ACTA STEREOL 1990; 9/2: 207-218
ORIGINAL SCIENTIFIC PAPER

RANDOM ROTATIONS IN SIMULATION WITH COMPUTER 3-D RECONSTRUCTION

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ABSTRACT

Simulation is used to estimate the distribution of orientation-dependent measurements made on 3-dimensional objects. Various methods are examined for generating the orientations in which measurements are made. The different methods lead to ways of checking the distribution of the resulting rotation matrices. The most efficient in terms of the number of random variables required and the mechanism for constructing the matrix is chosen. The simulation is incorporated within an interactive user-friendly computer package referred to as GLOM. Objects are represented by their outlines on serial sections which are traced into the computer via a bitpad and reconstructed into a 3-dimensional polyhedral representation. A potato is used as an example. Caliper diameters are measured by giving the reconstructed potato an isotropically Uniform random (IUR) rotation and finding its length in a fixed direction. The distribution of caliper diameters is found and used to estimate the mean caliper diameter.

Key Words: diameter, random rotations, simulation, 3-dimensional reconstruction.

INTRODUCTION

The irregular structure of real objects can be explored by cutting them up into serial sections and reconstructing the information into a 3-dimensional computer model. The representation of the object can then be viewed as a whole or in parts in any orientation with different components highlighted, (see for example, Briarty and Jenkins, 1984). It can also be extensively measured using standard methods to find section perimeter, area and centroid (Bowyer and Woodwark, 1983) and more complex methods to estimate volume (Cook et al., 1980) and surface area (Marino et al., 1981). We can also take advantage of the computer representation to make further measurements.

Many 3-dimensional measurements, such as volume ratio can be estimated from lower dimensional probes using results from stereology (see for example, Weibel, (1980)). Some properties, however, can only be estimated from the whole object, for example overall shape and diameter (De Hoff, 1983).

The diameter of a 3-dimensional object indicates its size but can be defined in a number of different ways, for example as the average of the largest internal chord and one perpendicular to it, the average of the width in X, Y or Z directions or the diameter of a volume equivalent sphere (see, for example Rink, 1976). One that has no shape assumptions or dependence upon measuring orientation is the mean caliper diameter. This is the distance between two parallel planes tangential to the object averaged over all orientations of the planes. It can only be measured on the 3-dimensional object and is easier to carry out on a computer model than on the original object which may not be of manageable size and rigidity or on a physical model which then has to be held and measured in precise orientations. Hull and Houk (1953) did just this when computers were less available to measure random cross-sections of wire-frame models of various polyhedra. The mean caliper diameter can be estimated from the computer model by applying random rotations to the data set and recording the range of coordinates in a fixed direction (Woody et al.,1980).

There are various ways of randomly rotating the data set (Altmann, 1986). One way is to multiply the points by a rotation matrix. The matrix elements are formed from functions of random variables. The probability distribution of the random variables affects the random nature of the matrix. This in turn affects the distribution of an orientation-dependent measurement like the caliper diameter.

Simulation using random rotations was implemented in a 3-dimensional computer reconstruction package, GLOM (Coleman et al., 1988). The package performs a variety of tasks including:

(a) the control of input of outlines traced manually from suitably scaled photographs, computer assisted tomography (CAT) scans or any other representation of sections placed on a computer bitpad. The sections may contain outlines of several different components, such as body wall, backbone etc.

(b) the rationalisation of the outlines to form shapes data which have a maximum of 100 points ordered from the 9 o'clock position and which are free from artefacts such as loops and cusps. The rationalised shapes are stored as ordered lists of (X,Y) coordinates with their component category and layer number. A Z value is calculated from the layer number, the final magnification, a bitpad scaling factor and the section thickness. Thus profiles in sections are converted to shapes in layers and consist of ordered triplets of points (X,Y,Z).

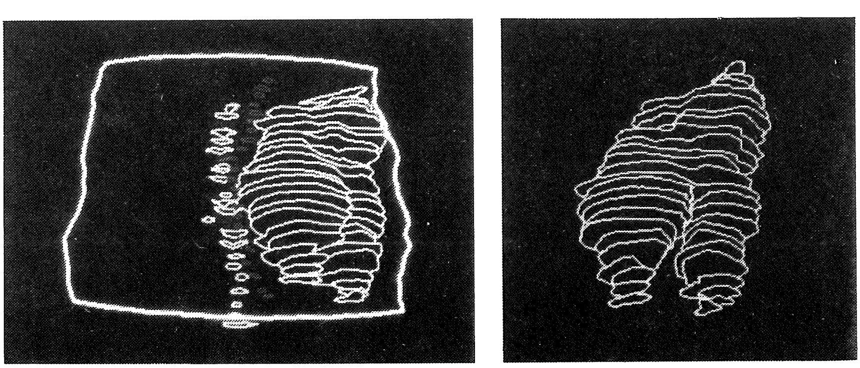

Figure 1 a) Computer reconstruction of a recurrent colonic tumour, backbone and ureter inside body wall b) the tumour in an alternative orientation.

(c) the automatic alignment of layers by minimising the distance between alignment markers, if they exist, or by superimposing centroids of key shapes. Additional adjustments can be made interactively by requesting small incremental changes in the rotation or position of one layer to make it coincide with a reference layer.

(d) the display of selected categories, layers or shapes in any colour and orientation. Figure 1a is a photograph of the 3-dimensional reconstruction of 23 CAT scan slices of a recurrent colonic tumour as displayed on a Tektronix 4107 computer graphics terminal. The outline of the body wall surrounds the tumour and outlines of the backbone and ureter are also shown. Hidden lines have been removed from the display. Figure 1b shows the same tumour rotated to show the bifurcation.

(e) the extensive mensuration of individual shapes, the whole data set or any sub-set. Measurements include those which are orientation-independent such as volume and surface area and those which depend on orientation such as caliper diameter. These are obtained by simulation with random rotations.

We consider here the estimation of the distribution of caliper diameters over random orientations. As a simple example a potato is sectioned and reconstructed into a 3-dimensional computer model. The following section discusses ways to construct rotation matrices. An efficient method is selected and incorporated into the interactive computer graphics environment and results using the potato are presented and discussed.

MATERIALS AND METHODS

A sample of orientations in which measurements are made can be obtained by taking small increments in the orientation variables, for example θ and ϕ in spherical polar coordinates. Hull and Houk (1953) used carefully chosen representative orientations to obtain the distribution of cross-sectional areas in wire-frame models of various polyhedra. In general, randomly chosen orientations give a more reliable coverage.

There are many criteria of randomness leading to different distributions of the orientation variables and the arbitrariness of the choice can lead to paradoxes, such as Bertrand's paradox (see, for example Weibel, 1980). The criterion of randomness chosen must be appropriate for the use to which it is put. The principle of invariance is expressed by Mackenzie (1958) as the requirement that the result of a calculation is unchanged or invariant for any displacement of the whole figure. Here, the measurements of interest are distances which are invariant and thus it seems reasonable to choose a criterion of randomness which is similarly invariant.

Three-dimensional invariant directions are selected such that if they were emanating from the centre of a unit sphere, they would intersect the surface of the sphere at points which are Uniformly distributed over the surface of the sphere. This is referred to as isotropic Uniform randomness (IUR). Kendall and Moran (1963) note that this is the only probability density function for random orientations which is invariant. The mean caliper diameter is defined over IUR orientations.

Rotation matrices can be generated a) by considering rotation about a random axis by a random angle, b) by specifying 3 random vectors and combining them into a rotation matrix or c) by creating an orthogonal matrix from one random vector and concatenating it with a rotation about a fixed axis by a random angle. These different methods provide ways of checking the distribution of the resulting matrices. The number of random variables required for each method varies as does the mechanism of generating the random variables so that the rotations are IUR. This is an important consideration where simulation is concerned.

The IUR criterion indicates how random directions can be generated for the rotation axis. The probability of the random line hitting a patch δs on the unit sphere surface must be $\delta s/4\pi$. In spherical polar coordinates the patch is approximately of length $\delta\theta$ and width $\sin\theta\delta\phi$ as shown in Figure 2, giving $\delta s = \sin\theta\delta\phi\delta\theta$.

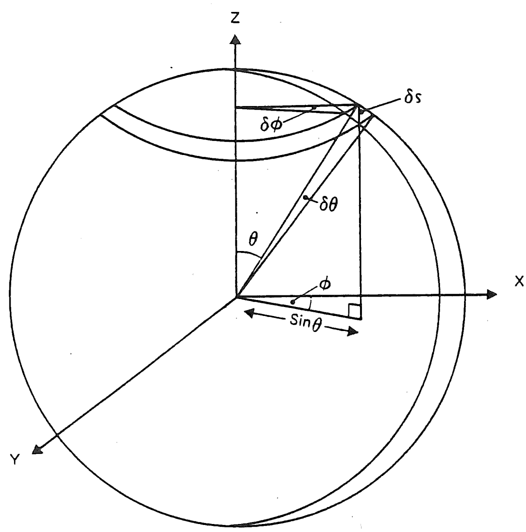

Figure 2 Probability element for an isotropic Uniform random direction.

Thus, the element of probability is

$$\sin\theta\delta\phi\delta\theta/(4\pi) \qquad 0 \le \theta \le \pi, \quad 0 \le \phi \le 2\pi$$

This represents a joint probability density function of independent variables, θ and ϕ with $f(\theta) = (1/2)\sin\theta$ and $g(\phi) = 1/(2\pi)$.
The distribution functions are

$$\int_0^\theta (1/2)\sin\theta d\theta = (1-\cos\theta)/2 \qquad \text{and} \qquad \int_0^\phi 1/(2\pi)d\phi = \phi/(2\pi)$$

Distribution functions are Uniformly distributed on (0,1) and so suitable random values of θ and ϕ may be generated by selecting Uniform random variables U_i and U_j from (0,1), and setting $U_i = (1-\cos\theta)/2$ and $U_j = \phi/(2\pi)$. From these, $1-2U_i = \cos\theta$ which is equivalent to equating $\cos\theta$ to U_i and hence $\theta = \arccos U_i$ and similarly, $\phi = 2\pi U_j$.

The equations of the direction cosines l,m,n of the random line depend upon the way θ and ϕ are defined with respect to Cartesian X, Y and Z axes. Figure 2 shows one arrangement. In this case, for the angle, XA, between the line and the X axis

$$l = \cos XA = \sin\theta\cos\phi$$

similarly for the angle, YA, with the Y axis

$$m = \cos YA = \sin\theta\sin\phi$$

and for the angle, ZA, with the Z axis

$$n = \cos ZA = \cos\theta$$

We now consider the choice of angle V to ensure that the rotation is IUR. Kendall and Moran (1963), following the work of Deltheil (1926), show that the probability element must be $(1/\pi)\sin^2(V/2)\,dV$, leading to the distribution function, F(V),

$$F(V) = \int_0^V (1/\pi)\sin^2(V/2)dV = (2\pi)^{-1}(V-\sin V)$$

Thus V is found by selecting a random variable, U_k, from the Uniform (0,1) distribution and solving $V - \sin V = 2\pi U_k$. Note that V is not chosen directly from the Uniform distribution.

The direction cosines l,m,n of the rotation axis and the angle, V, are now combined into the random rotation matrix,

$$\begin{bmatrix} l^2A+\cos V & lmA-n\sin V & lnA+m\sin V \\ lmA+n\sin V & m^2A+\cos V & mnA-l\sin V \\ lnA-m\sin V & mnA+l\sin V & n^2A+\cos V \end{bmatrix} \qquad (1)$$

where A = 1-cosV. Thus 3 independent random variables are required to find (1) but solving for V requires extra work as it involves an intrinsic equation in V.

The trace of the rotation matrix is Y = 1+2cosV. Kendall and Moran (1963) show that the probability density of W = cosV is proportional to

$$f(W)dW = 2\sin^2(V/2)dV = (1-\cos V)dV$$

and from this the distribution function of the trace, Y, can be obtained as

$$G(Y) = (1/\pi)(\sqrt{((3-Y)(Y+1)/2)} - \arccos((Y-1)/2)+\pi).$$

The traces of IUR matrices should have this distribution however they were constructed and so this provides a check that matrices used in simulation have the required distribution. This is only a check as it is possible for the traces of other types of matrices to have this distribution.

Random rotation matrices can also be generated by choosing three independent random vectors and combining them into an orthogonal 3x3 matrix (Kendall and Moran, 1963).

The independent random vectors, r, can be constructed from random angles via direction cosines as above giving r = (l,m,n), or they can be taken directly proportional to three independent Normal variables, X_1, X_2, X_3, with mean zero and unit variance,

$$\underline{r} = (X_1/C,\ X_2/C,\ X_3/C) \quad \text{where } C = \Sigma X_i^2$$

Choosing a vector in this way is equivalent to choosing a point with joint probability density function

$$(2\pi)^{-3/2}\exp(-\Sigma X_i^2 /2)$$

The equation $\Sigma X_i^2 = C$ defines the surface of a sphere. The joint probability density function

$$(2\pi)^{-3/2}\exp(-C^2/2)$$

is constant and so the direction of the vector (X_1, X_2, X_3) is Uniformly distributed on the surface of a sphere and IUR as required (Mackenzie and Thomson, 1957).

Random vectors can be combined into an orthogonal rotation matrix by vector algebra. If $\underline{a}$ and $\underline{b}$ are two independent random vectors, then the vector perpendicular to $\underline{a}$ in the plane defined by $\underline{a}$ and $\underline{b}$ is given by

$$\underline{c} = \underline{b} - \underline{a}(\underline{a}.\underline{b})$$

The vector product of $\underline{a}$ and $\underline{c}$ gives a third vector mutually perpendicular to $\underline{a}$ and $\underline{c}$

$$\underline{d} = \underline{a} \times \underline{c}$$

and the three vectors $\underline{a}$, $\underline{c}$ and $\underline{d}$ can be used as the columns or rows in a random orthogonal rotation matrix. This method requires the generation of 6 random variables per matrix.

The construction using Normal variables can be used to show that each element in the matrix is Uniformly distributed (Cramer, 1946, p240). The variable

$$Z = X_j / \surd(\Sigma X_i^2/n), \quad 0 < Z < \surd n$$

has a modified t distribution

$$f(Z) = \frac{\Gamma(n/2).(1-Z^2/n)^{(n-3)/2}}{\surd(n\pi).\Gamma((n-1)/2)}$$

When n=3 this reduces to the Uniform distribution.

$$f(Z) = 1/(2\surd 3) \quad 0 < Z < \surd 3$$

In rotation matrices, the variable of interest is $\pm Z/\surd 3$. Thus each element in the rotation matrix is Uniformly distributed on (-1,1). The elements are not independent and only 3 are needed to specify the matrix (Jeffreys and Jeffreys, 1946, p51).

The construction of the rotation matrix can also be interpreted in a different way. The direction cosines of one vector make up the first row or column of the matrix directly. Two other orthogonal unit vectors are then formed from the sines and cosines and make up the rest of the matrix. For example,

$$\begin{bmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ -\cos\theta\cos\phi & -\cos\theta\sin\phi & \sin\theta \\ \sin\phi & -\cos\phi & 0 \end{bmatrix}$$

Although this matrix is orthogonal it only provides rotation in two planes. Full rotation is attained by choosing a third angle, α, Uniformly on $(0,2\pi)$ and multiplying the matrix for rotation about the X axis by this angle, (see below) by the above matrix. The resulting rotation matrix is

$$\begin{bmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ -\cos\theta\cos\phi\cos\alpha+\sin\phi\sin\alpha & -\cos\theta\sin\phi\cos\alpha-\cos\phi\sin\alpha & \sin\theta\cos\alpha \\ \cos\theta\cos\phi\sin\alpha+\sin\phi\cos\alpha & \cos\theta\sin\phi\sin\alpha-\cos\phi\cos\alpha & -\sin\theta\sin\alpha \end{bmatrix} \quad (2)$$

This construction only requires the generation of 3 random variables per matrix. It is the most efficient of the 3 methods of constructing IUR rotation matrices discussed above and it can also be used to express the rotation matrix as a rotation about the X, Y and Z axes.

In the three-dimensional reconstruction package, GLOM, data can be displayed in any orientation by specifying angles of rotation about the X, Y and Z axes. This method of requesting views is preferred to the alternative of giving a rotation axis and angle as it is easier to visualise. As a further aid, rotations can be specified in any of the orders XYZ, ZYX and XZX. These angles are referred to by names such as pitch, tilt and roll in commercial 3-dimensional reconstruction packages, for example VIDEOPLAN by Kontron Bildanalyse GMBH, Breslauer Str. 2, D-8057 Eching/Munich, FRG.

The three methods of constructing IUR rotations discussed above involve the generation of 3 random variables and solving 1 equation, 6 random variables and 3 random variables respectively. The last method is the most efficient and can also be adapted to take the same form as rotations requested by the user.

A 3-dimensional rotation of a point (x,y,z) by an angle, X, about the X axis is performed by

$$(x,y,z)\begin{bmatrix}1 & 0 & 0\\ 0 & \cos X & \sin X\\ 0 & -\sin X & \cos X\end{bmatrix} = (x',y',z')$$

in a left-handed Cartesian coordinate system (see, for example, Newman and Sproull, 1979) where a positive angle causes a clockwise rotation as viewed from the positive axis. Rotation about the Y axis and the Z axis are given by the matrices

$$\begin{bmatrix}\cos Y & 0 & -\sin Y\\ 0 & 1 & 0\\ \sin Y & 0 & \cos Y\end{bmatrix} \quad \text{and} \quad \begin{bmatrix}\cos Z & \sin Z & 0\\ -\sin Z & \cos Z & 0\\ 0 & 0 & 1\end{bmatrix}$$

respectively.

A 3-dimensional rotation about the X, then Y, then Z axes is effected by the matrix multiplication of the simple rotation matrices and results in the matrix (3) which is of a similar form to (2) above.

$$\begin{bmatrix}\cos Y.\cos Z & \cos Y.\sin Z & -\sin Y\\ \sin X.\sin Y.\cos Z-\cos X.\sin Z & \sin X.\sin Y.\sin Z+\cos X.\cos Z & \sin X.\cos Y\\ \cos X.\sin Y.\cos Z+\sin X.\sin Z & \cos X.\sin Y.\sin Z-\sin X.\cos Z & \cos X.\cos Y\end{bmatrix} \qquad (3)$$

There are six permutations of X,Y and Z rotations and a further six of the form X then Z then X again which will all produce a 3-dimensional rotation. Each composite rotation matrix has one element with a single trigonometric ratio in the row corresponding to the first rotation axis (X=1, Y=2, Z=3) and the column corresponding to the last rotation axis. The particular trigonometric ratio is the sine of the middle rotation angle for a rotation about 3 different axes and the cosine of this angle if the rotation was about only 2 axes, that is of the XZX type.

The construction of the random matrix, (2), can be made to comply with any of the 12 permutations by altering the order of the initial vector, placing it in a different row or column of the matrix and relating θ, ϕ and α to the X, Y and Z angles. For example, (2) corresponds to (3) if

$X = \alpha + \pi/2$

$Y = \theta - \pi/2$

and $Z = \phi$.

Thus, the rotation matrix for simulation can be constructed in the same way as that for chosen rotations in whichever order they are defined. Two of the X,Y or Z rotation angles are taken as Uniform random variables, as is the trigonometric function of the third angle. As each element in the rotation matrix must be Uniformly distributed, the nature and position of the single trigonometric function in the rotation matrix dictates which of the trigonometric functions must be Uniformly distributed to obtain the correct orientation distribution.

Random XYZ rotations were generated by considering the composite matrix for an XYZ rotation ((3)above) and choosing the X and Z angles from the Uniform $(0,2\pi)$ distribution and sinY from the Uniform (-1,1) distribution. The trigonometric ratios were entered into the rotation matrix. A sample of 150 random matrices was generated in this way and the goodness of fit of the elements to the Uniform distribution was assessed using the chi-square test.

To demonstrate the application of simulation with random rotations, a potato was chosen for 3-dimensional reconstruction as it is an example of a real object of irregular shape and manageable size. Figure 3a shows the potato and its diameter measured in an arbitrary direction. The potato was cut into 9 serial sections in a plane perpendicular to the measured diameter. The outlines on serial sections were copied onto paper, traced on a computer bitpad and stored in the computer. The section thickness was calculated by dividing the measured diameter by the number of sections and Z values were allocated to each outline. Figure 3b is a photograph of the reconstructed potato.

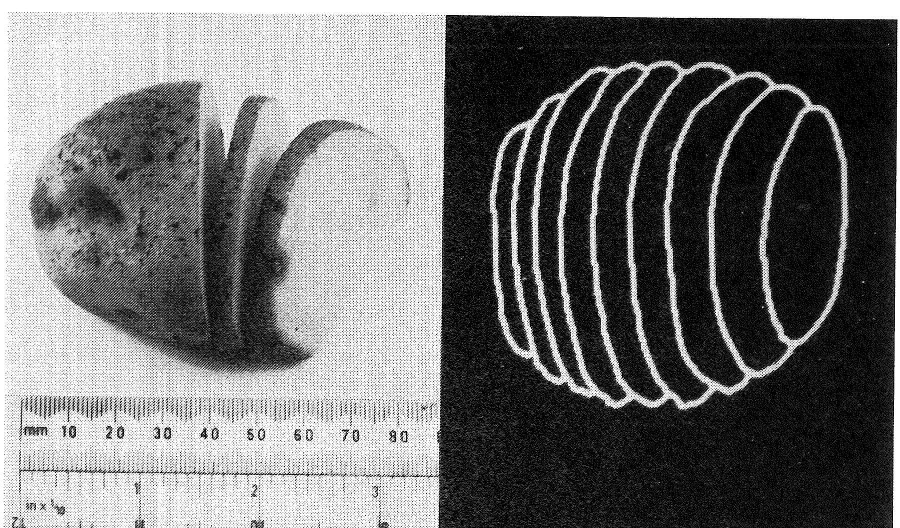

Figure 3 a) The potato being measured and sectioned b) computer reconstruction of 9 serial sections through potato.

A sample of 500 random matrices was generated and applied to the potato data set. The range of X values was found for each rotation and the frequency distribution and summary statistics of the simulated caliper diameters were found.

RESULTS

From the initial sample of 150 random rotation matrices, the goodness of fit of the matrix elements to the Uniform distribution was assessed using the chi-square test. The range of chi-square values for the 9 elements was 3.8 to 13.5 (on 9 degrees of freedom). Although these random variables are difficult to assess formally as they are not independent, they do not indicate any serious discrepancy. The trace of the matrices was similarly compared with the theoretical distribution and the value of chi-square with 7 degrees of freedom was 11.3 which shows no lack of fit.

The frequency distribution and summary statistics of the caliper diameters generated by the sample of 500 random matrices is given in Table 1.

Table 1 Frequency distribution of 500 randomly-orientated caliper diameters of the reconstructed potato.

Caliper diameter (mm)	Frequency
44-45	3
45-46	8
46-47	16
47-48	23
48-49	29
49-50	39
50-51	44
51-52	41
52-53	46
53-54	52
54-55	51
55-56	43
56-57	45
57-58	28
58-59	30
59-60	2
Total	500

mean = 52.78mm
standard deviation = 3.42mm
standard error of the mean = .0068mm
minimum = 44.52mm
maximum = 59.10mm

The caliper diameters range from 45.5mm to 59.1 mm. The standard deviation is large as the diameters include the longest and the shortest. The standard error of the mean can be made as small as required by increasing the number of simulated measurements.

The corresponding histogram is in Figure 4. The distribution is slightly skewed to the left reflecting the assymetric shape of the potato.

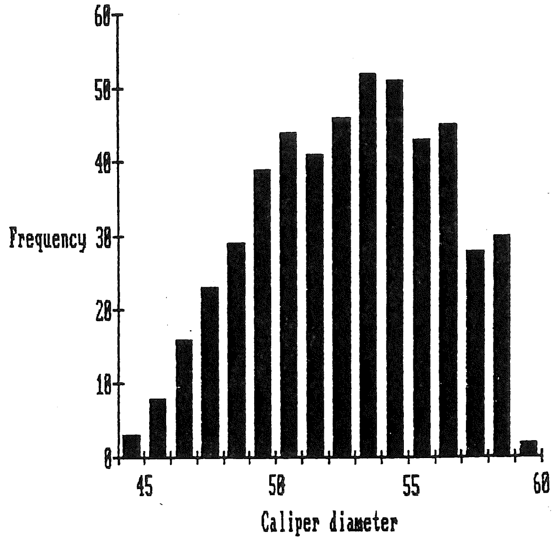

Figure 4 Histogram of 500 randomly-orientated caliper diameters of the reconstructed potato.

DISCUSSION

The 3-dimensional reconstruction gives a polyhedral approximation to any real structure. The closeness of the approximation depends upon the number of sections originally taken and the number of points used to represent them.

The advantage of using IUR rotations in which to measure caliper diameters is that their distribution corresponds to that of caliper diameters of randomly-orientated objects, for example, when cutting through rock or in computer-assisted tomography (CAT) scans. The results of the simulation can be compared with those obtained by slicing through a large number of separate structures with a single section. The results can also be used in formulae for which IUR is the standard. For example, the mean caliper diameter estimated from IUR rotations is used to predict the number of particles per unit volume from the number of profiles per unit area. It is also used in shape parameters having a value which can be calculated for many analytic objects (Weibel, 1980).

Although there are various methods for generating rotations, they are not all equally efficient for use in simulation. An interesting alternative uses quaternions (Martin, 1985) but although this method is efficient for computing compound rotations it requires more operations to rotate each point. By making the random rotations compatible with user-chosen orientations the interactive nature of the computer package can be maintained so that any simulated measurement can be examined by displaying the object on the computer screen rotated to the exact orientation.

The observed distribution of orientation-dependent measurements can be compared with any suitable theoretical model to aid interpretation of the structure. For example, caliper diameters of hypothetical ellipsoids, cylinders or rectangles can be generated.

The accuracy of the empirical distribution obtained from a sample of IUR rotations increases with the number of simulations used but also depends upon the simplicity of the objects involved. Woody et al. (1980) make 500 measurements to estimate the mean caliper diameter of the polyhedral approximation to a sphere. Warren and Durand (1981) find 5,000 to 10,000 random sections in their analysis of shape parameters for various analytic solids including rods and tetrakaidecahedra. Warren and Naumovich (1977) calculate at least 10,000 random intercepts through ellipsoids, rounded cubes and prisms.

Simulation with random rotations provides an interesting and versatile way to improve the evaluation of any object represented by serial sections. GLOM has been used to analyse 3-dimensional structures from light microscope slides of kidney biopsies, electron microscope sections of cockroach brains, CAT scans of human tumours and mathematically-defined outlines representing the region that a person can reach from a restricted seated position.

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