International Tables for Crystallography (2006). Vol. B, Section 3.3.1.2.1, pp. 361–363.

Hardware systems which use true floating-point representations have less need of homogeneous coordinates and for these N and W may normally be set to unity.

3.3.1.1.3. *Notation*

In this chapter the conventions of matrix algebra will be adhered to except where it is convenient to show operations on elements of vectors, matrices and tensors, where a subscript notation will be used with a modified summation convention in which summation is over lower-case subscripts *only*. Thus the equation

$$x_I = A_{Ij}X_j$$

is to be read 'For any I, x_I is $A_{Ij}X_j$ summed over j'.

Subscripts using the letter i or later in the alphabet will relate to the usual three dimensions and imply a three-term summation. Subscripts a to h are not necessarily so limited, and, in particular, the subscript a is used to imply summation over atoms of which there may be an arbitrary number.

We shall use the superscript T to denote a transpose, and also use the Kronecker delta, δ_{IJ}, which is 1 if $I = J$ and zero otherwise, and the tensor ε_{IJK} which is 1 if I, J and K are a cyclic permutation of 1, 2, 3, -1 if an anticyclic permutation, and zero otherwise.

$$\varepsilon_{IJK} = (I - J)(J - K)(K - I)/2 \quad 1 \leq I, J, K \leq 3.$$

A useful identity is then

$$\varepsilon_{iJK}\varepsilon_{iLM} = \delta_{JL}\delta_{KM} - \delta_{JM}\delta_{KL}.$$

Single modulus signs surrounding the symbol for a square matrix denote its determinant, and around a vector denote its length.

The symbol $\simeq$ is defined in the previous section.

3.3.1.1.4. *Standards*

The sections of this chapter concerned with graphics are primarily concerned with the mathematical aspects of graphics programming as they confront the applications programmer. The implementations outlined in the final section have all, so far as the author is aware, been developed *ab initio* by their inventors to deal with these aspects using their own and unrelated techniques and protocols. It is clear, however, that standards are now emerging, and it is to be hoped that future developments in applications software will handle the graphics aspects through one or other of these standards.

First among these standards is the Graphical Kernel System, GKS, defined in *American National Standards Institute, American National Standard for Information Processing Systems – Computer Graphics – Graphical Kernel System (GKS) Functional Description* (1985) and described and illustrated by Hopgood *et al.* (1986) and Enderle *et al*. (1984). GKS became a full International Standards Organization (ISO) standard in 1985, and its purpose is to standardize the interface between application software and the graphics system, thus enhancing portability of software. Specifications for Fortran, Pascal and Ada formulations are at an advanced stage of development. Its value to crystallographers is limited by the fact that it is only two-dimensional. A three-dimensional extension known as GKS-3D, defined in *International Standards Organisation, International Standard Information Processing Systems – Computer Graphics – Graphical Kernel System for Three Dimensions (GKS-3D), Functional Description* (1988) became an ISO standard in 1988. Perhaps of greatest interest to crystallographers, however, is the Programmers' Hierarchical Interactive Graphics System (PHIGS) (Brown, 1985; Abi-Ezzi & Bunshaft, 1986) since this allows hierarchical segmentation of picture content to exist in both the applications software and the graphics device in a related manner, which GKS does not. Some graphics devices now available support this type of working and its exploitation indicates the choice of PHIGS. Furthermore, Fortran implementations of GKS and GKS-3D require points to be stored in arrays dimensioned as *X*(*N*), *Y*(*N*), *Z*(*N*) which may be equivalenced (in the Fortran sense) to *XYZ*(*N*, 3) but not to *XYZ*(3, *N*), which may not be convenient. PHIGS also became an International Standard in 1988: *American National Standards Institute, American National Standard for Information Processing Systems – Computer Graphics – Programmer's Hierarchical Graphics System (PHIGS) Functional Description, Archive File Format, Clear-Text Encoding of Archive File* (1988). PHIGS has also been extended to support the capability of raster-graphics machines to represent reflections, shadows, see-through effects *etc.* in a version known as PHIGS+ (van Dam, 1988).

Increasingly, manufacturers of graphics equipment are orienting their products towards one or other of these standards. While these standards are not the subject of this chapter it is recommended that they be studied before investing in equipment.

In addition to these standards, related standards are evolving under the auspices of the ISO for defining images in a file-storage, or metafile, form, and for the interface between the device-independent and device-dependent parts of a graphics package. Arnold & Bono (1988) describe the ANSI and ISO Computer Graphics Metafile standard which provides for the definition of (two-dimensional) images. The definition of three-dimensional scenes requires the use of (PHIGS) archive files.

3.3.1.2. *Orthogonal (or rotation) matrices*

It is a basic requirement for any graphics or molecular-modelling system to be able to control and manipulate the orientation of the structures involved and this is achieved using orthogonal matrices which are the subject of these sections.

3.3.1.2.1. *General form*

If a vector $\mathbf{v}$ is expressed in terms of its components resolved onto an axial set of vectors $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ which are of unit length and mutually perpendicular and right handed in the sense that $(\mathbf{X} \times \mathbf{Y}) \cdot \mathbf{Z} = +1$, and if these components are v_I, and if a second set of axes $\mathbf{X}'$, $\mathbf{Y}'$, $\mathbf{Z}'$ is similarly established, with the same origin and chirality, and if $\mathbf{v}$ has components v'_I on these axes then

$$v'_I = a_{Ij}v_j,$$

in which a_{IJ} is the cosine of the angle between the ith primed axis and the jth unprimed axis. Evidently the elements a_{IJ} comprise a matrix $\boldsymbol{R}$, such that any row represents one of the primed axial vectors, such as $\mathbf{X}'$, expressed as components on the unprimed axes, and each column represents one of the unprimed axial vectors expressed as components on the primed axes. It follows that $\boldsymbol{R}^T = \boldsymbol{R}^{-1}$ since elements of the product $\boldsymbol{R}^T\boldsymbol{R}$ are scalar products among perpendicular unit vectors.

A real matrix whose transpose equals its inverse is said to be *orthogonal.*

Since $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$ can simultaneously be superimposed on $\mathbf{X}'$, $\mathbf{Y}'$ and $\mathbf{Z}'$ without deformation or change of scale the relationship is one of rotation, and orthogonal matrices are often referred to as rotation matrices. The operation of replacing the vector $\mathbf{v}$ by $\boldsymbol{R}\mathbf{v}$ corresponds to rotating the axes from the unprimed to the primed set with $\mathbf{v}$ itself unchanged. Equally, the same operation corresponds to retaining fixed axes and rotating the vector in the opposite sense. The second interpretation is the one more frequently helpful since conceptually it corresponds more closely to rotational operations on objects, and it is primarily in this sense that the following is written.

If three vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ form the edges of a parallelepiped, then its volume V is

$$V = \mathbf{u}\cdot(\mathbf{v}\times\mathbf{w}) = \varepsilon_{ijk}u_i v_j w_k$$

and if these vectors are transformed by the matrix $\boldsymbol{R}$ as above, then the transformed volume V' is

$$V' = \varepsilon_{lmn}u'_l v'_m w'_n = \varepsilon_{lmn}a_{li}a_{mj}a_{nk}u_i v_j w_k.$$

But the determinant of $\boldsymbol{R}$ is given by

$$|\boldsymbol{R}|\varepsilon_{IJK} = \varepsilon_{lmn}a_{lI}a_{mJ}a_{nK}$$

so that

$$V' = |\boldsymbol{R}|V$$

and the determinant of $\boldsymbol{R}$ must therefore be +1 for a transformation which is a pure rotation. Nevertheless orthogonal matrices with determinant -1 exist though these do not describe a pure rotation. They may always be described as the product of a pure rotation and inversion through the origin and are referred to here as improper rotations. In what follows all references to orthogonal matrices refer to those with positive determinant only, unless stated otherwise.

An important general form of an orthogonal matrix in three dimensions was derived as equation (1.1.4.32) and is

$$\boldsymbol{R} = \begin{pmatrix} l^2+(m^2+n^2)\cos\theta & lm(1-\cos\theta)-n\sin\theta & nl(1-\cos\theta)+m\sin\theta \\ lm(1-\cos\theta)+n\sin\theta & m^2+(n^2+l^2)\cos\theta & mn(1-\cos\theta)-l\sin\theta \\ nl(1-\cos\theta)-m\sin\theta & mn(1-\cos\theta)+l\sin\theta & n^2+(l^2+m^2)\cos\theta \end{pmatrix}$$

or

$$R_{IJ} = (1-\cos\theta)l_I l_J + \delta_{IJ}\cos\theta - \varepsilon_{IJk}l_k\sin\theta,$$

in which l, m and n are the direction cosines of the axis of rotation (which are the same when referred to either set of axes under either interpretation) and θ is the angle of rotation. In this form, and with $\boldsymbol{R}$ operating on column vectors on the right, the sign of θ is such that, when viewed along the rotation axis *from* the origin *towards* the point lmn, the object is rotated clockwise for positive θ with a fixed right-handed axial system. If, under the same viewing conditions, the axes are to be rotated clockwise through θ with the object fixed then the components of vectors in the object, on the new axes, are given by $\boldsymbol{R}$ with the same lmn and with θ negated. This is the transpose of $\boldsymbol{R}$, and if $\boldsymbol{R}$ is constructed from a product, as below, then each factor matrix in the product must be transposed and their order reversed to achieve this. Note that if, for a given rotation, the viewing direction from the origin is reversed, l, m, n and θ are all reversed and the matrix is unchanged.

Any rotation about a reference axis such that two of the direction cosines are zero is termed a *primitive rotation*, and it is frequently a requirement to generate or to interpret a general rotation as a product of primitive rotations.

A second important general form is based on Eulerian angles and is the product of three such primitives. It is

$$\boldsymbol{R} = \begin{pmatrix} \cos\varphi_3 & -\sin\varphi_3 & 0 \\ \sin\varphi_3 & \cos\varphi_3 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \cos\varphi_2 & 0 & \sin\varphi_2 \\ 0 & 1 & 0 \\ -\sin\varphi_2 & 0 & \cos\varphi_2 \end{pmatrix}\begin{pmatrix} \cos\varphi_1 & -\sin\varphi_1 & 0 \\ \sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} (\cos\varphi_3\cos\varphi_2\cos\varphi_1 - \sin\varphi_3\sin\varphi_1) & -(\cos\varphi_3\cos\varphi_2\sin\varphi_1 + \sin\varphi_3\cos\varphi_1) & \cos\varphi_3\sin\varphi_2 \\ (\sin\varphi_3\cos\varphi_2\cos\varphi_1 + \cos\varphi_3\sin\varphi_1) & (-\sin\varphi_3\cos\varphi_2\sin\varphi_1 + \cos\varphi_3\cos\varphi_1) & \sin\varphi_3\sin\varphi_2 \\ -\sin\varphi_2\cos\varphi_1 & \sin\varphi_2\sin\varphi_1 & \cos\varphi_2 \end{pmatrix}$$

which is commonly employed in four-circle diffractometers for which $\varphi = -\varphi_1$, $\chi = \varphi_2$ and $\omega = -\varphi_3$. In terms of the fixed-axes–moving-object conceptualization this corresponds to a rotation φ_1 about Z followed by φ_2 about Y followed by φ_3 about Z. In the familiar diffractometer example, when $\chi = 0$ the φ and ω axes are both vertical and equivalent. If φ is altered first, then the χ axis is still in the direction of a fixed Y axis, but if ω is altered first it is not. Since all angles are to be rotations about fixed axes to describe a rotating object it follows that it is φ rather than ω which corresponds to φ_1. In general, when rotating parts are mounted on rotating parts the rotation closest to the moved object must be applied first, forming the right-most factor in any multiple transformation, with the rotation closest to the fixed part as the left-most factor, assuming data supplied as column vectors on the right.

Given an orthogonal matrix, in either numerical or analytical form, it may be required to discover θ and the axis of rotation, or to factorize it as a product of primitives. From the first form we see that the vector

$$v_I = \varepsilon_{Ijk}a_{jk},$$

consisting of the antisymmetric part of $\boldsymbol{R}$, has elements $-2\sin\theta$ times the direction cosines l, m, n, which establishes the direction immediately, and normalization using $l^2+m^2+n^2=1$ determines $\sin\theta$. Furthermore, the trace is $1+2\cos\theta$ so that the quadrant of θ is also fixed. This method fails, however, if the matrix is symmetrical, which occurs if $\theta=\pi$. In this case only the direction of the axis is required, which is given by

$$l:m:n = (a_{23})^{-1}:(a_{31})^{-1}:(a_{12})^{-1}$$

for non-zero elements, or $l = \sqrt{\tfrac{1}{2}(a_{11}+1)}$ *etc.*, with the signs chosen to satisfy $a_{12} = 2lm$ *etc.*

The Eulerian form may be factorized by noting that $\tan\varphi_1 = -a_{32}/a_{31}$, $\tan\varphi_3 = a_{23}/a_{13}$, $\cos\varphi_2 = a_{33}$. There is then freedom to choose the sign of $\sin\varphi_2$, but the choice then fixes the quadrants of φ_1 and φ_3 through the elements in the last row and column, and the primitives may then be constructed. These expressions for φ_1 and φ_3 fail if $\sin\varphi_2 = 0$, in which case the rotation reduces to a primitive rotation about Z with angle $(\varphi_1+\varphi_3), \varphi_2 = 0$, or $(\varphi_3-\varphi_1), \varphi_2 = \pi$.

Eulerian angles are unlikely to be the best choice of primitive angles unless they are directly related to the parameters of a system, as with the diffractometer. It is often more important that the changes to primitive angles should be quasi-linearly related to θ for any small rotations, which is not the case with Eulerian angles when the required rotation axis is close to the X axis. In such a case linearized techniques for solving for the primitive angles will fail. Furthermore, if the required rotation is about Z only $(\varphi_1+\varphi_3)$ is determinate.

Quasi-linear relationships between θ and the primitive rotations arise if the primitives are one each about X, Y and Z. Any order of the three factors may be chosen, but the choice must then be adhered to since these factors do not commute. For sufficiently small rotations the primitive rotations are then $l\theta$, $m\theta$ and $n\theta$, whilst for larger θ linearized iterative techniques for finding the primitive rotations are likely to be convergent and well conditioned.

The three-dimensional space of the angles φ_1, φ_2 and φ_3 in either case is non-linearly related to θ. In the Eulerian case the worst non-linearities occur at the origin of φ-space. Equally severe non-linearities occur in the quasi-linear case also but are 90° away from the origin and less likely to be troublesome.

Neither of the foregoing general forms of orthogonal matrix has ideally convenient properties. The first is inconvenient because it uses four non-equivalent variables l, m, n and θ, with a linking equation involving l, m and n, so that they cannot be treated as independent variables for analytical purposes. The second form (the product of primitives) is not ideal because the three angles, though independent, are not equivalent, the non-equivalence arising from the non-commutation of the primitive factors. In the remainder of this section we give two further forms of orthogonal matrix which each use three variables which are independent and strictly equivalent, and a third form using four whose squares sum to unity.

The first of these is based on the diagonal and uses the three independent variables p, q, r, from which we construct the auxiliary variables

$$P = \pm\sqrt{1+p-q-r},\ Q = \pm\sqrt{1-p+q-r},$$
$$R = \pm\sqrt{1-p-q+r},\ S = \pm\sqrt{1+p+q+r},$$

then

$$\boldsymbol{R} = \begin{pmatrix} p & \tfrac{1}{2}[PQ-RS] & \tfrac{1}{2}[PR+QS] \\ \tfrac{1}{2}[PQ+RS] & q & \tfrac{1}{2}[QR-PS] \\ \tfrac{1}{2}[PR-QS] & \tfrac{1}{2}[QR+PS] & r \end{pmatrix}$$

is orthogonal with positive determinant for any of the sixteen sign combinations. The signs of P, Q, R and S are, respectively, the signs of the direction cosines of the rotation axis and of $\sin\theta$. Using also $T = \sqrt{4-S^2}$, which may be deemed positive without loss of generality,

$$l = P/T, m = Q/T, n = R/T,\ \sin\theta = ST/2,$$
$$\cos\theta = 1 - T^2/2 = S^2/2 - 1.$$

Although p, q and r are independent, the point $[pqr]$ is bound, by the requirement that P, Q, R and S be real, to lie within a tetrahedron whose vertices are the points $[111]$, $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$ and $[\bar{1}\bar{1}1]$, corresponding to the identity and to 180° rotations about each of the axes. The facts that the identity occurs at a vertex of the feasible region and that $(1-\cos\theta)$, rather than $\sin\theta$, is linear on p, q and r in this vicinity make this form suitable only for substantial rotations.

The second form consists in defining a rotation vector $\mathbf{r}$ with components u, v, w such that $u = lt$, $v = mt$, $w = nt$ with $t = \tan(\theta/2)$ and $\mathbf{r}\cdot\mathbf{r} = t^2$. Then the matrix

$$\boldsymbol{R} = \begin{pmatrix} \dfrac{1+u^2-v^2-w^2}{1+t^2} & \dfrac{2(uv-w)}{1+t^2} & \dfrac{2(uw+v)}{1+t^2} \\ \dfrac{2(uv+w)}{1+t^2} & \dfrac{1-u^2+v^2-w^2}{1+t^2} & \dfrac{2(vw-u)}{1+t^2} \\ \dfrac{2(uw-v)}{1+t^2} & \dfrac{2(vw+u)}{1+t^2} & \dfrac{1-u^2-v^2+w^2}{1+t^2} \end{pmatrix}$$
$$R_{IJ} = (1+t^2)^{-1}[\delta_{IJ}(1-u_k u_k) + 2(u_I u_J - \varepsilon_{IJl} u_l)]$$

is orthogonal and the variables u, v, w are independent, equivalent and unbounded, and, unlike the previous form, small rotations are quasi-linear on these variables. As examples, $\mathbf{r} = [100]$ gives 90° about X, $\mathbf{r} = [111]$ gives 120° about [111].

$\boldsymbol{R}$ then transforms a vector $\mathbf{d}$ according to

$$\boldsymbol{R}\mathbf{d} = \mathbf{d} + \frac{2}{1+t^2}\{(\mathbf{r}\times\mathbf{d}) + [\mathbf{r}\times(\mathbf{r}\times\mathbf{d})]\}.$$

Multiplying two such matrices together allows us to establish the manner in which the rotation vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ combine.

$$\mathbf{r} = \frac{\mathbf{r}_2 + \mathbf{r}_1 + \mathbf{r}_2\times\mathbf{r}_1}{1-\mathbf{r}_2\cdot\mathbf{r}_1}$$

for a rotation $\mathbf{r}_1$ followed by $\mathbf{r}_2$, so that rotations expressed in terms of rotation angles and axes may be compounded into a single such rotation without the need to form and decompose a product matrix.

Note that if $\mathbf{r}_1$ and $\mathbf{r}_2$ are parallel this reduces to the formula for the tangent of the sum of two angles, and that if $\mathbf{r}_1\cdot\mathbf{r}_2 = 1$ the combined rotation is always 180°. Note, too, that reversing the order of application of the rotations reverses only the vector product.

If three rotations $\mathbf{r}_1, \mathbf{r}_2$ and $\mathbf{r}_3$ are applied successively, $\mathbf{r}_1$ first, then their combined rotation is

$$\begin{aligned}\mathbf{r} = [&\mathbf{r}_3(1-\mathbf{r}_1\cdot\mathbf{r}_2) + \mathbf{r}_2(1+\mathbf{r}_3\cdot\mathbf{r}_1) + \mathbf{r}_1(1-\mathbf{r}_3\cdot\mathbf{r}_2) \\ &+ \mathbf{r}_3\times\mathbf{r}_2 + \mathbf{r}_3\times\mathbf{r}_1 + \mathbf{r}_2\times\mathbf{r}_1] \\ &\times[1-\mathbf{r}_1\cdot\mathbf{r}_2 - \mathbf{r}_2\cdot\mathbf{r}_3 - \mathbf{r}_3\cdot\mathbf{r}_1 - \mathbf{r}_3\cdot(\mathbf{r}_2\times\mathbf{r}_1)]^{-1}.\end{aligned}$$

Note the irregular pattern of signs in the numerator.

Similar ideas, using a vector of magnitude $\sin(\theta/2)$, are developed in Aharonov *et al.* (1977).

The third form of orthogonal matrix uses four variables, λ, μ, ν and σ, which comprise a four-dimensional vector $\boldsymbol{\rho}$, such that $\lambda = ls$, $\mu = ms$, $\nu = ns$ with $s = \sin(\theta/2)$ and $\sigma = \cos(\theta/2)$. In terms of these variables

$$\boldsymbol{R} = \begin{pmatrix} (\lambda^2-\mu^2-\nu^2+\sigma^2) & 2(\lambda\mu-\nu\sigma) & 2(\lambda\nu+\mu\sigma) \\ 2(\mu\lambda+\nu\sigma) & (-\lambda^2+\mu^2-\nu^2+\sigma^2) & 2(\mu\nu-\lambda\sigma) \\ 2(\lambda\nu-\mu\sigma) & 2(\mu\nu+\lambda\sigma) & (-\lambda^2-\mu^2+\nu^2+\sigma^2) \end{pmatrix}.$$

Two further matrices $\boldsymbol{S}$ and $\boldsymbol{T}$ may be defined (Diamond, 1988),

$$\boldsymbol{S} = \begin{pmatrix} -\sigma & \nu & -\mu & \lambda \\ -\nu & -\sigma & \lambda & \mu \\ \mu & -\lambda & -\sigma & \nu \\ \lambda & \mu & \nu & \sigma \end{pmatrix} \text{ and } \boldsymbol{T} = \begin{pmatrix} \sigma & -\nu & \mu & \lambda \\ \nu & \sigma & -\lambda & \mu \\ -\mu & \lambda & \sigma & \nu \\ -\lambda & -\mu & -\nu & \sigma \end{pmatrix},$$

which are themselves orthogonal (though $\boldsymbol{S}$ has determinant -1) and which have the property that

$$\boldsymbol{S}^2 = \begin{pmatrix} \boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix}$$

so that, for example, if homogeneous coordinates are being employed (Section 3.3.1.1.2)

$$\begin{pmatrix} x' \\ y' \\ z' \\ w \end{pmatrix} = \begin{pmatrix} -\sigma & \nu & -\mu & \lambda \\ -\nu & -\sigma & \lambda & \mu \\ \mu & -\lambda & -\sigma & \nu \\ \lambda & \mu & \nu & \sigma \end{pmatrix} \begin{pmatrix} -\sigma & \nu & -\mu & \lambda \\ -\nu & -\sigma & \lambda & \mu \\ \mu & -\lambda & -\sigma & \nu \\ \lambda & \mu & \nu & \sigma \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix}$$

is a rotation of (x, y, z, w) through the angle θ about the axis (l, m, n). With suitably pipelined hardware this forms an efficient means of applying rotations since the 'overhead' of establishing $\boldsymbol{S}$ is so trivial.

$\boldsymbol{T}$ has the property that the rotation vector $\boldsymbol{\rho}$ arising from a concatenation of n rotations is

$$\boldsymbol{\rho} = \boldsymbol{T}_n\boldsymbol{T}_{n-1}\ldots\boldsymbol{T}_1\boldsymbol{\rho}_0,$$

in which $\boldsymbol{\rho}_0^T$ is the vector (0, 0, 0, 1) which defines a null rotation. This equation may be used as a basis for factorizing a given rotation into a concatenation of rotations about designated axes (Diamond, 1990*a*).

Finally, an exact rotation of the vector $\mathbf{d}$ may be obtained without using matrices at all by writing

$$\mathbf{d} = \sum_0^\infty \mathbf{d}_n$$

in which

$$\mathbf{d}_n = \frac{1}{n}(\boldsymbol{\theta}\times\mathbf{d}_{n-1})$$

and $\mathbf{d}_0$ is the initial position which is to be rotated. Here $\boldsymbol{\theta}$ is a vector with direction cosines l, m and n, and magnitude equal to the required rotation angle in radians (Diamond, 1966). This method is particularly efficient when $|\boldsymbol{\theta}| \ll 1$ or when the number of vectors to be transformed is small since the overhead of establishing $\boldsymbol{R}$ is eliminated and the process is simple to program. It is the three-dimensional analogue of the power series for $\sin\theta$ and $\cos\theta$ and has the same convergence properties.

references