

3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING

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

$$\mathbf{S} = \mathbf{VUTX};$$

hence data-space coordinates are given by

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

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

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

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

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

and

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

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

$$\mathbf{U}^{-1} \simeq \begin{pmatrix} \frac{R-L}{2} & 0 & 0 & \frac{R+L}{2} \\ 0 & \frac{T-B}{2} & 0 & \frac{T+B}{2} \\ 0 & 0 & F-N & N \\ 0 & 0 & 0 & V \end{pmatrix}.$$

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 \mathbf{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 \mathbf{M}_A of order 3 is formed as

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

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

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

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

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

which is