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ATOMLLL—A THREE-D OPAQUE MOLECULE SYSTEM (LAWRENCE LIVERMORE LABORATORY VERSION)

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LIVERMORE

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LABORATORY VERSION)**

N. L. May

Manuscript date: January 11, 1979

DISCLAIMER

AVAILABILITY

This document is available online as follows:

```
XPORT RD .717675:UCRL:UCRL52645 / 1 1
RD .717675:UCRL:UX52645
```

View the file on the TMDS using the TRIX AC command:

```
TVmm,1,8,851NN!T
```

To print the file, type:

```
TRIX AC / 1 1
.PRINT!NIP UCRL52645 BOX ann identification
.END
```

To view this file on the TMDS with full font capabilities and pictures, use REDPP as described in UCID-30125. To print the file with full font capabilities and pictures, use the REDPP execution line:

```
REDPP filename NIPS. / 2 2.2
```

Remember, the TRIX AC commands use far less computer time than the REDPP command.

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ATOMLLL—A THREE-D OPAQUE MOLECULE SYSTEM (LAWRENCE LIVERMORE LABORATORY VERSION)

ABSTRACT

The program ATOMLLL draws color, shaded, hidden-surface pictures and movies of "ball-and-stick" and "space-filling" molecular models. From a file containing the colors and radii of the atoms, the coordinates of their centers, and the descriptions of bonds, if any, the program computes the visible portions of each atom. ATOMLLL then writes their descriptions into a file that can be copied to tape. The tape is read by a Varian minicomputer, which controls the plotting on the Dicomed D-48 color-film recorder.

INTRODUCTION

Steve Levine (Lawrence Livermore Laboratory Computer Graphics Group) adapted the ATOMLLL program from an earlier program, ATOMS, written at Bell Laboratories by Ken Knowlton and Lorinda Cherry.¹ I added the information for shading and highlights to the output and wrote the program to produce the shading on the Dicomed. Bell Telephone Laboratories and Lawrence Livermore Laboratory take no responsibility for maintaining exported copies of the codes described here.

The first section gives the teletype interaction and input data format. In section 2, the sample data and interactions in Appendix A, and the list of error messages in Appendix B, are all that a user of ATOMLLL need read. Section 2 discusses output data format; section 3 outlines the strategy of the shading algorithm; and section 4 describes the shading program "DN1" on the Varian. These three sections will be of use to those who wish to plot the output on other devices. Finally, section 5 partially describes the structure of the subroutines in ATOMLLL, and Appendix C lists its common blocks and variables. This information may be of help to those who wish to adapt the program to other installations; possible modifications are mentioned.

1. INFORMATION FOR THE USER

The source program ATOMLLL and the load module ATOMC are available in the directory .026123:GGPUBLIC. When you start ATOMC, it will ask

OUTLINES ON TMS? Y or N

If you type Y you will be asked

MONITOR NO?

In this mode, the outlines of the visible portions of each atom or bond in the picture will appear on the monitor in addition to the more complete description in the output file. This feature can be used to debug a picture or movie file. The system will prompt

>

when a new frame is ready and hold the current frame on the screen until a carriage return is supplied.

The next prompt is

INPUT FILE NAME:

which should be answered by the name, up to 10 characters, of the input file. Finally the program asks for the

OUTPUT FILE NAME:

which can have up to 9 characters.

The program requests 670,000 60-bit words on disk for the output file. When the current file is filled, ATOMLLL automatically increments the name by one (changing the last character to the following letter or number) and opens a new file. The program reports each new file created to the terminal. The files can be copied to tape by TAPECOPY. Each takes about one-third of a 2200-ft reel of 800-bpi tape.

Carry the tapes to the rack outside the Dicomed room and attach a white instruction slip, with your box number, for film delivery. Request the tape to be run by DNI (see section 4). If you want the results to be mountable as full-frame 35mm slides, request IFDA=1. This will not increase the image size, but will have unexposed black film fill the frame of the 8 perforated slide mounts. The same tape may be plotted at 1024, 2048, or 4096 pixels resolution. The higher resolutions give cleaner edges, but take longer to plot. Generally, 2048 is good enough for movies. The 4096 resolution should be used only for 4-by 5-in. sheet film.

The picture is clipped in the CDC 7600 computer to a height of 0.75 times its width, which is the aspect ratio of movie film. Thus parts of the picture hidden by the camera aperture plate will not be drawn. If you want the full square frame [which can only be plotted on Polaroid sheet film or on the television monitor display system (TMDS) screen], you must change the line ARATIO=.75 in the subroutine SETDAT to specify the desired aspect ratio (1.0 for a square).

The input file lists the information necessary to describe each frame of the movie. The first line for each frame lists the numbers, NATOMS, of atoms for the frame, and the perspective ratio PRATIO. These are given in the format

16, F6.2. (Note that the .2 in F6.2 is only a default if the input has no decimal point. Any decimal point in the 8-character input field takes priority.) The number PRATIO is the ratio of screen width to viewer's distance from the screen. A value of PRATIO between 0.3 and 0.5 gives a reasonably comfortable perspective.

The next NATOMS lines give the X, Y, and Z coordinates of each atom, the radius of the sphere used to represent it, and the color of that sphere in the format 4F6.2, I3. The color is an integer from 1 to 7, corresponding to the seven colors on the Dicomed filler wheel, in this order: red, green, yellow, blue, magenta, cyan, and white. If two spheres interpenetrate, their intersection will be computed, and only the visible portions rendered. By choosing radii near the Van der Waals radii of the atoms, a realistic simulation of the plastic "CPK space-filling models" is produced. The viewpoint is assumed to be at the origin, so all atoms must have positive Z coordinates to be visible.

If smaller radii are used, so there is space between atoms, covalent bonds can be represented by cylinders or "sticks" connecting atomic centers. This results in ball-and-stick models. Again, although the sticks intersect the spheres, only the visible portions are rendered. However, the spheres must be large enough to cover any potential intersections of sticks, since the program will not correctly render such intersections. In this report, the word "part" refers either to a sphere representing an atom or to a cylinder representing a bond. Parts are numbered by the order in which they appear in the input file, with the first bond following the last atom.

The next line of the input file contains the number, NBONDS, of these sticks and their default radius, BONDR, in the format 16, F6.2. If there are no bonds, this line must still be given, with NBONDS=0. If BONDR=0, the radii of the various bonds are taken from the succeeding lines.

The next NBONDS lines contain the part numbers of the two atoms connected by each bond, and the radius of the bond, in the format 2I3, F6.2. The current color for all bonds is magenta but can be modified by changing the Varian program DNI. If BONDR is nonzero, it takes priority, and the radii need not be listed on each line.

After the bond description, the line with NATOMS and PRATIO may be entered for the next frame, and the process repeated. Successive frames of a movie are thus concatenated in the input file. When the program sees the end of file after the last frame: (1) an end-of-job indicator is written on the output; (2) the output buffer is cleared to disk; (3) the number of 660-word records written to the last output file is reported on the terminal; and (4) the program exits, typing ALL DONE.

2. OUTPUT FORMAT

As described in Ref. 1, ATOMLLL keeps track of the visible portions of each part in terms of a list of "trapezoids." Each trapezoid (Fig. 1) has two straight vertical sides.

Fig. 1. A trapezoid, whose top arc is concave downward and whose bottom arc is a straight line.

The other two sides may be straight lines, or arcs of circles, and the term "arc" will refer to either of these. The circular arcs can be convex down, as the top arc in Fig. 1, or convex up. In addition, each arc must be monotone, with Y either nonincreasing or nondecreasing. Thus, a sphere is initially represented as two trapezoids, each having one degenerate vertical side (Fig. 2(a)). Occlusions or intersections of this sphere with other spheres or cylinders will result in subdividing, reducing, or removing some trapezoids in this list (Figs. 2(b) and 2(c)), and perhaps joining adjacent ones (Fig. 2(d)).

Fig. 2.(a) Initial subdivision of an atom.

Fig. 2.(b) Subdivision caused by intersecting atom.

Fig. 2.(c) Further subdivision caused by occluding atom.

Fig. 2.(d) Subdivision after COMPACT has joined adjacent trapezoids.

After all potential occlusions have been taken into account, the final list of trapezoids for each part is written to the output file.

It takes 11 numbers to describe each trapezoid, arranged on output as a row in the 200 x 11 matrix KOUT. Inside ATOMLLL and DNI, they are called J, KT, KB, XL, XR, XCT, YCT, RT, XCB, YCB, and RB. The first three are integers: J is the atom or bond number from which the trapezoid comes (used only for debugging) and KT and KB describe the type of the upper and lower arcs, 1 for convex downward, 2 for convex upward, and ? for straight. The next eight are real numbers: XL and XR are the X-coordinates of the left and right vertical sides (Fig. 1); XCT, YCT, and RT are the center and radius of the upper arc; and XCB, YCB, and RB are

the center and radius of the lower arc. The screen is assumed to have boundaries at $X = -1$, $X = 1$, $Y = -ARATIO$, and $Y = ARATIO$. The program ATOMLLL also keeps track of YTL, YBL, YTR, and YBR (the Y-coordinates of the corners) as an aid in processing the trapezoid list; but these are not needed in the output.

Since it is easier and quicker for the Varian to read fixed point binary data, all real coordinates and radii are multiplied by 2^{14} and converted to integers for output. This "normalization" allows a range from -2 to 2 for these real numbers, and the resulting integers become screen coordinates for the bicomod.

Circular arcs of small curvature, requiring centers or radii outside this range, are converted to straight lines on output. In addition, lines of slope greater than 1 or less than -1 are represented by their reciprocal slopes and X-intercepts, again to keep the numbers in range. This gives a new class of arc, type 4, used only in the output.

If the bottom arc is of type 3, as in Fig. 1, the ninth number, XCB, will be $[(2^{15})-1]$ times its slope; the tenth number, YCB, will be meaningless; and the last, RB, will be the normalized Y-intercept. Similarly, if it is of type 4, XCB indicates the reciprocal of the slope and RB indicates the X-intercept. The corresponding interpretations hold for the top arc. (This applies only to the output file. Internally, in ATOMLLL, these are reversed: R denotes the slope and XC denotes the Y-intercept.)

A tape record contains 200 rows of the 200×11 matrix KOUT in columnwise order by FORTRAN conversion. If the first entry, J, of a row is positive, a trapezoid is indicated, arising from part J. A negative J indicates one of four other kinds of information. A J of -5 tells the Varian that a frame has been completed, and the film is advanced before further plotting. A J of -4 indicates the end of the run, and the job is terminated.

A J of -3 indicates the beginning of a new sphere, and other entries in the row give data necessary to compute its shading. Specifically, the second entry is the color, the next two entries are the normalized X and Y coordinates of the center, and the fifth entry is the normalized radius.

Finally, a J of -2 indicates the beginning of a cylinder for a bond. The shading algorithm needs to know the top edge, bottom edge, and center line of the cylinder; these are given in three groups of three numbers. In each group, the first number indicates the kind of line. If it is 1, the next number is $[(2^{15})-1]$ times the slope, and what follows is the normalized Y-intercept. If the first number is 2, the reciprocal slope and X-intercept are used instead. The eleventh entry gives the highlight intensity of the bond, which depends on the angle between the axis of the cylinder and the light source. It is maximum, at $(2^{15})-1$, when the bond is parallel to the picture plane.

As a ball-and-stick model rotates, bond highlights flash on and off appropriately. Simultaneously, atom highlights turn correctly, remaining at the centers of the projected spheres.

3. SHADING AND HIGHLIGHTS

Atoms are shaded as if they diffusely reflect the illuminating light, which is assumed to come from an infinitely distant point directly behind the viewer. Thus intensity is a monotone-decreasing function, $f(\theta)$, of the angle θ between the normal PN to a point P on the sphere and the Z axis (Fig. 3). A suitable function might be "Lambert's law":

$$f(\theta) = A + D \cos \theta \quad (1)$$

where D represents the diffuse reflectivity of the illuminating light from the surface and A represents reflection of ambient light coming from all directions, so the sphere does not become totally black at the edges.

This function, $f(\theta)$, could be used to multiply the three color components (red, green, blue) for any sphere. In the current version, one of the seven colored filters is used, taking one pass to shade each sphere instead of three passes. However, the plotting program could be modified to use three passes if more than seven colors were required. In this case, the second pass now used to add the highlights could be eliminated.

The highlights represent specular reflection from the surfaces of the spheres and cylinders and are added in white, with a separate pass through the clear filter. Here, a function that concentrates the intensity at small angles of θ is appropriate, for example,

$$g(\theta) = C \cos^{28} \theta \quad (2)$$

(This particular expression gave an unpleasant Mach band around the central highlight, so several other terms were added in the current implementation.)

The Dicomod contains a loadable color-lookup table, designed to compensate for nonlinearities in the output scope and the film, which takes an 8-bit input intensity and gives an 8-bit output intensity to the scope. (Actually, the plotting intensity is kept constant, and the output of the table controls the plotting time instead.) After a record of 200 x 11 words is read from tape, the shading function, $f(\theta)$, is entered into the table and the listed trapezoids are shaded in their appropriate colors. Then $g(\theta)$ is entered and the highlights are added through the clear filter.

The functions f and g are actually tabulated in terms of $\cos^2 \theta$. I now demonstrate how $\cos \theta$ can be efficiently computed along a vertical scan line, using finite differences.

Fig. 3. Section of a sphere normal to the viewing plane, showing angle of incidence, θ , between illuminating ray and normal vector, PN.

Fig. 4. Projection of sphere on a viewing plane. The dotted line is the projection of the plane of Fig. 3.

Figure 4 shows the projection of a sphere onto the picture plane. The point $P = (X, Y, Z)$ is on the sphere's surface, $C = (X_C, Y_C, Z_C)$ is the center, and R is the radius. Figure 3 shows a section of this sphere, in a plane perpendicular to the dotted line.

From triangle PDC in Fig. 3, one finds

$$\cos^2 \theta = \frac{\overline{PD}^2}{\overline{PC}^2} = \frac{(Z - Z_C)^2}{R^2}. \quad (3)$$

Solving the equation of the sphere,

$$(X - X_C)^2 + (Y - Y_C)^2 + (Z - Z_C)^2 = R^2, \quad (4)$$

for $(Z - Z_C)^2$, and substituting in Eq. (3), I get

$$\cos^2 \theta = \frac{R^2 - (X - X_C)^2 - (Y - Y_C)^2}{R^2}. \quad (5)$$

Since the trapezoids have vertical sides, they are colored in vertical raster-scan lines. Along a vertical line such as the one shown in Fig. 4, the quantities R, X, XC, and YC are constant, so Eq. (5) represents a quadratic polynomial in Y. This polynomial is evaluated at successive points along the scan line, using finite differences. The second difference for any quadratic polynomial is a constant, equal to its second derivative. Thus only two differences are required, and the value accumulated from the differences will be exact.

4. THE VARIAN PROGRAM DNI

The Varian program DNI initializes the value K1 of $\cos^2\theta$ at the lowest point Q of the scan line, its first difference K2, its second difference K3, and the number N of points to be plotted. Then successive values of K1 can be plotted by the FORTRAN loop

```
DO 1 I = 1, N
  PLOT (K1)
  K1 = K1 + K2
1 K2 = K2 + K3. (6)
```

Here, PLOT takes the higher order 8 bits of K1 and stores them in a buffer, which is sent through the color-lookup table when full. Double buffering is used so the Dicomed can plot one buffer while the Varian fills another.

Since a vertical scan line may have N greater than 1000, and K3 is added effectively $N^2/2$ times in determining the last K1, double precision integer arithmetic is required. Double-word integers on the Varian have a sign bit and 30 data bits. (The sign bit in the lower order word is not used.)

If $\cos^2\theta$, which varies from 0 to 1, is multiplied by $(2^8-1) \cdot 2^{22}$, the higher order 8 data bits will be in the appropriate range. Therefore, if $B = (2^8-1) \cdot 2^{22}/R^2$ and X and Y are the coordinates, for Q, one has

$$K1 = B \cdot (R^2 - (X - XC)^2 - (Y - YC)^2). \quad (7)$$

The Dicomed is capable of coloring in an $n \times m$ raster rectangle for each byte in the data buffer, and this feature is used for plotting at less than maximum resolution. Thus, if JSP is the number of raster positions skipped on each step through the loop, K2 can be found by evaluating Eq. (7) at Y + JSP and subtracting the value at Y, giving

$$K2 = -2 \cdot B \cdot JSP \cdot (Y - YC) - B \cdot JSP^2. \quad (8)$$

The first term corresponds to the derivative of Eq. (7) and the second can be interpreted as a correction to get a secant line instead of a tangent. An equation for K3 can be determined similarly:

These equations will not actually be found in the Varian program, since the constants like $K3$, which are independent of the scan line, are computed when the sphere is initialized rather than just before the loop. The current version does not contain loop (6) either. Because the machine instructions for double precision arithmetic are quite inefficient and a writeable control store was available, the whole loop was replaced by a single new microcoded instruction. The assembly language routine QCAD ($K1, K2, K3, X$) loads the initial values into registers and calls this new instruction, which can execute the loop in eight 195-ns microinstructions per iteration. For atoms that fill up a substantial area of the screen, the microcode can generate the data faster than the Dicomod can plot it; but for smaller atoms, computing the upper and lower boundary arcs of trapezoids becomes the bottleneck.

Ideally, the shading for a cylinder is also a quadratic polynomial along a vertical scan line. However, after perspective projection, cylinders become cones and the shading is no longer so simple, especially when the directions of the projected edges lie in different quadrants.

In Fig. 5, QA and QC are the extensions of the projected edges of a bond and QB is the projected center line, all meeting at the "vanishing point" Q.

Fig. 5. Regions of picture plane formed by extended bond edges, QA and QC, and centerline QB.

For this case, the part of the bond lying in AQB will be shaded using quadratic polynomials on horizontal scan lines. The part in BQC will be shaded using different polynomials on vertical scan lines. These polynomials are adjusted to have their maximum value (as specified by the eleventh entry in the row initializing the bond) along the line QB and to be zero along QA and QC. Thus, they agree smoothly along QB and give a close approximation to the true shading. In a movie, the assignment of scan directions may switch as a bond rotates. This may cause a slight change in the shading, but it is not noticeable.

The following briefly describes the use and structure of the DSI program. The MAIN program starts by asking for two integers, IWAIT and IDFA, in format 211. If IWAIT is 1, the system pauses between frames so sheet film can be changed and continues when a carriage return is entered on the teletype. If IDFA is 1, a double advance is called between frames to produce 35mm pictures suitable for mounting in full-frame slides. If one of these options is not wanted, the operator should enter 0; if neither is wanted, the prompt can be answered with just a carriage return.

Next SETABL is called, which reads a list of measured film densities from the card reader and computes three sets of color-lookup tables: (1) for the color shading; (2) for the highlights; and (3) for the standard linear compensation, replaced when the program exits. The desired intensities, D1 for shading and D2 for highlights, are computed in terms of $EK = \cos^2\theta$. The formulas for D1 and D2 can be easily changed to give a different surface appearance. To get the lookup table output that will result in a desired brightness when the film is viewed, the program interpolates between the brightness resulting from the measured densities. (By definition, the density of film is the negative of the base 10 logarithm of the fraction of light the film transmits.)

Next, the computer asks for the integer -1096/RESOLUTION, which specifies how large a square pixel should be plotted for each data byte. This number must be either 1, 2, or 4.

Each new tape is requested by the message

MOUNT NEW TAPE AND PRESS RETURN

A record containing a 200 x 11 array of specifications is read as a block by the assembly language routine REED. Part-initialization rows of the matrix are processed by MAIN, while TRAPEZE is called to shade the trapezoids, as described above. The parameter KIND is 1 if the trapezoid arises from an atom sphere and 2 if it arises from a bond cylinder.

Each time a part of a new color is encountered, NEWCOL is called to switch the color filter wheel and to specify a new minimum value, AP, and range, BP, of the color table input for that color. Color plotting terminates when either the end of the input arrays is reached ($I = 201$) or an end-of-frame indicator is encountered ($NCI = -5$). Then the clear filter is put in place, the color table for the highlights is entered, and the same output data is regenerated and sent to the Dicomod to render the highlights. The variable KSTART saves the index of

the first data row for the next frame, which begins after the highlights have been plotted and the film advanced. The complete control flow to achieve all this is somewhat complex (as illustrated in the flowchart of Fig. 6).

If film is being recorded in three passes (red, green, and blue) for a greater variety of atom colors, the tables should be reloaded for each atom color. Also, the three tables should include a component of white (equal parts of red, green, and blue) near the center to give the highlight.

Similarly, if the output is being displayed on a frame buffer, a portion of the color table should be used to shade each color and the white component for the highlights should be included in the table entries.

Fig. 6. Flowchart for section of a minicomputer program DNI that processes input buffer from tape. Each frame in the buffer has its atoms and bond trapezoids rendered (a) for shading, in color, and (b) for highlights, in white.

5. STRUCTURE OF ATOMLLL

Appendix C contains a table of subroutines in ATOMLLL. This table has a short phrase describing their functions and shows their page number in the listing. Further information is available from the comments at the beginning of each subroutine, from the variables identified in Appendix D, and from the partial description below.

The ATOMS program has been considerably debugged and revised since the version reported in Ref. 1. The pseudo-code in Fig. 6 of Ref. 1 was a simplification of the actual code even at the time of writing, and some of the limitations in Ref. 1 do not apply. In particular, bonds will overlap each other correctly in the picture plane, contrary to statement 4 in the first section of Ref. 1, although they still must not intersect in space. Also, the curved edges, where bonds intersect their atoms, are rendered more realistically than the method suggested by Fig. 3 of Ref. 1. The coordinate transformations have been removed to conserve memory, but may easily be replaced.

The MAIN program gets the appropriate file names from the user and opens the input and output files. For each frame, it calls SETDAT to read the atomic coordinates and bond data from the input file, it calls INITL to initialize the data structure, and it calls PICTUR to do everything else. If the variable IWR, currently set equal to 0, is changed to 1, a file named TEXT of intermediate data will be created. TEXT can be used for debugging purposes to trace the progress of the calculations.

Subroutine SETDAT reads in the atomic coordinates from the input file. Users who want to interact with their picture on the TMDS by changing the point of view or the coordinates of the atoms, might replace SETDAT by their own routine to define or transform coordinates.

The first dimensions of many of the data arrays, currently 0605, can be easily decreased to save space or increased to render more atoms and bonds. Simply replace all symbols 0605 in the program by an alternate number, which is at least as large as the total number of parts: NATOMS plus NBONDS.

The quantity DELTAR is the half-width of the black line between different atoms and bonds regions. Since the TMDS shows the outline of these regions, its picture will consist mostly of double lines if DELTAR is positive; a more pleasing picture will result if DELTAR is zero. However, a positive value is needed for colored photographs to prevent adjacent differently colored regions from bleeding together. A positive value is also useful to accentuate the outlines.

Subroutine INITL eliminates atoms and bonds that lie outside the picture plane and locates the circles where bonds intersect the atoms they join.

A linked list of potential picture-plane interactions is maintained in common arrays IWHERE, NEXT, and LAST. For each part B, LAST(B) points to the beginning of B's list. If L is an index on B's list, IWHERE(L) gives the number

F of this interacting part and NEXT(L) points to the next item on the list for part B. If F is positive, part F may hide part B. If F is negative, part (-F) may "truncate" part B; i.e., parts (-F) and B intersect in space and this intersection may affect the way they hide each other. These lists are initialized to zeros at the beginning of INITL. As INITL processes bonds, their interactions with the atoms they join are added to the list.

The next routine, PICTURE, processes the array of parts, one color at a time. For each part J of the correct color NC, KSCAN is called to add to the interaction list any succeeding parts that might interact with J. At the same time, the reverse interactions of J with any other parts M are also noted, so J may be skipped when KSCAN considers the interactions for M. This avoids almost half the comparisons and saves significant time in the case of complex pictures, at the expense of a lot of memory. For smaller pictures, the size of IWHERE and NEXT, currently 4700, could be decreased. (Note also the 4700's in the seventh and ninth executable statements of INITL.) Alternatively, at the expense of some extra computer time, all three arrays could be eliminated and KSCAN combined with DIGEST to find the interactions as they are processed.

After the current version of KSCAN updates the interaction list to include all interactions with part J, the list is processed by DIGEST, resulting in a list of visible trapezoids for part J. The first step is done by CTRAP, which outputs the shading information for a part and which creates its initial list of trapezoids: two for an atom and up to seven for a bond. The parameters for these trapezoids are stored in the arrays in common block TRAPP, starting with index 8. Then for each part in the list of potential interactions for part J, a list of "mask" trapezoids is created using the first seven entries in these arrays. The two lists are compared, trapezoid by trapezoid. If a mask trapezoid overlaps a part trapezoid the routines TRAP, ATRAP, and ALIST are called to remove the part trapezoid and replace it with the pieces into which it is chopped (Figs. 2b and 2c). If any such interaction has occurred for a masking part, COMPACT is called to rejoin trapezoids adjacent in the picture and also in the list. This may happen if the reason for their separation has now become hidden (Fig. 2(d)).

The details of the routines DIGEST, TRAP, ATRAP, and ALIST, which form the heart of the hidden-surface algorithm, are beyond the scope of this report.

The routine OUTPUT takes the final list of visible trapezoids for a part, loads the data for each into an integer array KO of length 11, and modifies it into the output format described in section 2. It then calls WRTBUF to copy KO into the output buffer, KOUT. The nonvertical sides of each trapezoid are also drawn on the TMDS, if requested.

The routine WRTBUF is also called when frames are completed or when the job is completed. In addition, when new parts are created by CTRAP, WRTBUF is called to set up the proper row of KOUT as described in section 2. In this case, the information is taken from array LO instead of KO. When a record has been filled and output to disk, the old array LO is copied as the first row of KOUT for the new record. Thus the Varian minicomputer can regain the initialization of the part if it is drawing after the input buffer is overwritten.

The Varian reads 7-track tape in a mode requiring three 6-bit tape frames to fill up a 16-bit word; it disregards the two higher order bits of the 18 read in.

On the other hand, the 7600 writes 10 tape frames per 60-bit word, wasting nothing. Thus the 200 x 11 array KOUT of 18-bit bytes is equivalent to the 660 60-bit word array KEQU for output. Actually, KEQU is first block-copied to LEQU, which lies in the 7600's large core memory. LEQU is then transferred to disk. This double transfer speeds up the 7600, since the second transfer can take place in parallel with other computations. On other computers, this will not be useful, so KEQU should be output directly, and the first two lines after the comments in WRTBUF should be deleted.

Another quirk concerns the representation of negative numbers. The 7600 is a two's-complement machine, with the possibility of negative zeros. However the output file must be read by the Varian, which is a one's-complement machine. Thus the statement

$MO(M,KIND) = MO(M,KIND) + ZERO$

is required to eliminate the negative zeros and the following statement

$IF(MO(M,KIND).LT.0) MO(M,KIND) = MO(M,KIND) + 1$

is required to adjust negative numbers to their one's-complement form. On other installations, different methods may be required to account for word size and form. The problem of conversion could be avoided by using two machines with compatible floating-point formats or using one machine to do everything.

The only constructions that are not standard FORTRAN are an occasional IF ... THEN ... ELSE ... ENDIF, and the input and output in MAIN, SETDAT, and WRTBUF. Unit 6 is used for output of the data for the Varian; unit 12 is used for output of the debugging information, if requested; and unit 10 is used for the input file. Unit 59 is the terminal used both for input of specifications and output of messages.

The variable ITM in main, currently set equal to 8, may be changed to 9 to write the output directly to tape instead of to disk. For this case, the prompt TAPE NAME replaces OUTPUT FILE NAME. When the name is supplied, the program halts until the tape is mounted. In this latter case, consistent parity errors can be expected and error-recovery procedures should be added to the routine WRTBUF.

The subroutine NEWFIL is called to open the output file and subsequently, each time a file is full, to open a new one.

REFERENCE

1. K. Knowlton and L. Cherry, "ATOMS -- A Three-D Opaque Molecule System -- for Color Pictures of Space-Filling or Ball-and-Stick Modules," *Computers and Chemistry* 1, 161 (1977).

APPENDIX A. SAMPLE DATA AND INTERACTIONS

Below is the data file LLL, containing three atoms and no bonds.

```

3      15
9.1    15    13.1  1.46  3
-1.1    9.1  12.6    .9  2
.17    1.76  39.6  1.07  1

```

0

The following is the teletype interaction to create (1) a picture on the TMB, and (2) an output file LD. Figures 2a through 2d show intermediate stages in rendering the first atom. A carriage return was entered after the computer displayed the TMB picture and typed ">".

```

NAME / L L L
GETFILE OK TMB? Y OR N
Y
MONTAGE 0, 200
ENDFILE NAME:
111
GETFILE NAME:
LD
OR SAVE L L L FILE LD
>

```

1.16 COLD WRITTEN.

ALL DONE.

Next, the file LD was copied to a blank tape named LD1, using TAPECOPY. The prompt OPTIONS OR CARRIAGE RETURN was answered with simply a carriage return, since no options had to be specified.

```

TAPECOPY
OK
LD # LD1 1
OPTIONS OR CARRIAGE-RETURN

```

WAITING ON TAPE ASSIGNMENT
ALL TAPES ASSIGNED.

1 END-OF-FILES READ. TYPE 1 (NEW INPUT FILE), 0 (NEW OUTPUT FILE), CARRIAGE-RETURN (CONTINUE), END (TERMINATE), OR OPTIONS: END

ALL DONE

Below is the completed Dicomed job request form, which should be attached to the tape when it is submitted.

job length (approx):	1 frames	3 minutes
check camera to use:	35mm	16mm low 16mm x 4x5 inch
film to use:	x color	black and white 4x5 type
check PROGRAM to use; check or fill in values for OPTIONS to use:		
FR80	POINT	SRI.
options:	#X, #Y	scale
	scale	# picture
	# pictures	# colors
	# colors	linear?
	filter #	compensated?
x OTHER DNI	invert intensities?	double frame?
options:	linear?	filter seq
1024 resolution	compensated?	(if different)
	double frame?	
	6 or 8 bit?	

REMARKS:

date & time plotted	# frame	time used
---------------------	---------	-----------

REQUEST TO PLOT DICOMED JOB

tape name	LDI	date	12 April 1979
submitter	Nelson Max	box #	P23
dept or dev	comp	classification (UNCL, PARD, etc)	UNCL
phone ext	2-4074		

Below is the interaction that took place when the Dicomed operator ran the program DNI. Figure 7 shows the resulting 4- by 5-in. color Polaroid.

```
/LOAD,DNI
IWAIT,HDA, 244

4096/RESOLUTION, 13
4
MOUNT NEW TAPE AND PRESS RETURN .

FINISHED FRAME 1
JC**
```

Fig. 7. Color Polaroid output for Example 1.

Next, we consider the file SDATA, which describes three different views of a three-atom structure, including bonds. Here is the data file:

```

3      .37
-1.    -1.    10.    .7  1
-1.     2.    12.    1.2 2
 2.    -2.    14.     1. 3
 2      .2
1 2
1 3
 3      .37
-1.    -1.    20.    .7  1
-1.     2.    24.    1.2 2
 2.    -2.    24.     1. 3
 2      .2
1 2
1 3
 3      .37
-1.    -1.    20.    1.4 1
-1.     2.    24.    2.4 2
 2.    -2.    24.     1. 3
 2      .2
1 2
1 3

```


Again, the three frames appeared on the TMDS. The output file SD1 was copied to tape and run on the Dicomed.

```
ATOMC / 1 1.1
OUTLINES ON TMDS? Y OR N
Y
MONITOR NO.?362
INPUT FILE NAME:
SDATA
OUTPUT FILE NAME:
SDA
CREATED DISC FILE      SDA
>
>
>
```

1 RECORDS WRITTEN.

ALL DONE

```
TAPECOPY
OK
SDA Ø +SD2 1
OPTIONS OR CARRIAGE-RETURN
```

```
WAITING ON TAPE ASSIGNMENT
ALL TAPES ASSIGNED.
```

1 END-OF-FILES READ. TYPE 1 (NEW INPUT FILE), 0 (NEW OUTPUT FILE), CARRIAGE-RETURN (CONTINUE), END (TERMINATE), OR OPTIONS
END

ALL DONE

The TMDS pictures are in Fig. 8 and the first two color output pictures are shown in Fig. 9. Note that the pictures have been clipped at the frame boundaries. Figure 10 shows six base pairs of DNA, including approximately 400 atoms. It took 2 seconds on the CDC 7600 for ATOMLLL to compute the visible parts of this structure, and 100 seconds for the picture to be shaded by DN1 and plotted on the Dicomed.

Fig. 8.(a) Line-drawing output for Example 2, first frame, showing closeup. The television monitor display system (512- by 512-pixels resolution) has been rescanned at higher resolution for this report.

Fig. 8.(b) Line-drawing output for Example 2, second frame.
The molecule has been moved farther away.

Fig. 8.(c) Line-drawing output for Example 2, third frame.
The atom radii have been increased.

Fig. 9 (Top) Color Polaroid output corresponding to Fig. 8(a). (Bottom) Color Polaroid output corresponding to Fig. 8(b).

Fig. 10. A six-base-pair segment of DNA, containing over 400 atoms.

APPENDIX B. ERROR MESSAGES

The following error conditions are reported on the user's terminal. If they are fatal, the program will exit prematurely. Other ORDERLIB, TV80LIB, and system error messages may also occur.

n BAD TRAP PASSED

Subroutine ALIST has been asked to add to part n's list of visible trapezoids a trapezoid for which $XTL < YBL$, $YTR < YBR$, or $XR < XL$. This trapezoid will not be added and a black gap may appear in the picture. This could be caused by a round-off error or, more likely, a bug in the program logic. The error is not your fault, and there is nothing you can do except complain to the author.

BAD TRAP CREATED BY BRAKUP

This message will appear, with circumstances and consequences similar to the one above, when BRAKUP creates a bad trapezoid by subdividing a convex region. It could be caused by a bug in BRAKUP or by incorrect input to BRAKUP. Again, there is nothing you can do about this.

MORE THAN 7 TRAP FOR MASK

Only seven spaces are allowed in the common arrays in /TRAPP/ for mask trapezoids. This message indicates that BRAKUP has found more than this, probably due to an incorrect counterclockwise tour of the boundary of the projection of a bond. Again, nothing can be done. The above three errors will cause a (hopefully small) trapezoid to be left out and should not seriously affect the final picture.

NELSON CANNOT CREATE <name>

Fatal

The system was unable to create the output data file <name> requested by NEWFIL, probably because not enough disk space or file index space was available. Rerun the program after files have been released by you and other users.

ERROR WRITING OUTPUT FILE.

Fatal

Subroutine WRTBUF found an error condition after writing the output buffer. This is unlikely for a disk file, but parity errors may be expected consistently if ITM was changed to 9 so that the output goes directly to tape. Error recovery procedures should be added to WRTBUF.

BOND LOST FROM BAD TRUNCATION n

Subroutine CTRAP tried to shrink by DELTA the region that it created for a bond. It found that an end arc did not intersect the bond profile line at corner n. The bond will be missing from the picture. This would be due to a software bug, and there is nothing a user can do but report it.

LIST OF INTERACTIONS EXCEEDED

Fatal

(From subroutine ADDA.) The linked lists of interactions in IWHERE and NEXT are not large enough. Increases their size as suggested in section 5.

TOO MANY BOUNDARY ARCS

Fatal

Subroutine BRKUP required more than 14 upper and lower boundary arcs in temporary storage when breaking up a convex region into trapezoids. This is probably due to a bad specification of the boundary in its input. Again, a software bug that is not the user's fault.

APPENDIX C. SUBROUTINES

MAIN	assigns input and output files	1
SETDAT	reads input data	3
PICTUR	loops by color	4
INITL	calculates picture plane coordinates	6
KSCAN	lists possible interactions	13
IBOA	bond-atom interaction	15
IBB	bond-bond interaction	19
IAA	atom-atom interaction	24
DIGEST	processes list of interactions	26
CIRCIR	finds intersection of two circular arcs	32
KIND	kind of arc	34
POINT	calculates Y-coordinate of arc	35
SLOPE	calculates slope of arc	36
ERASE	makes part invisible	37
IBOX	preliminary bond-atom overlap	38
ICCPAR	compares two circles	39
DIST	square of distance from origin	40
BLOCK DATA		41
FREE	returns an interaction list to free storage	42
ALIST	adds trapezoid to list for part	43
CINT	intersection of two arcs	45
CIRLIN	intersection of circular arc and line	46
TRUNC	3-space intersection of two spheres	48
ADDA	adds to interaction list	50
TTRUNC	makes mask trapezoids for truncation	51
BRKUP	turns convex region into trapezoids	55
TRAP	compares mask and part trapezoids	61
ATRAP	does non-trivial trapezoid interactions	66
CTRAP	creates trapezoids for part or mask	70
OUTPUT	formats trapezoid list for output	78
COMPACT	rejoins adjacent trapezoids	81
WRITBUF	adds a row to output array	82
NEWFIL	creates a new disk file	84

APPENDIX D. VARIABLES AND ARRAYS IN COMMON

COMMON /VCONST/NCOL, NATOMS, NBONDS, CAMX, CAMY, CAMZ, AIMX, AIMY, AIMZ, ZMIN,
PRATIO, ARATIO, DELTAR, NTRPPZ, VIMX, VIMY, VIMZ, IFIRST, NTOTRP, ITV, IWV,
FINISHED

NCOL = number of colors
NATOMS = number of atoms
NBONDS = number of bonds
CAMX, CAMY, CAMZ
- obsolete
AIMX, AIMY, AIMZ
- obsolete
ZMIN = cut-off plane in front of camera - things closer than zmin are invisible
PRATIO = ratio of picture plane width to picture plane distance from camera
DELTAR = 1/2 width of black line between overlapping things
NTRPPZ = number of trapezoids thus far in current frame arising from atoms (not used in calculations; at one time it was output on teletype)
VIMX, VIMY, VIMZ
- obsolete
IFIRST
- obsolete
NTOTRP = number of trapezoids thus far in current frame (not used in calculations)
ITV = 1 if TMDS picture requested; 0 otherwise
ITM = 1 if supplementary output requested on unit 12 for debugging; 0 otherwise
FINISHED = 1 if end of job, so that output buffer should be flushed to output file after current WRTBUF transfer; 0 otherwise

COMMON/ MINW/WMIN

WMIN = minimum width of trapezoid

COMMON /TOUT/NOUT, KEQU(600), LO(11), KO(11), TAPENAME, RECORDS

KEQU is equivalenced to the byte(18) array KOUT(200,11); LO and KO are equivalenced to the array MO(11,2)

NOUT = the current row number in KOUT
KEQU = the output buffer
LO = the new row, if a part identifier
KO = the new row otherwise

TAPENAME = name (or bin number) of current output tape
 NRECORDS = number of records on current output file
 ISCNAME = name of current disk output file
 ITM = 8 for disk output or 9 for tape output

COMMON /COM/ZPICT,NSUM,NBS

ZPICT = distance of 2-wide picture plane from camera, = 2/PRATIO
 NSUM = total number of things (NATOMS+NBONDS)
 NBS = where bonds start (NATOMS+1)

COMMON /MCOORD/COORD/(0605,8)

Contains atoms and bond coordinates. Coord is always equivalenced to arrays
 CIR, ATOMS, BONDS, and always indexed as in column 3 below to improve
 clarity of code

atoms:

COORD(*,1) = ATOMS(*,1) = ATOMS(*,1R) = 3d radius
 COORD(*,2) = ATOMS(*,2) = ATOMS(*,1X) = 3d X center
 COORD(*,3) = ATOMS(*,3) = ATOMS(*,1Y) = 3d Y center
 COORD(*,4) = ATOMS(*,4) = ATOMS(*,1Z) = 3d Z center
 COORD(*,5) = CIR(*,5) = CIR(*,CR) = pp radius
 COORD(*,6) = CIR(*,6) = CIR(*,CX) = pp X center
 COORD(*,7) = CIR(*,7) = CIR(*,CY) = pp Y center
 COORD(*,8) unused

bonds:

COORD(*,1) = BONDS(*,1) = BONDS(*,NR) = near-end pp radius
 COORD(*,2) = BONDS(*,2) = BONDS(*,NX) = near-end pp X
 COORD(*,3) = BONDS(*,3) = BONDS(*,NY) = near-end pp Y
 COORD(*,4) = BONDS(*,4) = BONDS(*,NZ) = near-end 3d Z
 COORD(*,5) = BONDS(*,5) = BONDS(*,FR) = far-end pp radius
 COORD(*,6) = BONDS(*,6) = BONDS(*,FX) = far-end pp X
 COORD(*,7) = BONDS(*,7) = BONDS(*,FY) = far-end pp Y
 COORD(*,8) = BONDS(*,8) = BONDS(*,FZ) = far-end 3d Z

COMMON /MCONST/IR,IX,IY,IZ,CR,CX,CY,IA1,IA2,NR,NX,NY,NZ,FR,FX,FY,FZ

constants for indexing into coord and its equivalent arrays as described
 above

COMMON /MCOL/ICOL(0605,3)

ICOL is equivalenced to NAC and MBONDS

atoms:

ICOL(*,1) = NAC(*,1) = color of atom
 (in same order as coord)
 ICOL(*,2) - unused
 ICOL(*,3) - unused

bonds:

ICOL(*,1) = color of bond

ICOL(*,2) = MBONDS(*,1) = new index of near end atom

ICOL(*,3) = MBONDS(*,2) = new index of far end atom

COMMON /I1/IWHERE(4700)

COMMON /I2/NEXT(4700)

COMMON /I3/LAST(0605),LEPTR

linked list of possible interactions

LAST(*) is indexed by atom-bond number and points to the last entry for that atom or bond or 0 if none

NEXT(*) points to the next entry - indexed by number obtained from LAST or NEXT

WHERE(*) contains the number of the atom or bond to interact, negative number if truncation or 0 for picture plane mask

LEPTR is next empty place in NEXT and IWHERE

COMMON /TRAPP/IPTRM(7),IPTRP(50),KTBM(7),KTBP(50),KBBM(7),KBBP(50),

RTM(7),RTP(50),RBM(7),RBP(50),XCTM(7),XCTP(50),

XCBM(7),XCBP(50),YCTM(7),YCTP(50),YCBM(7),YCBP(50),

YTLM(7),YTLP(50),YBLM(7),YBLP(50),YTRM(7),YTRP(50),

YBRM(7),YBRP(50),XLM(7),XLP(50),XRM(7),XRP(50), LTPTR,LT,INDEX,ITOP,IBOT

TRAPP contains the parameters that describe the trapezoids. In most routines it appears as above where names ending in "m" describe masks and where names ending with "p" describe parts. In subroutine BRAKUP, the mask and part names are put together into 1 array, so IPTRM(7),IPTRP(50) becomes IPTR(57), etc., in routines POINT, SLOPE, ALIST, CINT the top and bottom arrays are also combined so RTM,RTP,RBM,RBP are combined into R(114).

IPTRM = contains the index of the next mask trapezoid or 0 for last

IPTRP = contains the index of the next part trapezoid or 0 for last

KTBM,KTBP,KBBM,KBBP

- kind of top(KTP) or bottom (KBB) boundary - 1=convex up,
2=concave up, 3=line

RTM,RTP,RBM,RBP

- radius of top(RT) or bottom(RB) arc if boundary curved, or slope
if boundary is a line

XCTM,XCTP,XCBM,XCBP

- X-coordinate of center of top(XCT) or bottom(XCB) arc if
boundary is curved; or Y-intercept if boundary is a line

YCTM,YCTP,YCBM,YCBP

- Y-coordinate of center of top(YCT) or bottom(YCB) arc if
boundary is curved; unused if boundary is a line

YTLM,YTLP,YBLM,YBLP

- Y-coordinate of top left(YTL) or bottom left(YBL) corner of
trapezoid

YTRM,YTRP,YBRM,YBRP

- Y-coordinate of top right(YTR) or bottom right(YBR) corner of

trapezoid
 XLM,XLP,XRM,XRP
 - X-coordinate of left(XL) and right(XR) edge of trapezoid
 LTPTR - next empty place in arrays
 LT - index of trapezoid pointing to 1 (for linking in alist)
 INDEX - index of boundary for point of slope
 ITOP - index of top boundary for new trap passed to ALIST
 IBOT - index of bottom boundary for new trap passed to ALIST

COMMON /LFIR/LFIRST

LFIRST is index of first part trapezoid or 0 if none

COMMON /ATRAPP/XR,YTL,YBL,TYTL,TYBL,XR,YTR,YBR,TYTR,TYBR

contains the corner coordinates of the mask- and part-overlap regions found by digest and passed to TRAP

XR,XL = left and right X-coordinates

YTL,YBL,YTR,YBR

= top and bottom left and top and bottom right Y-coordinates for part

TYTL,TYBL,TYTR,TYBR

= top and bottom left and top and bottom right Y-coordinates for mask

COMMON /INTERC/IFLQB,XLBB,XRBB,YRBB,IFLGT,XLTB,YLTB,XRTB,YRTB,I,K,I7,I7B,KB

used primarily to pass parameters from TRAP to ATRAPP

IFLQB = number of intersections between either top of part and top of mask or bottom of part and bottom of mask or 3 if none
 (XLBB,YLBB),(XRBB,YRBB) are the intersections

IFLGT = number of intersections between either the top of part and bottom of mask or bottom of part and top of mask, or 3 if none
 (XLTB,YLTB),(XRTB,YRTB) are the intersections

I = index of part trapezoid

K = index of mask trapezoid

I7 = index of part if mask and part arrays combined

I7B = index of bottom of part if mask and part arrays combined and top and bottom arrays combined

KB = index of bottom of mask if mask and part arrays combined and top and bottom arrays combined

COMMON /LOOPS/INARC(14),XC(14),YC(14),RA(14),XI(14),YI(14),

IFLG,IPREV

defines boundaries of enclosed area for brakup

INARC = index of next arc or line (clockwise)

XC,YC = center of arc or slope and Y-intercept of line
 RA = radius of arc or 0 for line
 XI,YI = end point of arc or line
 IFLG = index of starting trapezoid (i.e. 1=mask, 8=part)
 IPREV = number of arcs and lines

COMMON/JBALL/J

J = part number of current part

COMMON /BTRUNK/XTRUNK,YTRUNK,RTRUNK

used to store definition of concave truncation arc on the end of a bond,
caused by intersection with near atom.

XTRUNK,YTRUNK

= X- and Y-coordinates of the center of arc

RTRUNK = the radius of arc

COMMON /TEMPL

used to store some temporary variables in subroutines; vestige of a
minicomputer implementation with space limitations