		Major axis parallel to Z-axis	$\frac{(z - \bar{z})^2}{B^2} + \frac{(\sqrt{(x - \bar{x})^2 + (y - \bar{y})^2} - A)^2}{C^2} = 1$	$\bar{x},\bar{y},\bar{z}$,A,B,C

$$B^t = B^{-1} \tag{5}$$

$$AB = BD \tag{6}$$

where

$$D = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \text{, and}$$

λ_i = eigenvalues of A.

If $\lambda_1 \neq \lambda_2 \neq \lambda_3$ the surface is symmetric, but not rotationally symmetric. Therefore, two eigenvalues must be identical for rotational symmetry. We arbitrarily choose the y'-axis as the axis of rotational symmetry, and therefore require $\lambda_1 = \lambda_3$ for the sake of analysis. Actually, in MCNP the x'-axis is chosen.

The appropriate choice for $\vec{x}_o$ is

$$\vec{x}_o = -\frac{1}{2} A^{-1}\vec{b} \quad , \tag{7}$$

except for the following three cases where A is singular and hence has no inverse. If A represents a parabola, then $\lambda_2 = 0$, A is singular, and we have found that

$$\vec{x}_o = -\frac{1}{2\lambda_1} \vec{b} \tag{8}$$

is a suitable translation vector. If $\lambda_1 = \lambda_3 = 0$, then A represents a two-sheet plane which is disallowed. And if $\lambda_1 = \lambda_2 = \lambda_3 = 0$, then A represents a plane, $\vec{x}_o$ may have any arbitrary or convenient value, and a suitable choice for the rotation matrix is

$$B = \begin{bmatrix} v/t & u & -uw/t \\ -u/t & v & -vw/t \\ 0 & w & t \end{bmatrix}$$

where

$$t = \sqrt{u^2 + v^2} \quad ,$$

$$u = G/\sqrt{G^2 + H^2 + J^2} \quad ,$$
$$v = H/\sqrt{G^2 + H^2 + J^2} \quad , \text{ and}$$
$$w = J/\sqrt{G^2 + H^2 + J^2} \quad .$$

If t = 0 an appropriate substitute B-matrix is chosen.

There are many ways to determine the orthonormal modal matrix, B, of A. In the MCNP volume and surface area calculation B is found using a standard system routine which finds the eigenvalue and eigenvectors of A.

This routine is only infrequently used because most MCNP problems consist of many cells rotationally symmetric about a single common axis. Therefore, for each cell the values of B and $\vec{x}_o$ from the previous cell are tried, and only if they fail to rotate and translate the present cell surfaces into Q-form are a new B and $\vec{x}_o$ calculated. For the first cell in a problem an initial guess of $B = I$ (identity matrix) and $\vec{x}_o = 0$ is tried before a calculation of B and $\vec{x}_o$ is attempted. Thus for problems fully symmetric about the y-axis, B and $\vec{x}_o$ are never calculated because the initial guess always works. For rotational symmetry about the other major axes the calculation of B and $\vec{x}_o$ is also avoided.

C. Step 3: Rotation and Translation

The third step in converting surfaces to Q-form is to rotate and translate the coordinate system by substituting Eq. (4) into Eq. (3):

$$\vec{x}^t A\vec{x} + \vec{b}^t\vec{x} + c = (B\vec{y} + \vec{x}_o)^t A(B\vec{y} + \vec{x}_o) + \vec{b}^t(B\vec{y} + \vec{x}_o) + c$$
$$= \vec{y}^t B^t AB\vec{y} + 2\vec{y}^t B^t A\vec{x}_o + \vec{x}_o^t A\vec{x}_o + \vec{b}^t B\vec{y} + \vec{b}^t\vec{x}_o + c = 0$$

Letting

$$e = \vec{x}_o^t A\vec{x}_o + \vec{b}^t\vec{x}_o + c \text{ (a scalar quantity)}$$
$$\vec{y}^t B^t AB\vec{y} + 2\vec{y}^t B^t A\vec{x}_o + \vec{b}^t B\vec{y} + e = 0 \quad .$$

From Eqs. 5 and 6 this becomes

$$\vec{y}^t D\vec{y} + 2\vec{y}^t B^t A\vec{x}_o + \vec{b}^t B\vec{y} + e = 0 \quad . \tag{9}$$

If $\lambda_2 \neq 0$, let $\vec{x}_o = -\frac{1}{2} A^{-1}\vec{b}$ and then Eq. (9) becomes

$$\vec{y}^t D\vec{y} - \vec{y}^t B^t \vec{b} + \vec{b}^t B\vec{y} + e \quad ,$$
$$= \vec{y}^t D\vec{y} + e \quad ,$$
$$= \lambda_1 x'^2 + \lambda_2 y'^2 + \lambda_3 z'^2 + e \quad , \text{ and}$$
$$= ar^2 + cs^2 + e = 0$$

which is in Q-form. If $\lambda_2 = 0$, let $\vec{x}_o = -\frac{1}{2\lambda_1}\vec{b}$ and then Eq. (9) becomes

$$\vec{y}^t D\vec{y} - \frac{1}{\lambda_1}\vec{y}^t B^t A\vec{b} + \vec{b}^t B\vec{y} + e \quad ,$$
$$= \vec{y}^t D\vec{y} - \frac{1}{\lambda_1}\vec{b}^t BD\vec{y} + \vec{b}^t B\vec{y} + e \quad ,$$
$$= \vec{y}^t D\vec{y} + \vec{b}^t B\left[I - \frac{1}{\lambda_1} D\right]\vec{y} + e \quad ,$$
$$= \lambda_1 x'^2 + \lambda_1 z'^2 + \vec{b}^t \vec{v}_2 y' + e \quad , \text{ and}$$
$$= ar^2 + ds + e = 0$$

which is in Q-form. Note that $\vec{v}_2$ is the eigenvector corresponding to λ_2.

As mentioned earlier, one-sheet cones and tori are exceptions to the above procedure. However, as shown in TABLE I, these surfaces are limited to axes parallel to major axes in the MCNP (x,y,z) coordinate system. Hence there is no need to compute B and $\vec{x}_o$ since these quantities are known at the time of input. The rotation matrix is either the identity matrix or a permutation thereof; the translation vector is simply

$$\vec{x}_o = (\bar{x},\bar{y},\bar{z}) \quad ,$$

where $\bar{x}$, $\bar{y}$, and $\bar{z}$ are input parameters. Thus both one-sheet cones and tori can be checked for common symmetry with other surfaces in the cell and then put directly into Q-form.

For a one-sheet cone, Q-form is

$$r - ts + e = 0 \quad ,$$

where t is an input parameter. The value of the constant, e, is different for different kinds of cones. For a K/X cone

$$e = t(\overline{x} - y') \quad ,$$

where $\overline{x}$ is an input parameter (see TABLE I) and y' is offset distance between the $\vec{x}$ and $\vec{y}$ coordinate system origins. For a torus, Q-form is

$$r^2 - 2Ar + \left(\frac{C}{B}\right)^2 s^2 + ds + e = 0 \quad ,$$

where C, B and A are input parameters. For a TX torus

$$d = -2(\overline{x} - y')\frac{C^2}{B^2}$$

and

$$e = A^2 - C^2 + (\overline{x} - y')^2 \frac{C^2}{B^2} \quad ,$$

where $\overline{x}$ is again an input parameter and y' is an offset.

Once the bounding surfaces of a cell are converted to Q-form they may be recast in the form

$$r = f(s) \quad .$$

Then the cell volumes and surface areas are computed from integrals of the form

$$V_i = \pi \int r^2 \, ds = \pi \int [f(s)]^2 \, ds$$

and

$$A_i = 2\pi \int r\sqrt{1 + \left(\frac{\partial r}{\partial s}\right)^2}\, ds = 2\pi \int f(s)\sqrt{1 + \left(\frac{\partial f}{\partial s}\right)^2}\, ds$$

III. DETERMINATION OF INTERSECTIONS AND CORNERS

In order to deterministically compute the volumes of cells and the areas of surfaces the limits of integration must be found. For the integrals in the MCNP cell volume and surface area calculator, these limits are the coordinates of cell corners in the (r,s) coordinate system.

A. Calculation of Intersections

In order to find the corners of cells it is first necessary to find the intersection of each cell-bounding surface with all other surfaces bounding the cell. Note that the axis of rotational symmetry is automatically added to the list of cell-bounding surfaces. Thus a simple cell with only a single surface, such as a sphere, will still have intersections and be properly treated.

When the surfaces are written in Q-form, the intersections of any two surfaces are simply the coordinates found by solving the following two simultaneous quadratic equations:

$$a_1r^2 + b_1r + c_1s^2 + d_1s + e_1 = 0 \quad , \tag{10a}$$

$$a_2r^2 + b_2r + c_2s^2 + d_2s + e_2 = 0 \quad , \tag{10b}$$

where a_1, b_1, c_1, d_1, and e_1 are the Q-form coefficients of the first surface and a_2, b_2, c_2, d_2, and e_2 are the Q-form coefficients of the second surface. Three possible cases arise in the solution of Eq. (10):

1. Quartic Case [$(a_1b_2 - a_2b_1) \neq 0$; and $(a_1c_2 - a_2c_1) \neq 0$]. This case arises when neither surface is a plane and at least one surface is either a torus or a one-sheet cone. Equation (10a) is multiplied by a_2 and Eq. (10b) is multiplied by a_1 and then the resulting equations are subtracted to give

$$t_1r + t_2s^2 + t_3s + t_4 = 0 \quad , \tag{11}$$

where

$$t_1 = a_1b_2 - a_2b_1 \quad ,$$

$$t_2 = a_1 c_2 - a_2 c_1 \quad ,$$

$$t_3 = a_1 d_2 - a_2 d_1 \quad , \text{ and}$$

$$t_4 = a_1 e_2 - a_2 e_1 \quad .$$

Equation (11) is then inserted into Eq. (10a) which results in the quartic equation

$$As^4 + Bs^3 + Cs^2 + Ds + E = 0 \quad , \tag{12}$$

where

$$A = a_1 t_2^2 \quad ,$$

$$B = 2a_1 t_2 t_3 \quad ,$$

$$C = a_1\left(2t_2 t_4 + t_3^2\right) + t_1\left(c_1 t_1 - b_1 t_2\right) \quad ,$$

$$D = 2a_1 t_3 t_4 + t_1(d_1 t_1 - b_1 t_3) \quad , \text{ and}$$

$$E = a_1 t_4^2 + t_1(e_1 t_1 - b_1 t_4) \quad .$$

If $a_1 = 0$ then $a_2 \neq 0$ and Eq. (11) is inserted into Eq. (10b) instead with similar results. In either case, the quartic equation is solved for s by an iterative nth order polynomial solver system routine and then the corresponding values of r are found by substituting these values of s back into Eq. (11).

2. Quadratic Case [$t_1 \neq 0, t_2 = 0$; or $t_1 = 0$, a_1 or $a_2 \neq 0$]. This case arises when at least one surface is a torus or quadratic. If $t_1 = a_1 b_2 - a_2 b_1 = 0$, then Eq. (11) becomes a quadratic equation in s. If $t_1 \neq 0$ but $t_2 = 0$ from the quartic case, then the quartic equation reduces to a quadratic equation [$A = B = 0$ in Eq. (12)] in s. In either case, the quadratic equation is solved for s and then these values are substituted back into Eq. (10a) [Eq. (10b) if $a_1 = 0$] to form a second quadratic equation to find the corresponding values of r.

3. Linear or Quadratic Case ($a_1 = a_2 = 0$). This case arises when both surfaces are either planes or one-sheet cones. Whichever, Eq. (10a) is multiplied by b_2 and Eq. (10b) is multiplied by b_1 and then the resulting equations are subtracted to give a linear or quadratic equation in s. This equation is then solved (by the quadratic formula if it is quatratic and by substitution if

it is linear) and the resulting value of s, if any, is substituted back into Eq. (10a) [Eq. (10b) if $b_1 = 0$] to find the corresponding value(s) of r by the quadratic formula.

B. Determination of Corners

Once the intersection of two cell-bounding surfaces is calculated it is necessary to determine if this intersection is an actual corner of the cell. If the intersection occurs somewhere outside of the cell then, of course, it is not a corner of the cell. Also, if the r-coordinate of the intersection point in the (r,s) coordinate system is negative then the intersection is also rejected. Note that this exclusion gets rid of points on the unwanted arc of a degenerate torus and on the wrong leg of a one-sheet cone.

Intersections with $r \geqslant 0$ are identified as corners by a complicated procedure involving Boolean Algebra. Consider the intersection of the two surfaces in Fig. 1. The two surfaces divide space into four zones, i = 1, 4; and the cell could conceivably be within any combination of zones. The intersection defines a corner only if

$$f = \sum_{i=1}^{4} \delta_i \cdot 2^{(i-1)} \tag{13}$$

is not divisible by 3. Here,

$$\delta_i = 0 \text{ if the cell is not present in zone i;}$$
$$= 1 \text{ if the cell is present in zone i.}$$

For example, if the cell is present in zones 1 and 3 but not zones 2 and 4 ($\delta_1 = \delta_3 = 1$; $\delta_2 = \delta_4 = 0$) the intersection is a corner because f = 5. But if the cell is present in zones 1 and 2 but not zones 3 and 4 ($\delta_1 = \delta_2 = 1$; $\delta_3 = \delta_4 = 0$) then f = 3 and the intersection is not a corner. Note that if the intersection is outside the cell then f = 0 and the intersection is rejected.

Whether or not a cell is present in a zone is determined by the Boolean functions δ_i.[3] These are functions of the Boolean parameter v_j, j = 1, n where n is the number of cell bounding surfaces, and

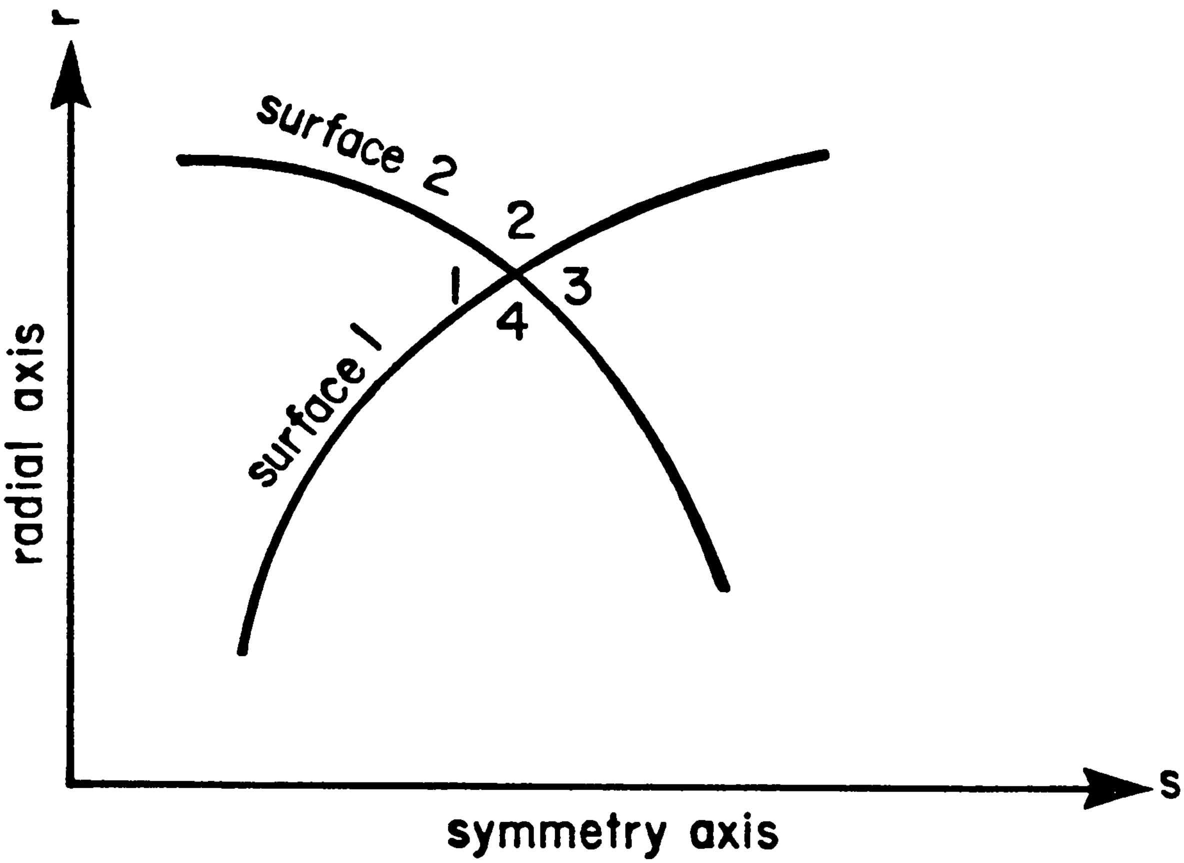

Fig. 1. Intersection of Two Surfaces

v_j = 1 if the sense of the intersection point to surface j is the same as the user-input sense of the cell to surface j;

v_j = 0 otherwise.

The sense of the intersection to surface j is positive if

$$a_j r^2 + b_j r + c_j s^2 + d_j s + e_j > 0 \quad ,$$

where r, s are the intersection coordinates and a_j, b_j, c_j, d_j, e_j are the surface coefficients of surface j. If

$$a_j r^2 + b_j r + c_j s^2 + d_j s + e_j < 0 \quad ,$$

then the sense of the intersection point to the surface is negative. For the two surfaces which form the intersection

$$a_j r^2 + b_j r + c_j s^2 + d_j s + e_j = 0 \quad ,$$

and the initial value of v_j is arbitrarily set to 1 if the user-input cell-surface sense is positive and 0 otherwise.

The Boolean functions, δ_i, are formed from the v_j's as illustrated in the example of Fig. 2. The user input surface relations for cell 1 in Fig. 2 are

-3(2:-1) ,

where : is the union operator. The Boolean function of v_j's for point 1 in Fig. 2 is then, for example

$$\delta = v_3 \cap (v_2 \cup v_1) \quad ,$$
$$= 1 \cap (0 \cup 0) = 1 \cap 0 = 0 \quad .$$

That is, point 1 is outside cell 1. For point 2,

$$\delta = v_3 \cap (v_2 \cup v_1) \quad ,$$
$$= 1 \cap (1 \cup 0) = 1 \cap 1 = 1 \quad .$$

That is, point 2 is inside cell 1.

For the intersection of surfaces 1 and 2 (point 3),

$$\delta = 1 \cap (1 \cup 0) = 1 \quad ,$$

where the values of v_j were arbitrarily set for the intersecting surfaces, j = 1, 2. To determine if this point is a corner, v_1 and v_2 are arbitrarily alternated to determine if the cell is present in the various zones of Fig. 1:

$$\delta_1 = 1 \cap (1 \cup 0) = 1 \quad \text{(zone 1)},$$
$$\delta_2 = 1 \cap (0 \cup 0) = 0 \quad \text{(zone 2)},$$

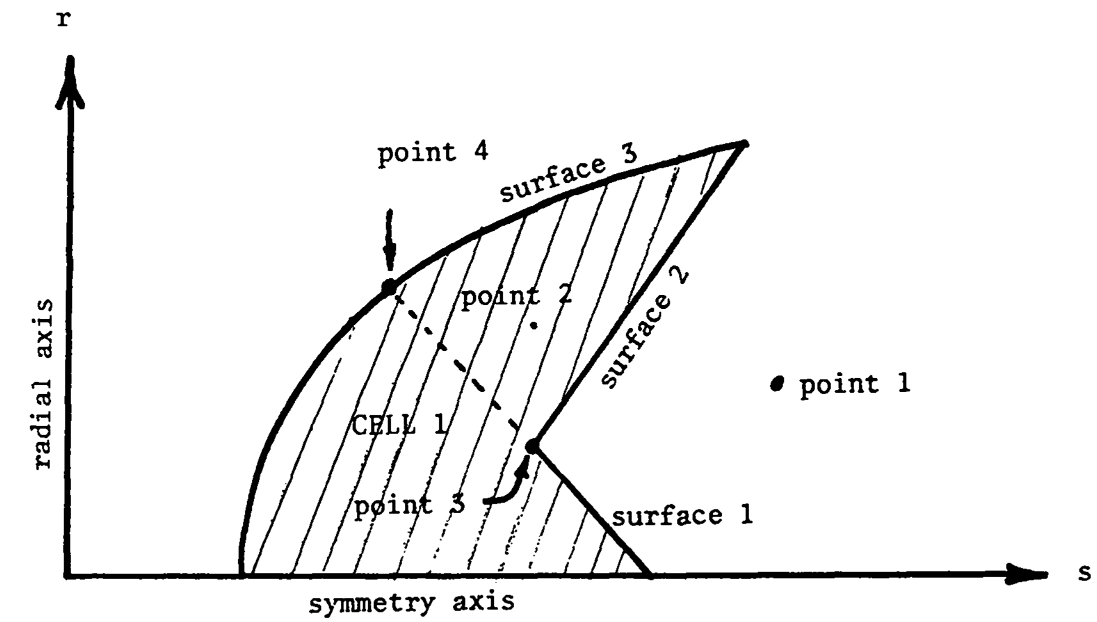

Fig. 2. The Cell -3(2:-1)

$$\delta_3 = 1 \cap (0 \cup 1) = 1 \quad \text{(zone 3), and}$$

$$\delta_4 = 1 \cap (1 \cup 1) = 1 \quad \text{(zone 4).}$$

When these values are inserted in Eq. (13),

$$f = 1 \cdot 1 + 0 \cdot 2 + 1 \cdot 4 + 1 \cdot 8 = 13 \quad .$$

Since f = 13 is not divisible by 3, the intersection of surfaces 1 and 2 is a corner.

As another example, consider the intersection of surfaces 1 and 3 (point 4)

$$\delta_1 = 0 \cap (1 \cup 0) = 0 \quad ,$$

$$\delta_2 = 1 \cap (1 \cup 0) = 1 \quad ,$$

$$\delta_3 = 1 \cap (1 \cup 1) = 1 \quad ,$$

$$\delta_4 = 0 \cap (1 \cup 1) = 0 \quad ,$$

and

$$f = 0 \cdot 1 + 1 \cdot 2 + 1 \cdot 4 + 0 \cdot 8 = 6 \quad .$$

Since f = 6 is divisible by 3 the intersection of surfaces 1 and 3 does not form a corner of cell 1.

C. Determination of Star Corners

The above procedure for determination of corners sometimes fails when more than two surfaces intersect at a point to form a "star." As an example, consider the intersection of surfaces 2 and 3 in Fig. 3. Surface 1 also passes through this intersection thus forming a star as illustrated in Fig. 4. Since

$$a_1r^2 + b_1r + c_1s^2 + d_1s + e_1 = 0 \quad ,$$

the value of v_1 is ambiguous and the corner determination procedure fails.

To remedy this situation, each corner is checked for the presence of additional surfaces passing through it. If

$$a_jr^2 + b_jr + c_js^2 + d_js + e_j < \varepsilon \, \mathrm{Max}[|2a_jr + b_j|,|2c_js + d_j|]$$

$$\varepsilon = \text{fractional permissible error in } r \text{ or } s \quad ,$$

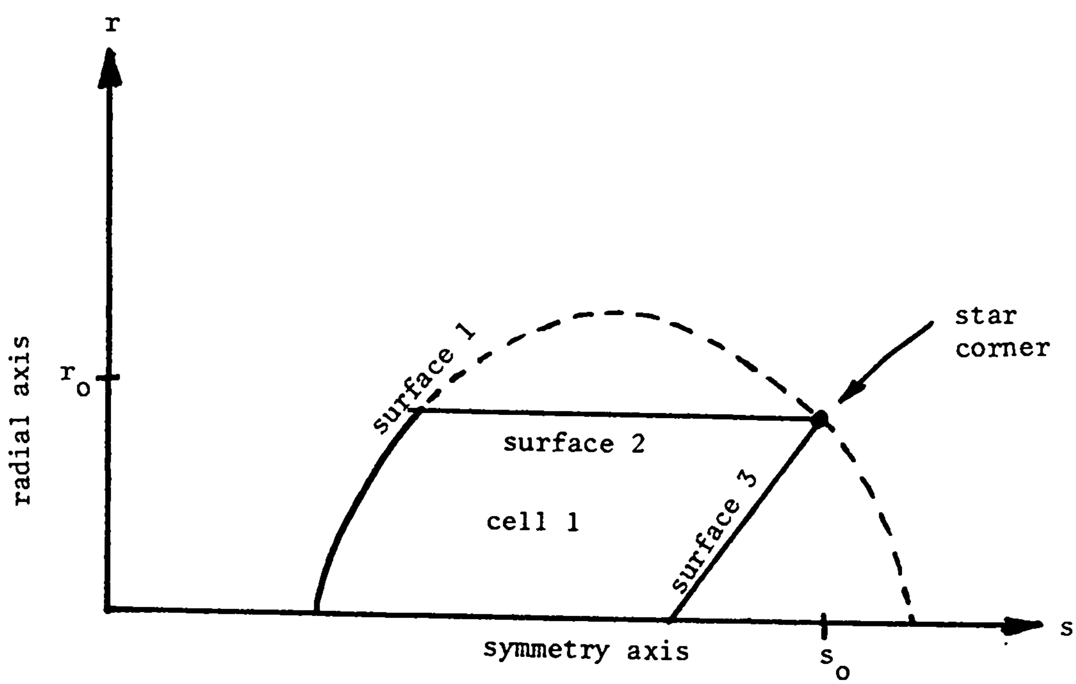

Fig. 3. Star Corner for the Cell -1 -2 3

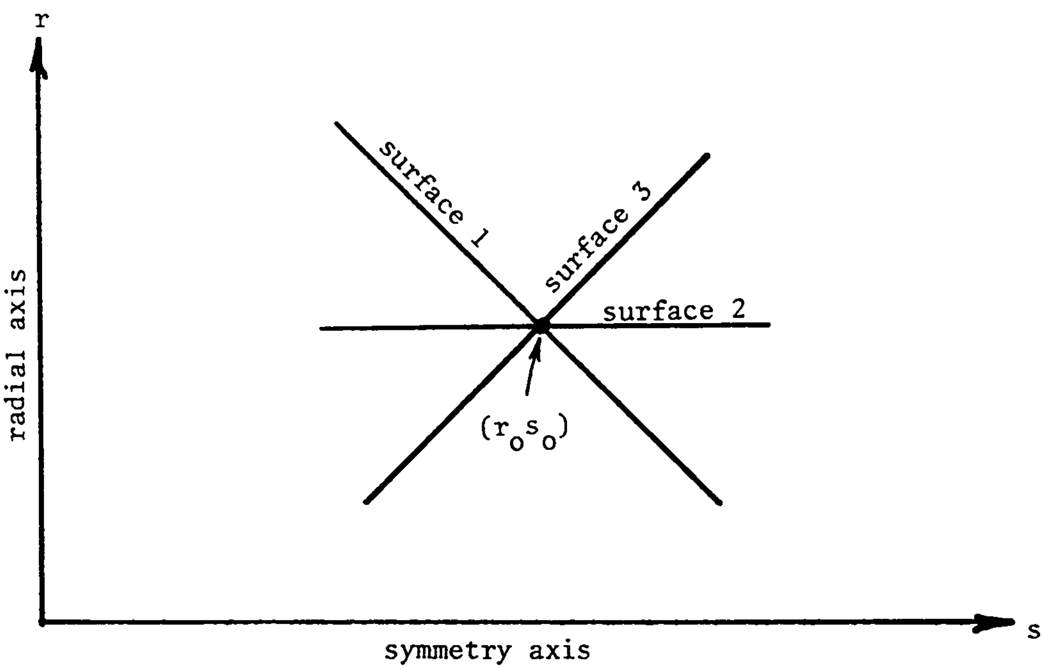

Fig. 4. Star Corner

then surface j passes through the intersection to form a star. If this condition is not satisfied for any surface other than the two forming the intersection then the star checking routine is bypassed.

To determine if surfaces i and k form a corner when another surface, j, also passes through the i-k intersection, each point on surfaces i and k is checked for the proper sense with respect to the other two surfaces in the neighborhood of the i-k intersection. In the neighborhood of the intersection point all surfaces, ℓ = i, j, k approach linearity and can thus be written as

$$(r - r_o) = \partial_\ell (s - s_o) \quad , \tag{14}$$

where r_o and s_o are the intersection coordinates and ∂_ℓ is the slope of surface ℓ near (r_o, s_o). If (r_j, s_i) is a point on surface i then

$$(r_i - r_o) = \partial_i (s_i - s_o) \quad .$$

If these points satisfy the user input sense, S_j to surface j then

$$S_j[(r_i - r_o) - \partial_j(s_i - s_o)] > 0 \quad .$$

Inserting Eq. (14),

$$S_j[\partial_i - \partial_j](s_i - s_o) > 0 \quad .$$

If (r_i,s_i) also satisfy the user input sense, S_k to surface k,

$$S_k[\partial_i - \partial_k](s_i - s_o) > 0 \quad .$$

These equations may be combined so that if each point on surfaces i satisfies the user input senses to surfaces j and k:

$$S_k S_j[\partial_i - \partial_j][\partial_i - \partial_k] > 0 \quad .$$

Similarly, each point on surface k must satisfy the user input senses to surfaces i and j:

$$S_i S_j[\partial_k - \partial_i][\partial_k - \partial_j] > 0 \quad .$$

If these two relationships are satisfied then the intersection of surfaces i and k is accepted as a corner; otherwise it is rejected.

For example, consider the situation of Fig. 3. The standard procedure of Section IIB would indicate that the intersections of surfaces 1 and 2, 2 and 3 and 3 and 1 all form corners of cell 1 at (r_o,s_o). But only surfaces 2 and 3 form a true corner at this star corner. The user input senses for the cell -1 -2 3 are $S_1 = -1$, $S_2 = -1$, $S_3 = +1$; from Fig. 4 it is seen that the slopes of the surfaces in the neighborhood of the intersection are $\partial_1 = -1$, $\partial_2 = 0$, $\partial_3 = 1$. Therefore,

Intersecting Surfaces:

1 & 2	$(-1)(1)[-1 -0][-1 -1] < 0$
	$(-1)(1)[0 - (-1)][0 - 1] > 0$
	intersection rejected,

Intersecting Surfaces:

2 & 3	(-1)(1)[0 - (-1)][0 - 1] > 0
	(-1)(-1)[1 - (-1)][1 - 0] > 0
	intersection accepted as corner,
1 & 3	(-1)(1)[-1 -0][-1 -1] < 0
	(-1)(-1)[1 - (-1)][1 - 0] > 0
	intersection rejected.

Hence the only legitimate corner at the star (three or more surfaces) intersection at (r_o,s_o) is the intersection of surfaces 2 and 3.

IV. INTEGRATION OF VOLUMES AND AREAS

Once the corners of a cell are identified in the (r,s) coordinate system of rotational symmetry the surfaces are integrated between corners if the midpoint of the surface between the corners is on the cell boundary.

The midpoint (r_m,s_m) of surface i,

$$a_i r^2 + b_i r + c_i s^2 + d_i s + e_i = 0 \quad , \tag{15}$$

between the corners (r_j,s_j) and (r_k,s_k) is

$$r_m = \frac{1}{2}(r_j + r_k)$$

$$s_m = \frac{1}{2}(s_j + s_k)$$

for linear surfaces ($a_i = 0$). For nonlinear surfaces r_m is found by plugging s_m into Eq. (15). A Boolean function, δ, (Section IIIB) is then formed for surface i where $v_i = 0$ and then alternately $v_i = 1$. If $\delta(v_i = 0) + \delta(v_i = 1) = 1$ then the midpoint, (r_m,s_m), is on the cell boundary. The integration limits are then s_j and s_k.

A. Determination of Volumes

The volume of the region formed by rotating surface i about the symmetry axis, A, is simply

$$V_i = \pi \int_{s_j}^{s_k} r^2 \, ds \quad .$$

For linear surfaces, $a_i = c_i = 0$; $b_i = 1$

$$V_i = \pi \int_{s_j}^{s_k} (d_i s + e_i)^2 \, ds$$

$$= \pi \left[\frac{1}{3} d_i^2 \left(s_k^3 - s_j^3 \right) + d_i e_i \left(s_k^2 - s_j^2 \right) + e_i^2 \left(s_k - s_j \right) \right] \quad .$$

For non-linear surfaces, $a_i \neq 0$

$$r = \bar{r} + q \sqrt{\left(\frac{b_i}{2a_i} \right)^2 - \frac{1}{a_i} \left[c_i s^2 + d_i s + e_i \right]} \quad ,$$

where

$q = -1$ for lower portion of a torus,

$= 1$ otherwise,

and

$\bar{r} = - \frac{b_i}{2a_i} =$ for a torus,

$= 0$ for other surfaces,

$$V_i = \pi \int_{s_j}^{s_k} \left[\bar{r} + q \sqrt{\bar{r}^2 - \frac{1}{a_i} \left(c_i s^2 + d_i s + e_i \right)} \right]^2 ds \quad ,$$

$$= \pi \int_{s_j}^{s_k} \left[2\bar{r}^2 + 2\bar{r} q \sqrt{\bar{r}^2 - \frac{1}{a_i} \left(c_i s^2 + d_i s + e_i \right)} - \frac{1}{a_i} \left(c_i s^2 + d_i s + e_i \right) \right] ds,$$

$$= \pi \left\{ 2\bar{r}^2 \left(s_k - s_j \right) - \frac{1}{a_i} \left[\frac{c_i}{3} \left(s_k^3 - s_j^3 \right) + \frac{d_i}{2} \left(s_k^2 - s_j^2 \right) + e_i \left(s_k - s_j \right) \right] \right\} \quad ,$$

$$+ 2\pi\bar{r}q \int_{s_i}^{s_k} \sqrt{\bar{r}^2 - \frac{1}{a_i}\left(c_i s^2 + d_i s + e_i\right)}\, ds \quad .$$

The integral,

$$I = \int_{s_j}^{s_k} \sqrt{\bar{r}^2 - \frac{1}{a_i}\left(c_i s^2 + d_i s + e_i\right)}\, ds$$

is of the form

$$I = \int \sqrt{A + Bx + Cx^2}\, dx \quad . \tag{16}$$

If

$$B^2 - 4AC = 0 \ (C > 0) \quad ,$$

then

$$\sqrt{A + Bx + Cx^2} = \sqrt{C}\left(x + \frac{B}{2C}\right) \quad ,$$

and

$$I = \sqrt{C} \int \left(x + \frac{B}{2C}\right) dx$$

which is solved trivially. If

$$B^2 - 4AC \neq 0 \quad ,$$

then

$$I = \int \sqrt{A + Bx + Cx^2}\, dx$$

$$= \frac{1}{8C}\left[2(2Cx + B)\sqrt{A + Bx + Cx^2} + (4AC - B^2)\int \frac{dx}{\sqrt{A + Bx + Cx^2}}\right]$$

and

$$\int \frac{dx}{\sqrt{A + Bx + Cx^2}} = \frac{1}{\sqrt{C}}\,\ell n\left[\sqrt{A + Bx + Cx^2} + x\sqrt{C} + \frac{B}{2\sqrt{C}}\right] \text{ if } C > 0$$

or

$$\int \frac{dx}{\sqrt{A + Bx + Cx^2}} = \frac{1}{\sqrt{-C}} \sin^{-1}\left[\frac{-2Cx - B}{\sqrt{B^2 - 4AC}}\right] \text{ if } C < 0,\ B^2 - 4AC > 0 \quad .$$

B. Determination of Areas

The area of any planar surface i [Eq. (15)] rotated about the symmetry axis, s, is

$$A_i = \left|\pi\left(r_k^2 - r_i^2\right)\right| \text{ plane.}$$

For a cylinder or one legged cone, $a_i = c_i = 0$

$$A_i = \left|2\pi \int_{s_j}^{s_k} r\sqrt{1 + \frac{\partial r}{\partial s}^2}\, ds\right|$$

$$= \left|2\pi \int_{s_j}^{s_k} \left[-\frac{1}{b_i}(d_i s + e_i)\sqrt{1 + \left(\frac{d_i}{b_i}\right)^2}\right] ds\right|$$

$$= \left| \frac{\pi}{b_i} \sqrt{1 + \left(\frac{d_i}{b_i}\right)^2} \left[d_i \left(s_k^2 - s_j^2 \right) + 2e_i \left(s_k - s_j \right) \right] \right|$$

For a quadratic surface, $a_i \neq 0$, $b_i = 0$

$$A_i = \left| 2\pi \int_{s_j}^{s_k} r \sqrt{1 + \left(\frac{\partial r}{\partial s}\right)^2} \, ds \right|$$

$$= \left| 2\pi \int_{s_j}^{s_k} \sqrt{- \frac{1}{a_i} \left(c_i s^2 + d_i s + e_i \right) \left[1 + \left\{ \frac{-(2c_i s + d_i)}{2\left[-a_i \left(c_i s^2 + d_i s + e_i \right) \right]^{1/2}} \right\}^2 \right]} \, ds \right|$$

$$= \left| 2\pi \int_{s_j}^{s_k} \sqrt{- \frac{1}{a_i} \left[c_i s^2 + d_i s + e_i \right] + \frac{1}{4a_i^2} \left[4c_i^2 s^2 + 4c_i d_i s + d_i^2 \right]} \, ds \right|$$

$$= \left| 2\pi \int_{s_j}^{s_k} \sqrt{\left(\frac{d_i}{2a_i}\right)^2 - \frac{e_i}{a_i} + \left(\frac{c_i}{a_i} - 1\right) \frac{d_i}{a_i} s + \left(\frac{c_i}{a_i} - 1\right) \frac{c_i}{a_i} s^2} \, ds \right| ,$$

which is of the same form and can be solved in the same way as Eq. (17).

For a toroidal surface, $a_i \neq 0$, $b_i \neq 0$,

$$r = - \frac{b_i}{2a_i} \pm \sqrt{\left(\frac{b_i}{2a_i}\right)^2 - \frac{1}{a_i} \left(c_i s^2 + d_i s + e_i \right)} ,$$

and the area integral

$$A_i = \left| 2\pi \int_{s_j}^{s_k} r \sqrt{1 + \left(\frac{\partial r}{\partial s}\right)^2} \, ds \right|$$

has no convenient integration formula. Therefore, let

$$\bar{r} = -\frac{b_i}{2a_i} \tag{17}$$

$$\bar{s} = -\frac{d_i}{2c_i}$$

$$r = \bar{r} + \alpha \sin \theta$$

$$s = \bar{s} + \beta \cos \theta$$

where

$$\beta = \alpha\sqrt{\frac{a_i}{c_i}} \quad .$$

Then

$$a_i r^2 + b_i r + c_i s^2 + d_i s + e_i = a_i(r - \bar{r})^2 + c_i(s - \bar{s})^2 + e_i - a_i\bar{r}^2 - c_i\bar{s}^2$$

$$= a_i\alpha^2 \sin^2 \theta + c_i\beta^2 \cos^2 \theta + e_i - a_i\bar{r}^2 - c_i\bar{s}^2$$

$$= a_i\alpha^2(\sin^2 \theta + \cos^2 \theta) + e_i - a_i\bar{r}^2 - c_i\bar{s}^2$$

$$= a_i\alpha^2 + e_i - a_i\bar{r}^2 - c_i\bar{s}^2 = 0 \quad .$$

Therefore

$$\alpha^2 = \bar{r}^2 - \frac{e_i}{a_i} + \frac{c_i}{a_i}\bar{s}^2$$

$$\beta^2 = \frac{a_i}{c_i}\bar{r}^2 - 1 + \bar{s}^2 \quad .$$

From Eq. (17),

$$dr = \pm\, \alpha \cos \theta \, d\theta$$

$$ds = \beta \sin \theta \, d\theta \quad .$$

Thus,

$$\sqrt{1 + \left(\frac{\partial r}{\partial s}\right)^2}\ ds = \sqrt{1 + \frac{\alpha^2\ \cos^2\ \theta}{\beta^2\ \sin^2\ \theta}}\ (\mp\ \beta\ \sin\ \theta)\ d\theta$$

$$= \mp\ \sqrt{\beta^2\ \sin^2\ \theta + \alpha^2\ \cos^2\ \theta}\ d\theta$$

$$= \mp\ \beta\sqrt{1 + \left(\frac{\alpha^2}{\beta^2} - 1\right)\ \cos^2\ \theta}\ d\theta$$

$$= \mp\ \beta\sqrt{1 + \left(\frac{c_i}{a_i} - 1\right)\ \cos^2\ \theta}\ d\theta \quad .$$

The area integral is then

$$A_i = \left|2\pi \int_{s_j}^{s_k} r\sqrt{1 + \left(\frac{\partial r}{\partial s}\right)^2}\ ds\right|$$

$$= 2\pi\beta \int_{\theta_1}^{\theta_2} (\bar{r} + \alpha\ \sin\ \theta)\ \sqrt{1 + \gamma\ \cos^2\ \theta}\ d\theta$$

$$= 2\pi\beta\bar{r} \int_{\theta_1}^{\theta_2} \sqrt{1 + \gamma\ \cos^2\ \theta}\ d\theta + 2\pi\alpha\beta \int_{\theta_1}^{\theta_2} \sqrt{1 + \gamma\ \cos^2\ \theta}\ \sin\ \theta\ d\theta \quad ,$$

where

$$\gamma = \frac{c_i}{a_i} - 1$$

and from Eq. (17)

$$\left(\frac{s_j - \bar{s}}{\beta}\right) = \cos\ \theta_1$$

$$\left(\frac{s_k - \bar{s}}{\beta}\right) = \cos\ \theta_2 \quad .$$

Letting $x = \cos\ \theta$, the last term of the area integral is readily solved by the method of Eq. (16):

$$2\pi\alpha\beta \int_{\theta_1}^{\theta_2} \sqrt{1 + \gamma \cos^2 \theta} \sin \theta \, d\theta = -2\pi\alpha\beta \int_{\frac{s_j - \bar{s}}{\beta}}^{\frac{s_k - \bar{s}}{\beta}} \sqrt{1 + \gamma x^2} \, dx \quad .$$

The first part of the area integral,

$$2\pi\beta\bar{r} \int_{\theta_1}^{\theta_2} \sqrt{1 + \gamma \cos^2 \theta} \, d\theta \quad ,$$

is a simple expression readily solvable by numerical integration.

V. SUMMATION OF VOLUMES AND AREAS

Once the volume and area integrals have been evaluated between the appropriate limits they must be added to determine the cell volumes and surface areas. Also, tally segments must be treated.

A. Adding Cell Volumes

The volume of a cell is simply the sum of its parts. If a bounding surface of the cell is above the cell its volume integral, $|V_i|$, between corners is added; if a surface is below the cell, its volume integral is subtracted. A surface is above the cell if the user-supplied sense of the cell to the surface is negative. Conversely, a surface is below a cell if the sense is positive. This rule is reversed for the lower branch $\left(r < \frac{-b_i}{2a_i}\right)$ of a torus.

B. Adding Surface Areas

The area of a surface is the sum of the absolute value of its parts. However, in MCNP the areas are computed twice for each surface: once when each of the cells with a positive sense with respect to the surface is calculated and once again when each of the cells with a negative sense with respect to the surface is calculated. In most cases the two areas are the same which provides a good check for the area calculation. But if any of the cells bounding the surface is not rotationally symmetric then the surface area bounding that cell is not computed invalidating the area calculation for one side of the surface. In this case only the area of the other side of the surface is used if the cells bounding that side are all rotationally symmetric. In this way rotationally symmetric surfaces bounding some non-symmetric cells may still be considered.

C. Calculation of Tally Segments

In MCNP cells and surfaces may be segmented into different geometric subregions for tallying purposes. Because the surfaces which define the tally segments are stored in the same way as cell bounding surface, calculation of the tally segments is trivial. For example, consider the geometry of Fig. 5. Cell 1 is the region of space with a negative sense to surface 1. Suppose we wish to segment the flux tally in cell 1 and across surface 2. In either case, the surface segmenting input card is

```
FSn -2 -3 .
```

This causes three volume segments to be computed:

Segment 1: volume bounded by surfaces -1 -2;

Segment 2: volume bounded by surfaces -1 2 -3;

Segment 3: volume bounded by surfaces -1 2 3.

Each of these segment volumes is computed as if it were for an actual cell; the only difference is the list of bounding surfaces.

Similarly, three surface segments are computed:

Segment 1: area of surface 1 satisfying -2 surface sense constraint;

Segment 2: area of surface 1 satisfying +2 and -3 surface sense constraint;

Segment 3: area of surface 1 satisfying +2 and +3 surface sense constraint.

VI. ACKNOWLEDGMENT

I wish to thank Ed Cashwell for his many helpful comments about this manuscript.

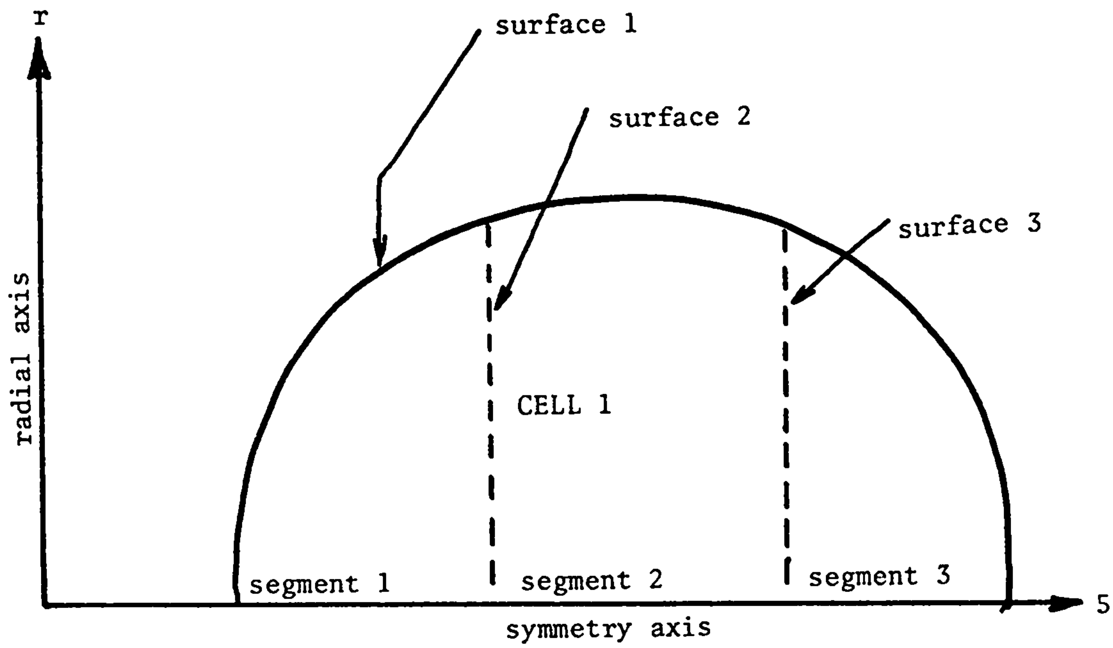

Fig. 5. Segmented Cell and Surface

REFERENCES

1. LASL Group X-6, "MCNP - A General Monte Carlo Code for Neutron and Photon Transport," Los Alamos Scientific Laboratory report, LA-7396-M, revised (November 1979).

2. B. Nobel, Applied Linear Algebra, p. 391, Prentice Hall, Englewood Cliffs, N. J. (1969).

3. Pfeiffer, Paul, Concepts of Probability Theory, p. 72, McGraw Hill, New York (1965).

Printed in the United States of America. Available from
National Technical Information Service
US Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

Microfiche $3.00

001-025	4.00	126-150	7.25	251-275	10.75	376-400	13.00	501-525	15.25
026-050	4.50	151-175	8.00	276-300	11.00	401-425	13.25	526-550	15.50
051-075	5.25	176-200	9.00	301-325	11.75	426-450	14.00	551-575	16.25
076-100	6.00	201-225	9.25	326-350	12.00	451-475	14.50	576-600	16.50
101-125	6.50	226-250	9.50	351-375	12.50	476-500	15.00	601-up	

Note: Add $2.50 for each additional 100-page increment from 601 pages up.