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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

$$\begin{pmatrix} c^2\psi s^2\varphi + (1-c^2\psi s^2\varphi)c\theta & -s\psi c\psi s\varphi(1-c\theta) - c\psi c\varphi s\theta & -c^2\psi s\varphi c\varphi(1-c\theta) + s\psi s\theta \\ -s\psi c\psi s\varphi(1-c\theta) + c\psi c\varphi s\theta & s^2\psi + c^2\psi c\theta & s\psi c\psi c\varphi(1-c\theta) + c\psi s\varphi s\theta \\ -c^2\psi s\varphi c\varphi(1-c\theta) - s\psi s\theta & s\psi c\psi c\varphi(1-c\theta) - c\psi s\varphi s\theta & c^2\psi c^2\varphi + (1-c^2\psi c^2\varphi)c\theta \end{pmatrix}$$

in which cos and sin are abbreviated to c and s, which is the standard form with $l = -\cos\psi\sin\varphi$, $m = \sin\psi$, $n = \cos\psi\cos\varphi$.

3.3.1.3.11. *Other useful rotations*

If rotations in display space are to be controlled by trackerball or tablet then there are two measures available, an x and a y, which can define an axis of rotation in the plane of the screen and an angle θ. If x and y are suitably scaled coordinates of a pen on a tablet then the rotation

$$\begin{pmatrix} \dfrac{y^2+x^2c}{x^2+y^2} & \dfrac{-xy(1-c)}{x^2+y^2} & x\sqrt{x^2+y^2} \\ \dfrac{-xy(1-c)}{x^2+y^2} & \dfrac{x^2+y^2c}{x^2+y^2} & y\sqrt{x^2+y^2} \\ -x\sqrt{x^2+y^2} & -y\sqrt{x^2+y^2} & c \end{pmatrix}$$

with $c = \sqrt{1-(x^2+y^2)^2}$ is about an axis in the xy plane (*i.e.* the screen face) normal to (x, y) and with $\sin\theta = x^2 + y^2$. Applied repetitively this gives a quadratic velocity characteristic. Similarly, if an atom at (x, y, z, w) in display space is to be brought onto the z axis by a rotation with its axis in the xy plane the necessary matrix, in homogeneous form, is

$$\begin{pmatrix} \dfrac{x^2z+y^2r}{x^2+y^2} & \dfrac{-xy(r-z)}{x^2+y^2} & -x & 0 \\ \dfrac{-xy(r-z)}{x^2+y^2} & \dfrac{x^2r+y^2z}{x^2+y^2} & -y & 0 \\ x & y & z & 0 \\ 0 & 0 & 0 & r \end{pmatrix}$$

with $r = \sqrt{x^2+y^2+z^2}$.

3.3.1.3.12. *Symmetry*

In Section 3.3.1.1.1 it was pointed out that it is usual to express coordinates for graphical purposes in Cartesian coordinates in ångström units or nanometres. Symmetry, however, is best expressed in crystallographic fractional coordinates. If a molecule, with Cartesian coordinates, is being displayed, and a symmetry-related neighbour is also to be displayed, then the data-space coordinates must be multiplied by

$$\begin{pmatrix} \mathbf{W} & \mathbf{T} \\ \mathbf{0}^T & W \end{pmatrix} \begin{pmatrix} \boldsymbol{M} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \mathscr{S} \begin{pmatrix} \boldsymbol{M}^{-1} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \begin{pmatrix} \mathbf{W} & -\mathbf{T} \\ \mathbf{0}^T & W \end{pmatrix},$$

where

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

are the data-space coordinates of the crystallographic origin, $\boldsymbol{M}$ and $\boldsymbol{M}^{-1}$ are as in Section 3.3.1.1.1 and $\mathscr{S}$ is a crystallographic symmetry operator in homogeneous coordinates, expressed relative to the same crystallographic origin.

For example, in $P2_1$ with the origin on the screw dyad along **b**,

$$\mathscr{S} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\begin{pmatrix} \boldsymbol{M} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \mathscr{S} \begin{pmatrix} \boldsymbol{M}^{-1} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2}b \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$\mathscr{S}$ comprises a proper or improper rotational partition, $\boldsymbol{S}$, in the upper-left 3×3 in the sense that $\boldsymbol{MSM}^{-1}$ is orthogonal, and with the associated fractional lattice translation in the last column, with the last row always consisting of three zeros and 1 at the 4, 4 position. See *IT* A (1983, Chapters 5.3 and 8.1) for a fuller discussion of symmetry using augmented (*i.e.* 4×4) matrices.

3.3.1.4. *Modelling transformations*

The two sections under this heading are concerned only with the graphical aspects of conformational changes. Determination of such changes is considered under Section 3.3.2.2.

3.3.1.4.1. *Rotation about a bond*

It is a common requirement in molecular modelling to be able to rotate part of a molecule relative to the remainder about a bond between two atoms.

If four atoms are bonded 1–2–3–4 then the dihedral angle in the bond 2–3 is zero if the four atoms are *cis* planar, and a rotation in the 2–3 bond is, by convention (IUPAC–IUB Commission on Biochemical Nomenclature, 1970), positive if, when looking along the 2–3 bond, the far end rotates clockwise relative to the near end. This is valid for either viewing direction. This sign convention, when applied to the $\boldsymbol{R}$ matrix of Section 3.3.1.2.1, leads to the following statement.

If one of the two atoms is selected as the near atom and the direction cosines are those of the vector from the near atom to the far atom, and if the matrix is to rotate material attached to the far atom (with the reference axes fixed), then a positive rotation in the foregoing sense is generated by a positive θ.

Rotation about a bond normally involves compounding $\boldsymbol{R}$ with translations in the manner of Section 3.3.1.3.8.

3.3.1.4.2. *Stacked transformations*

A flexible molecule may require to be drawn in any of a number of conformations which are related to one another by, for example, rotations about single bonds, changes of bond angles or changes of bond lengths, all of which changes may be brought about by the application of suitable homogeneous transformations during the drawing of the molecule (Section 3.3.1.3.8). With suitable organization, this may be done without necessarily altering the coordinates of the atoms in the coordinate list, only the transformations being manipulated during drawing.

The use of transformations in the manner shown below is straightforward for simply connected structures or structures containing only rigid rings. Flexible rings may be similarly handled provided that the matrices employed are consistent with the consequential constraints as described in Section 3.3.2.2.1, though this requirement may make real-time folding of flexible rings difficult.

Any simply connected structure may be organized as a tree with a node at each branch point and with an arbitrary number of sites of

references