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HIGH RESOLUTION COLOR RASTER COMPUTER ANIMATION OF SPACE FILLING MOLECULAR MODELS

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ABSTRACT

The ATOMLLL system efficiently produces realistic photographs of ball-and-stick or space-filling molecular models, with color shading, highlights, shadows, and transparency. The hidden surface problem for a scene composed of intersecting spheres and cylinders is solved on a CDC-7600, which outputs onto magnetic tape the outlines of the visible parts of each object. The outlines are then rendered, at up to 4096 x 4096 resolution, by a Dicomed D-48 color film recorder, controlled by a Varian V-75 minicomputer. The Varian computes the shading and highlights for each pixel in a fast microcoded loop. Recent modifications to give shadows and transparency are described.

Two films will be projected at the session. The first shows the intercalation of ethidium and adriamycin between the base pairs of DNA, as simulated by conformational energy minimization. The second shows the structure of the protein coat of the tomato bushy stunt virus, as determined by X-ray crystallography.

HIDDEN SURFACES

The ATOMLLL system is derived from the ATOMS code, written at Bell Telephone Laboratories by Ken Knowlton and Lorinda Cherry [1], and draws shaded raster pictures of molecules. The philosophy of the system is to separate the computation-intensive hidden-surface part of the task from the IO-intensive rendering of the visible surfaces on a film recorder.

In the Livermore version, (see [2], [3], [4]) the hidden surface calculation is done on a CDC 7600 computer. The input is a list of atoms, with their center coordinates and with either a chemical type or a color and radius, and a list of bonds, if any. The visible portion of each atom sphere or bond cylinder is divided up into trapezoid like shapes bounded above and below by circular arcs, as shown in figures 1a, 1b, and 1c. The hidden surface computation can then be reduced to comparing one of these "trapezoids" with a second, and if they overlap, modifying or subdividing the first to remove the part belonging to the second, as shown in figure 1b and 1c.

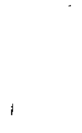

Fig. 1 (a) Initial subdivision of an atom.

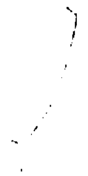

Fig. 1 (b) Subdivision caused by intersecting atom.

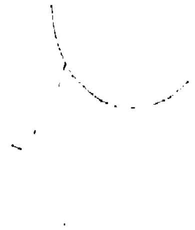

Fig. 1 (c) Further subdivision caused by occluding atom.

SHADING

When all such modifications are completed, the list of visible trapezoids for a sphere is copied to magnetic tape, with a header giving the center, color, radius, and highlight location. This tape is read by a Varian V-75 minicomputer, which controls a Dicomed D-48 color film recorder. Each trapezoid is rendered in raster mode along vertical scan lines. The intensities on a scan line are generated by a quadratic polynomial, which is calculated in a fast microcoded loop, at 1.35 μs per point, coupled with an appropriately loaded color look-up table (see [3] for details.) The Dicomed has a computer controlled color filter wheel with seven colors, and all the atoms of one color are rendered before the wheel is turned. After all colors are filled, the circular or elliptically shaped highlights are added through a clear filter, using the same microcode but a different look-up table.

SHADOWS

If a sphere is illuminated from the side, as is the moon by the sun, part of the sphere, bounded by an elliptical arc, is self shadowed, and is rendered dark. The shading on the rest can be approximated with the same microcode mentioned above. However, if another sphere casts a shadow on the first, the shadow would be bounded by a complicated algebraic curve of degree four, and would be difficult to break up into trapezoids.

Instead of rendering this cast shadow directly, I have chosen to dim the whole sphere by the proportion of its area which is shadowed by other spheres. To do this, a hidden surface picture is calculated from the point of view of the light source. The area of each sphere which is visible in this view is divided by the area which could be visible if other spheres were not in the way. The quotient is entered on the sphere's header, and used to multiply all shading intensities. A similar fraction for the highlight areas is computed to modify the highlight intensities. Since the highlight areas are fairly small, the highlights will turn on and off fairly accurately as an object moves or rotates into shadow.

TRANSPARENCY

For transparent molecules, only the exterior surfaces of the atom spheres are rendered, not the surfaces which lie inside other spheres. This exterior surface reveals the shape of the molecule, without confusing inner surfaces. The exterior surfaces are rendered in two passes; one for the forward facing pieces and one for the back facing pieces, which have opposite highlights. Each surface piece is bounded in part by the sphere's profile, and in part by ellipses. The ellipses are projections of the circles where the sphere intersects other spheres, and are approximated by circular arcs to make the trapezoids.

A third pass records the "front transparent surfaces", which would be visible even if the transparent surfaces were opaque. When this pass is added, these front transparent surfaces become brighter than the others, providing some depth cues to the viewer. If the scene contains any opaque molecules, these are rendered in a fourth pass.

As discussed in [5], optical printing can be used to partially mask one pass by the images in another. The forward and rear facing transparent surfaces are used to mask the opaque surfaces, and the front transparent surfaces are used to mask the other transparent surfaces. In addition, all passes can be used to mask a background, which may be any photograph or movie. This masking gives further information about the depth ordering of the surfaces. When combined with rotation, these transparent images can explain the relationship between the surfaces of two interacting molecules. Robert Langridge presented in the same session [6] a complementary method of viewing such interactions, using a real time color vector display.

FILMS

Two movies will be shown at the session. The first concerns the interaction of DNA with ethidium, a mutagenic DNA stain, and adriamycin, a cancer drug. Both of these molecules interact by intercalating, slipping between two base pairs, which have increased their separation to make room for the drug. Figure 2 shows a transparent DNA molecule, with an opaque ethidium ion intercalated between its center two base pairs. The conformation of the DNA was calculated by the method described in [7]. The interaction with adriamycin is described in [8] and [9].

The second film shows the structure of the protein coat of the tomato bushy stunt virus, as determined by x-ray crystallography [10]. The coat is made up of 180 chemically identical subunits, which are slightly deformed to fit together in three different symmetry environments. Figure 3 shows 90 of these subunits, as single large spheres, with different colors indicating the different symmetry environments. The small yellow spheres represent α-carbons of parts of these chains which are involved in linking the subunits up into a structure with dodecahedral symmetry. Note the highlights and shadows produced by a light source above the structure.

Acknowledgement

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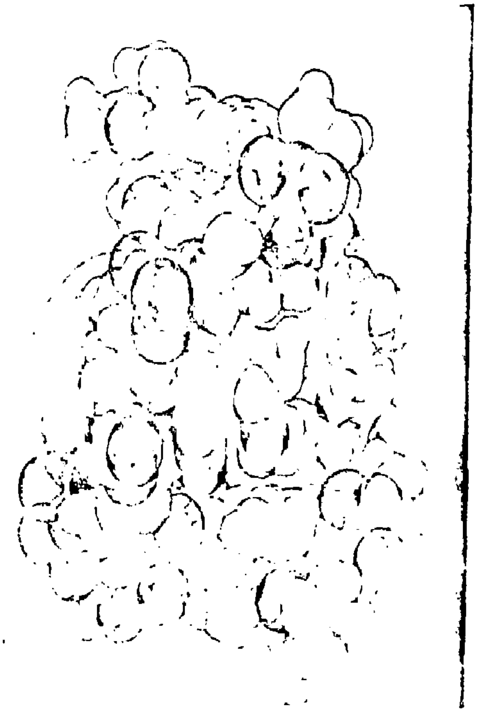

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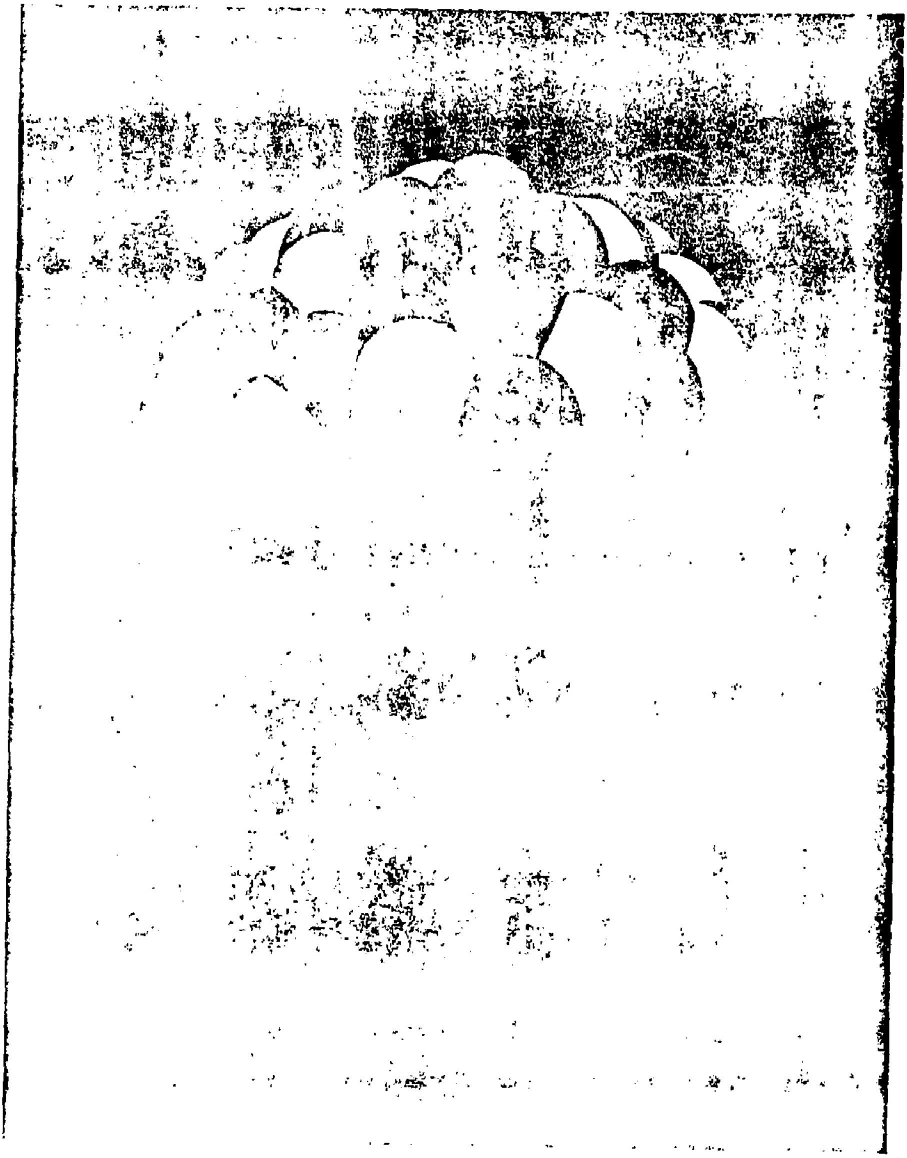

Figure 3. Protein coat of the tomato bushy stunt virus. Large spheres represent half of the 180 coat subunits, and small spheres represent chains which link the structure together.