International Tables for Crystallography (2006). Vol. B, Section 3.3.1.3.8, pp. 371–372.

by $\boldsymbol{V}$ and is used only to control intensity in a technique known as depth cueing.

It is necessary, of course, to arrange for the aspect ratio of the viewport, $(r - l)/(t - b)$, to equal that of the window otherwise distortions are introduced.

3.3.1.3.8. *Compound transformations*

In this section we consider the viewing transformation $\boldsymbol{T}$ of Section 3.3.1.3.1 and its construction in terms of translation, rotation and scaling, Sections 3.3.1.3.2–4. We use $\boldsymbol{T}'$ to denote a new transformation in terms of the prevailing transformation $\boldsymbol{T}$.

We note first that any 4×4 matrix of the form

$$\begin{pmatrix} U\boldsymbol{R} & \mathbf{V} \\ \mathbf{0}^T & W \end{pmatrix},$$

with U a scalar, may be factorized according to

$$\begin{pmatrix} U\boldsymbol{R} & \mathbf{V} \\ \mathbf{0}^T & W \end{pmatrix} \simeq \begin{pmatrix} U\boldsymbol{I} & \mathbf{0} \\ \mathbf{0}^T & W \end{pmatrix} \begin{pmatrix} U\boldsymbol{I} & \mathbf{V} \\ \mathbf{0}^T & U \end{pmatrix} \begin{pmatrix} U\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & U \end{pmatrix}$$

and also that multiplying

$$\begin{pmatrix} U\boldsymbol{R} & \mathbf{V} \\ \mathbf{0}^T & W \end{pmatrix}$$

by an isotropic scaling matrix, a rotation, or a translation, either on the left or on the right, yields a product matrix of the same form, and its inverse

$$\begin{pmatrix} W\boldsymbol{R}^T & -\boldsymbol{R}^T\mathbf{V} \\ \mathbf{0}^T & U \end{pmatrix}$$

is also of this form, *i.e.* any combination of these three operations in any order may be reduced by the above factorization to a rotation about the original origin, a translation (which defines a new origin) and an expansion or contraction about the new origin, applied in that order.

If

$$\begin{pmatrix} N\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & N \end{pmatrix}$$

is a rotation matrix as in Section 3.3.1.3.3, its application produces a rotation about an axis through the origin defined only in the space in which it is applied. For example, if

$$\boldsymbol{R} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\boldsymbol{T}'\begin{pmatrix} \mathbf{X} \\ W \end{pmatrix} = \boldsymbol{T}\begin{pmatrix} N\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & N \end{pmatrix}\begin{pmatrix} \mathbf{X} \\ W \end{pmatrix}$$

rotates the image about the z axis of data space, whatever the prevailing viewing transformation, $\boldsymbol{T}$.

Forming

$$\begin{pmatrix} N\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & N \end{pmatrix}\boldsymbol{T}\begin{pmatrix} \mathbf{X} \\ W \end{pmatrix}$$

rotates the image about the z axis of display space, *i.e.* the normal to the tube face under the usual conventions, whatever the prevailing $\boldsymbol{T}$. Furthermore, if this rotation is to appear to be about some chosen position in the picture, *e.g.* the centre, then the window transformation $\boldsymbol{U}$, Section 3.3.1.3.5, must place the origin of display space there by setting $F > S = R + L = T + B = 0 > N$, in the notation of that section.

If a rotation is to be about a point

$$\begin{pmatrix} \mathbf{V} \\ N \end{pmatrix}$$

then

$$\boldsymbol{T}' = \begin{pmatrix} N\mathbf{I} & \mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}\begin{pmatrix} N'\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & N' \end{pmatrix}\begin{pmatrix} N\boldsymbol{I} & -\mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}\boldsymbol{T}$$
$$\simeq \begin{pmatrix} N\boldsymbol{R} & \mathbf{V} - \boldsymbol{R}\mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}\boldsymbol{T}$$

or

$$\boldsymbol{T}' = \boldsymbol{T}\begin{pmatrix} N\boldsymbol{I} & \mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}\begin{pmatrix} N'\boldsymbol{R} & \mathbf{0} \\ \mathbf{0}^T & N' \end{pmatrix}\begin{pmatrix} N\boldsymbol{I} & -\mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}$$
$$\simeq \boldsymbol{T}\begin{pmatrix} N\boldsymbol{R} & \mathbf{V} - \boldsymbol{R}\mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix}$$

according to whether $\boldsymbol{R}$ and $\mathbf{V}$ are both defined in display space or both in data space. If the rotation is defined in display space and the position of the centre of rotation is defined in data space, then the first form of $\boldsymbol{T}'$ must be used, in which $\mathbf{V}$ is first computed from

$$\begin{pmatrix} \mathbf{V} \\ N \end{pmatrix} = \boldsymbol{T}\begin{pmatrix} \mathbf{U} \\ W \end{pmatrix}$$

for a rotation centre at

$$\begin{pmatrix} \mathbf{U} \\ W \end{pmatrix}$$

in data space.

For continuous rotations defined in display space it is usually worthwhile to bring the centre of rotation to the origin of display space and leave it there, *i.e.* to omit the left-most factor in the first expression for $\boldsymbol{T}'$. Incremental rotations can then be made by further rotational factors on the left without further attention to $\mathbf{V}$. When continuous rotations are implemented by repeated multiplication of $\boldsymbol{T}$ by a rotation matrix, say thirty times a second for a minute or so, the orthogonality of the top-left partition of $\boldsymbol{T}$ may become degraded by accumulation of round-off error and this should be corrected occasionally by one of the methods of Section 3.3.1.2.3.

It is sometimes a requirement, depending on hardware capabilities, to affect a transformation in display space when access to data space is all that is readily available. In such a case

$$\boldsymbol{T}' = \boldsymbol{T}_1\boldsymbol{T} = \boldsymbol{T}\boldsymbol{T}_2,$$

where $\boldsymbol{T}_1$ is the required alteration to the prevailing viewing transformation $\boldsymbol{T}$ and $\boldsymbol{T}_2$ is the data-space equivalent,

$$\boldsymbol{T}_2 = \boldsymbol{T}^{-1}\boldsymbol{T}_1\boldsymbol{T} = \begin{pmatrix} U\boldsymbol{R} & \mathbf{V} \\ \mathbf{0}^T & W \end{pmatrix}^{-1}\begin{pmatrix} U_1\boldsymbol{R}_1 & \mathbf{V}_1 \\ \mathbf{0}^T & W_1 \end{pmatrix}\begin{pmatrix} U\boldsymbol{R} & \mathbf{V} \\ \mathbf{0}^T & W \end{pmatrix}$$
$$\simeq \begin{pmatrix} UU_1\boldsymbol{R}^T\boldsymbol{R}_1\boldsymbol{R} & \boldsymbol{R}^T(U_1\boldsymbol{R}_1\mathbf{V} + W\mathbf{V}_1 - W_1\mathbf{V}) \\ \mathbf{0}^T & UW_1 \end{pmatrix}.$$

An important special case is when $\boldsymbol{T}_1$ is to effect a rotation about the origin of display space without change of scale, so that $\mathbf{V}_1 = 0, U_1 = W_1 = W$, for then

$$\boldsymbol{T}_2 \simeq \begin{pmatrix} U\boldsymbol{R}^T\boldsymbol{R}_1\boldsymbol{R} & \boldsymbol{R}^T(\boldsymbol{R}_1 - \boldsymbol{I})\mathbf{V} \\ \mathbf{0}^T & U \end{pmatrix}.$$

If $\mathbf{r}$ is the required axis of rotation of $\boldsymbol{R}_1$ in display space then the axis of rotation of $\boldsymbol{R}^T\boldsymbol{R}_1\boldsymbol{R}$ in data space is $\mathbf{s} = \boldsymbol{R}^T\mathbf{r}$ since $\boldsymbol{R}^T\boldsymbol{R}_1\boldsymbol{R}\mathbf{s} = \mathbf{s}$. This gives a particularly simple result if $\boldsymbol{R}_1$ is to be a primitive rotation for then $\mathbf{s}$ is the relevant row of $\boldsymbol{R}$, and $\boldsymbol{R}^T\boldsymbol{R}_1\boldsymbol{R}$

can be constructed directly from this and the required angle of rotation.

3.3.1.3.9. *Inverse transformations*

It is frequently a requirement to be able to identify a feature or position in data space from its position on the screen. Facilities for identifying an existing feature on the screen are in many instances provided by the manufacturer as a 'hit' function which correlates the position indicated on the screen by the user (with a tablet or light pen) with the action of drawing and flags the corresponding item in the drawing internally as having been hit. In other instances it may be necessary to be able to indicate a position in data space independently of any drawn feature and this may be done by setting two or more non-parallel sight lines through the displayed volume and finding their best point of intersection in data space.

In Section 3.3.1.3.1 the relationship between data-space coordinates and screen-space coordinates was given as

$$\mathbf{S} = \boldsymbol{VUT}\mathbf{X};$$

hence data-space coordinates are given by

$$\mathbf{X} = \boldsymbol{T}^{-1}\boldsymbol{U}^{-1}\boldsymbol{V}^{-1}\mathbf{S}.$$

A line of sight through the displayed volume passing through the point

$$\begin{pmatrix} x \\ y \end{pmatrix}$$

on the screen is the line joining the two position vectors

$$\boldsymbol{S} = \begin{pmatrix} x & x \\ y & y \\ o & n \\ n & n \end{pmatrix}$$

in screen-space coordinates, as in Section 3.3.1.3.7, from which the corresponding two points in data space may be obtained using

$$\boldsymbol{V}^{-1} \simeq \begin{pmatrix} \dfrac{2n}{r-l} & 0 & 0 & \dfrac{-(r+l)}{(r-l)} \\ 0 & \dfrac{2n}{t-b} & 0 & -\dfrac{(t+b)}{(t-b)} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\boldsymbol{U}^{-1} \simeq \begin{pmatrix} \dfrac{R-L}{2(S-E)} & 0 & \dfrac{-C(F-N)}{(F-E)(N-E)} & \dfrac{(R+L)(N-E)-2C(N-S)}{2(N-E)(S-E)} \\ 0 & \dfrac{T-B}{2(S-E)} & \dfrac{-D(F-N)}{(F-E)(N-E)} & \dfrac{(T+B)(N-E)-2D(N-S)}{2(N-E)(S-E)} \\ 0 & 0 & \dfrac{-E(F-N)}{(F-E)(N-E)} & \dfrac{N}{(N-E)} \\ 0 & 0 & \dfrac{-V(F-N)}{(F-E)(N-E)} & \dfrac{V}{(N-E)} \end{pmatrix}$$

in the notation of Section 3.3.1.3.5, and $\boldsymbol{T}^{-1}$ was given in Section 3.3.1.3.8. If orthographic projection is being used $(E = -\infty)$ then $\boldsymbol{U}^{-1}$ simplifies to

$$\boldsymbol{U}'^{-1} \simeq \begin{pmatrix} \dfrac{R-L}{2} & 0 & 0 & \dfrac{R+L}{2} \\ 0 & \dfrac{T-B}{2} & 0 & \dfrac{T+B}{2} \\ 0 & 0 & F-N & N \\ 0 & 0 & 0 & V \end{pmatrix}.$$

Each of these inverse matrices may be suitably scaled to suit the word length of the machine [Section 3.3.1.1.2 (iii)].

Having determined the end points of one sight line in data space the viewing transformation $\boldsymbol{T}$ may then be changed and the required position marked again through the screen in the new orientation. Each such operation generates a pair of points in data space, expressed in homogeneous form, with a variety of values for the fourth coordinate. Each such point must then be converted to three dimensions in the form $(X/W,\ Y/W,\ Z/W)$, and for each sight line any (three-dimensional) point $\mathbf{p}_A$ on the line and the direction $\mathbf{q}_A$ of the line are established. For each sight line a rank 2 projector matrix $\boldsymbol{M}_A$ of order 3 is formed as

$$\boldsymbol{M}_A = \boldsymbol{I} - \mathbf{q}_A\mathbf{q}_A^T/\mathbf{q}_A^T\mathbf{q}_A$$

and the best point of intersection of the sight lines is given by

$$\left(\sum_a \boldsymbol{M}_a\right)^{-1}\left(\sum_a \boldsymbol{M}_a\mathbf{p}_a\right),$$

to which three-vector a fourth coordinate of unity may be applied.

3.3.1.3.10. *The three-axis joystick*

The three-axis joystick is a device which depends on compound transformations for its exploitation. As it is usually mounted it consists of a vertical shaft, mounted at its lower end, which can rotate about its own length (the Y axis of display space, Section 3.3.1.3.1), its angular setting, φ, being measured by a shaft encoder in its mounting. At the top of this shaft is a knee-joint coupling to a second shaft. The first angle φ is set to zero when the second shaft is in some selected direction, *e.g.* normal to the screen and towards the viewer, and goes positive if the second shaft is moved clockwise when seen from above. The knee joint itself contains a shaft encoder, providing an angle, ψ, which may be set to zero when the second shaft is horizontal and goes positive when its free end is raised. A knob on the tip of the second shaft can then rotate about an axis along the second shaft, driving a third shaft encoder providing an angle θ. The device may then be used to produce a rotation of the object on the screen about an axis parallel to the second shaft through an angle given by the knob. The necessary transformation is then

$$\boldsymbol{R} = \begin{pmatrix} \cos\varphi & 0 & -\sin\varphi \\ 0 & 1 & 0 \\ \sin\varphi & 0 & \cos\varphi \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & \sin\psi \\ 0 & -\sin\psi & \cos\psi \end{pmatrix}$$
$$\times \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{pmatrix}$$
$$\times \begin{pmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{pmatrix}$$

which is

references