

3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING

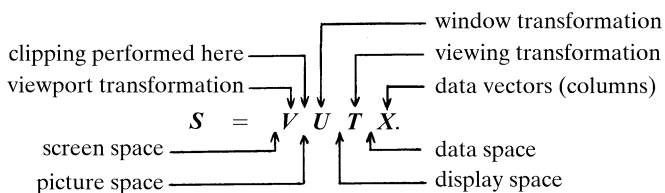
coordinates and this coordinate system is generally a constant aspect of the problem.

In order to view these data in convenient ways such coordinates may be subjected to a  $4 \times 4$  viewing transformation  $T$ , affecting orientation, scale etc., the resulting coordinates  $TX$  being then in display space. Here, and throughout what follows, we treat position vectors as columns with transformation matrices as factors on the left, though some writers do the reverse.

In general, only some portion of display space which lies inside a certain frustum of a pyramid is required to fall within the picture. The pyramid may be thought of as having the observer's eye at its vertex, with a rectangular base corresponding to the picture area. This volume is called a window. A transformation,  $U$ , which takes display-space coordinates as input and generates vectors  $(X, Y, Z, W)$  for which  $X/W$  and  $Y/W = \pm 1$  for points on the left, right, top and bottom boundaries of the window and for which  $Z/W$  takes particular values on the front and back planes of the window, is said to be a windowing transformation. In machines for which  $Z/W$  controls intensity depth cueing, the range of  $Z/W$  corresponding to the window is likely to be 0 to 1 rather than  $-1$  to 1. Coordinates obtained by multiplying display-space coordinates by  $U$  are termed picture-space coordinates. Mathematically,  $U$  is a  $4 \times 4$  matrix like any other, but functionally it is special. Declaring a transformation to be a windowing transformation implies that only resulting points having  $|X|, |Y| < W$  and positive  $Z < W$  are to be plotted. Machines with clipping hardware to truncate lines which run out of the picture perform clipping on the output from the windowing transformation.

Finally, the picture has to be drawn in some rectangular portion of the screen which is allocated for the purpose. Such an area is termed a viewport and is defined in terms of screen coordinates which are defined absolutely for the hardware in question as  $\pm n$  for full-screen deflection, where  $n$  is declared by the manufacturer. Screen coordinates are obtained from picture coordinates with a viewport transformation,  $V$ .\*

To summarize, screen coordinates,  $S$ , are given by



3.3.1.3.2. Translation

The transformation

$$\begin{pmatrix} NI & \mathbf{V} \\ \mathbf{0}^T & N \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ W \end{pmatrix} = \begin{pmatrix} \mathbf{X}N + \mathbf{V}W \\ NW \end{pmatrix} \simeq \begin{pmatrix} \mathbf{X} + \mathbf{V}W/N \\ W \end{pmatrix} \simeq \begin{pmatrix} \mathbf{X}/W + \mathbf{V}/N \\ 1 \end{pmatrix}$$

evidently corresponds to the addition of the vector  $\mathbf{V}W/N$  to the components of  $\mathbf{X}$  or of  $\mathbf{V}/N$  to the components of  $\mathbf{X}/W$ . ( $I$  is the identity.) Displacements may thus be affected by expressing the required displacement vector in homogeneous coordinates with any suitable choice of  $N$  (commonly,  $N = W$ ), with  $\mathbf{V}$  scaled to correspond to this choice, and loading the  $4 \times 4$  transformation matrix as indicated above.

\* In recent years it has become increasingly common, especially in two-dimensional work, to apply the term 'window' to what is here called a viewport, but in this chapter we use these terms in the manner described in the text.

3.3.1.3.3. Rotation

Rotation about the origin is achieved by

$$\begin{pmatrix} NR & \mathbf{0} \\ \mathbf{0}^T & N \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ W \end{pmatrix} = \begin{pmatrix} NR\mathbf{X} \\ NW \end{pmatrix} \simeq \begin{pmatrix} R\mathbf{X} \\ W \end{pmatrix},$$

in which  $R$  is an orthogonal  $3 \times 3$  matrix.  $R$  necessarily has elements not exceeding one in modulus. For machines using integer arithmetic, therefore,  $N$  would be chosen large enough (usually half the largest possible integer) for the product  $NR$  to be well represented in the available word length. Characteristically,  $N$  affects resolution but not scale.

3.3.1.3.4. Scale

The transformation

$$\begin{pmatrix} SNI & \mathbf{0} \\ \mathbf{0}^T & N \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ W \end{pmatrix} = \begin{pmatrix} SN\mathbf{X} \\ NW \end{pmatrix} \simeq \begin{pmatrix} S\mathbf{X} \\ W \end{pmatrix}$$

scales the vector  $(\mathbf{X}, W)$  by the factor  $S$ . For integer working and  $|S| < 1$ ,  $N$  should be set to the largest representable integer. For  $|S| > 1$  the product  $SN$  should be the largest representable integer,  $N$  being reduced accordingly.

3.3.1.3.5. Windowing and perspective

It is necessary at this point to relate the discussion to the axial system inherent in the graphics device employed. One common system adopts  $X$  horizontal and to the right when viewing the screen,  $Y$  vertically upwards in the plane of the screen, and  $Z$  normal to  $X$  and  $Y$  with  $+Z$  into the screen. This is, unfortunately, a left-handed system in that  $(\mathbf{X} \times \mathbf{Y}) \cdot \mathbf{Z}$  is negative. Since it is usual in crystallographic work to use right-handed axial systems it is necessary to incorporate a matrix of the form

$$\begin{pmatrix} W & 0 & 0 & 0 \\ 0 & W & 0 & 0 \\ 0 & 0 & -W & 0 \\ 0 & 0 & 0 & W \end{pmatrix}$$

either as the left-most factor in the matrix  $T$  or as the right-most factor in the windowing transformation  $U$  (see Section 3.3.1.3.1). The latter choice is to be preferred and is adopted here. The former choice leads to complications if transformations in display space will be required. Display-space coordinates are necessarily referred to this axial system.

Let  $L, R, T, B, N$  and  $F$  be the left, right, top, bottom, near and far boundaries of the windowed volume ( $L < R, T > B, N < F$ ),  $S$  be the  $Z$  coordinate of the screen, and  $C, D$  and  $E$  be the coordinates of the observer's eye position, all ten of these parameters being referred to the origin of display space as origin, which may be anywhere in relation to the hardware.  $L, R, T$  and  $B$  are to be evaluated in the screen plane. All ten parameters may be referred to their own fourth coordinate,  $V$ , meaning that the point  $(X, Y, Z, W)$  in display space will be on the left boundary of the picture if  $X/W = L/V$  when  $Z/W = S/V$ .  $V$  may be freely chosen so that all eleven quantities and all elements of  $U$  suit the word length of the machine. These relationships are illustrated in Fig. 3.3.1.1.

Since

$$(X, Y, Z, W) \simeq \left( \frac{XV}{W}, \frac{YV}{W}, \frac{ZV}{W}, V \right),$$

$XV/W$  is a display-space coordinate on the same scale as the window parameters. This must be plotted on the screen at an  $X$  coordinate (on the scale of the window parameters) which is the weighted mean of  $XV/W$  and  $C$ , the weights being  $(S - E)$  and

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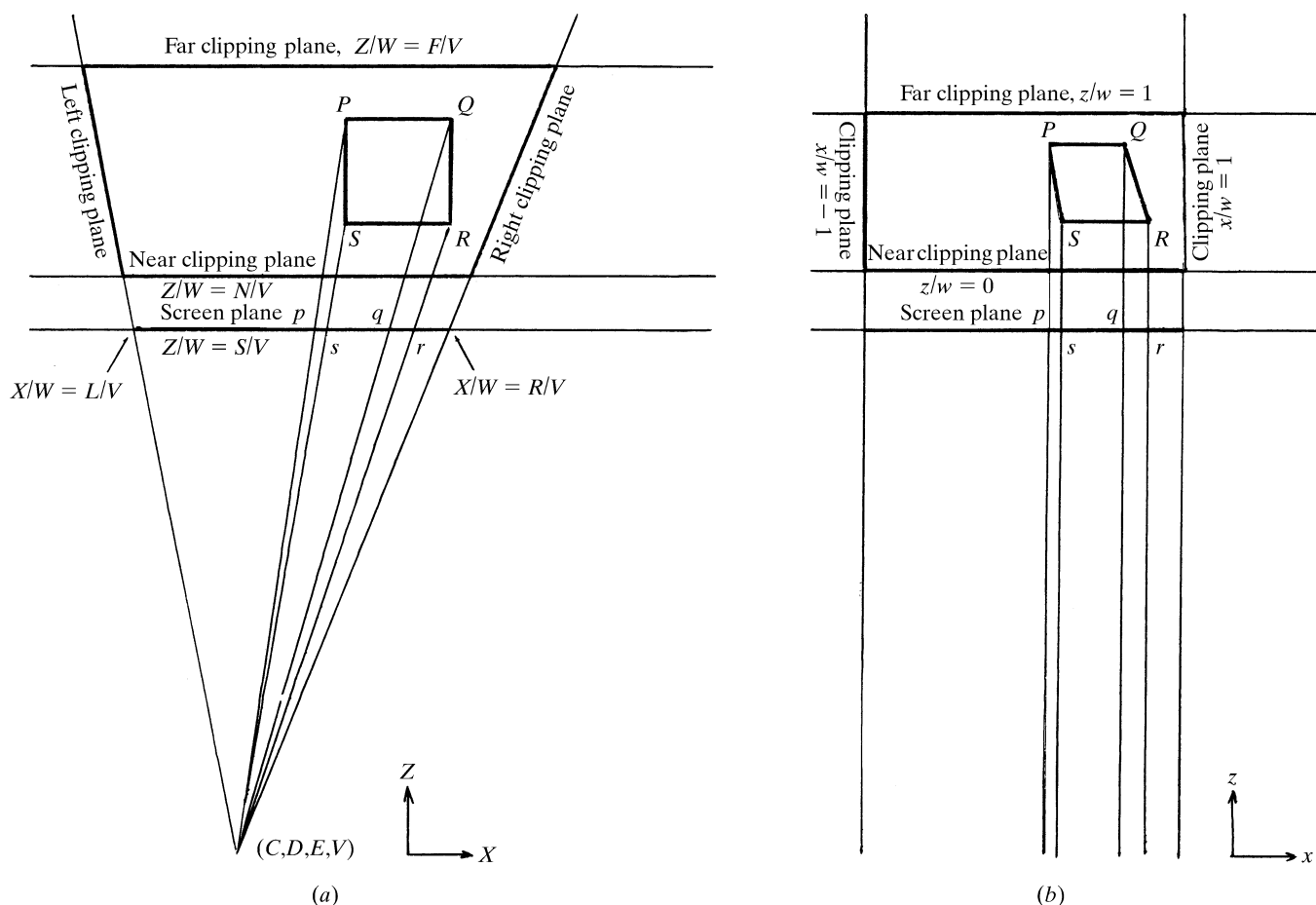


Fig. 3.3.1.1. The relationship between display-space coordinates ( $X, Y, Z, W$ ) and picture-space coordinates ( $x, y, z, w$ ) derived from them by the window transformation,  $U$ . (a) Display space (in  $X, Z$  projection) showing a square object  $P, Q, R, S$  for display viewed from the position  $(C, D, E, V)$ . The bold trapezium is the window (volume) and the bold line is the viewport portion of the screen. The points  $P, Q, R$  and  $S$  must be plotted at  $p, q, r$  and  $s$  to give the correct impression of the object. (b) Picture space (in  $x, z$  projection). The window is mapped to a rectangle and all sight lines are parallel to the  $z$  axis, but the object  $P, Q, R, S$  is no longer square. The distribution of  $p, q, r$  and  $s$  is identical in the two cases. Note that  $z/w$  values are not linear on  $Z/W$ , and that the origin of picture space arises at the midpoint of the near clipping plane, regardless of the location of the origin of display space. The figure is accurately to scale for coincident viewport positions. The words 'Left clipping plane', if part of the scene in display space, would currently be obscured, but would come into view if the eye moved to the right, increasing  $C$ , as the left clipping plane would pivot about the point  $L/V$  in the screen plane.

( $ZV/W - S$ ), respectively. This provides perspective because the weighted mean is at the point where the straight line from ( $X, Y, Z, W$ ) to the eye intersects the screen. This then has to be mapped into the  $L$ -to- $R$  interval, so that picture-space coordinates ( $x, y, z, w$ ) are given by

$$\begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \begin{pmatrix} \frac{2(S-E)V}{(R-L)} & 0 & \frac{(2C-R-L)V}{(R-L)} & \frac{(R+L)E-2SC}{(R-L)} \\ 0 & \frac{2(S-E)V}{(T-B)} & \frac{(2D-T-B)V}{(T-B)} & \frac{(T+B)E-2SD}{(T-B)} \\ 0 & 0 & \frac{(F-E)V}{(F-N)} & \frac{-N(F-E)}{(F-N)} \\ 0 & 0 & V & -E \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \\ W \end{pmatrix}$$

which provides for  $|x/w|$  and  $|y/w|$  to be unity on the picture boundaries, which is usually a requirement of the clipping hardware, and for  $0 < z/w < 1$ , zero being for the near-plane boundary. Even though  $z/w$  is not linear on  $Z/W$ , straight lines and planes in display space transform to straight lines and planes in picture space,

the non-linearity affecting only distances. Thus vector-drawing machines are not disadvantaged by the introduction of perspective.

Note that the dimensionality of  $X/W$  must equal that of  $S/V$  and that this may be regarded as length or as a pure number, but that in either case  $x/w$  is dimensionless, consistent with the stipulation that the picture boundaries be defined by the pure number  $\pm 1$ .

The above matrix is  $U$  and is suited to left-handed hardware systems. Note that only the last column of  $U$  (the translational part) is sensitive to the location of the origin of display space and that if the eye is on the normal to the picture centre then  $C = \frac{1}{2}(R+L)$ ,  $D = \frac{1}{2}(T+B)$  and simplifications result. If  $C, D$  and  $E$  can be continuously monitored then dynamic parallax as well as perspective may be obtained (Diamond *et al.*, 1982).

If data space is referred to right-handed axes, the viewing transformation  $T$  involves only proper rotations and the hardware uses a left-handed axial system then elements in the third column of  $U$  should be negated, as explained in the opening paragraph.

To provide for orthographic projection, multiply every element of  $U$  by  $-K/E$  and then let  $E \rightarrow -\infty$ , choosing some positive  $K$  to suit the word length of the machine [see Section 3.3.1.1.2 (iii)]. The

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result is

$$\mathbf{U}' \simeq \begin{pmatrix} \frac{2KV}{(R-L)} & 0 & 0 & \frac{-K(R+L)}{(R-L)} \\ 0 & \frac{2KV}{(T-B)} & 0 & \frac{-K(T+B)}{(T-B)} \\ 0 & 0 & \frac{KV}{(F-N)} & \frac{-KN}{(F-N)} \\ 0 & 0 & 0 & K \end{pmatrix},$$

which is the orthographic window.

It may be convenient in some applications to separate the functions of windowing and the application of perspective, and to write

$$\mathbf{U} = \mathbf{U}'\mathbf{P},$$

where  $\mathbf{U}$  and  $\mathbf{U}'$  are as above and  $\mathbf{P}$  is a perspective transformation given by

$$\mathbf{P} = (\mathbf{U}')^{-1}\mathbf{U} \simeq \begin{pmatrix} S-E & 0 & C & -SC/V \\ 0 & S-E & D & -SD/V \\ 0 & 0 & F-E+N & -NF/V \\ 0 & 0 & V & -E \end{pmatrix},$$

which involves  $F$  and  $N$  but not  $R, L, T$  or  $B$ . In this form the action of  $\mathbf{P}$  may be thought of as compressing distant parts of display space prior to an orthographic projection by  $\mathbf{U}'$  into picture space.

Other factorizations of  $\mathbf{U}$  are possible, for example

$$\mathbf{U} = \mathbf{U}''\mathbf{P}'$$

with

$$\mathbf{U}'' \simeq \begin{pmatrix} \frac{2KV}{R-L} & 0 & 0 & \frac{-K(R+L)}{(R-L)} \\ 0 & \frac{2KV}{T-B} & 0 & \frac{-K(T+B)}{(T-B)} \\ 0 & 0 & \frac{KV(N-E)(F-E)}{E^2(F-N)} & \frac{KN(F-E)}{E(F-N)} \\ 0 & 0 & 0 & K \end{pmatrix}$$

$$\mathbf{P}' \simeq \begin{pmatrix} S-E & 0 & C & -SC/V \\ 0 & S-E & D & -SD/V \\ 0 & 0 & -E & 0 \\ 0 & 0 & V & -E \end{pmatrix},$$

which renders  $\mathbf{P}'$  independent of all six boundary planes, but  $\mathbf{U}''$  is no longer independent of  $E$ . It is not possible to factorize  $\mathbf{U}$  so that the left factor is a function only of the boundary planes and the right factor a function only of eye and screen positions.

Note that as  $E \rightarrow -\infty$ ,  $\mathbf{U}'' \rightarrow \mathbf{U}'$ ,  $\mathbf{P}$  and  $\mathbf{P}' \rightarrow -\mathbf{I}E \simeq \mathbf{I}$ .

#### 3.3.1.3.6. Stereoviews

Assuming that left- and right-eye views are to be presented through the same viewport (next section) or that their viewports are to be superimposed by an external optical system, *e.g.* Ortony mirrors, then stereopairs are obtained by using appropriate eye coordinates in the  $\mathbf{U}$  matrix of the previous section. However,  $\mathbf{U}$  may be factorized according to

$$\mathbf{U} = \mathbf{U}'''\mathbf{S}$$

in which  $\mathbf{U}'''$  is the matrix  $\mathbf{U}$  obtained by setting  $(C, D, E, V)$  to correspond to the point midway between the viewer's eyes and

$$\mathbf{S} = \begin{pmatrix} 1 & 0 & c/(S-E) & -cS/(S-E)V \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\simeq \begin{pmatrix} V & 0 & cV/(S-E) & -cS/(S-E) \\ 0 & V & 0 & 0 \\ 0 & 0 & V & 0 \\ 0 & 0 & 0 & V \end{pmatrix}$$

in which  $(c, 0, 0, V)$  is the position of the right eye relative to the mean eye position, and the left-eye view is obtained by negating  $c$ .

Stereo is often approximated by introducing a rotation about the  $Y$  axis of  $\pm \sin^{-1}[c/(S-E)]$  to the views or  $\sin^{-1}[2c/(S-E)]$  to one of them. The first corresponds to

$$\mathbf{S} = \begin{pmatrix} \sqrt{1-\sigma^2} & 0 & \sigma & 0 \\ 0 & 1 & 0 & 0 \\ -\sigma & 0 & \sqrt{1-\sigma^2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with  $\sigma = c/(S-E)$ . The main difference is in the resulting  $Z$  value, which only affects depth cueing and  $z$  clipping. The  $X$  translation which arises if  $S \neq 0$  is also suppressed, but this is not likely to be noticeable.  $\sigma$  is often treated as a constant, such as  $\sin 3^\circ$ .

The distinction in principle between the true  $\mathbf{S}$  and the rotational approximation is that with the true  $\mathbf{S}$  the eye moves relative to the screen and the displayed object, whereas with the approximation the eye and the screen are moved relative to the displayed object, in going from one view to the other.

Strobing of left and right images may conveniently be accomplished with an electro-optic liquid-crystal shutter as described by Harris *et al.* (1985). The shutter is switched by the display itself, thus solving the synchronization problem in a manner free of inertia.

A further discussion of stereopairs may be found in Johnson (1970) and in Thomas (1993), the second of which generalizes the treatment to allow for the possible presence of an optical system.

#### 3.3.1.3.7. Viewports

The window transformation of the previous two sections has been constructed to yield picture coordinates  $(X, Y, Z, W)$  (formerly called  $x, y, z, w$ ) such that a point having  $X/W$  or  $Y/W = \pm 1$  is on the boundary of the picture, and the clipping hardware operates on this basis. However, the edges of the picture need not be at the edges of the screen and a viewport transformation,  $\mathbf{V}$ , is therefore needed to position the picture in the requisite part of the screen.

$$\mathbf{V} = \begin{pmatrix} (r-l)/2 & 0 & 0 & (r+l)/2 \\ 0 & (t-b)/2 & 0 & (t+b)/2 \\ 0 & 0 & n & 0 \\ 0 & 0 & 0 & n \end{pmatrix},$$

where  $r, l, t$  and  $b$  are now the right, left, top and bottom boundaries of the picture area, or viewport, expressed in screen coordinates, and  $n$  is the full-screen deflection value. Thus a point with  $X/W = 1$  in picture space plots on the screen with an  $X$  coordinate which is a fraction  $r/n$  of full-screen deflection to the right.  $Z/W$  is unchanged