RMS: programs for generating raster molecular surfaces

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RMS (Raster Molecular Surfaces) is a package of programs that offer the researcher a number of solid modeling techniques for presenting a macromolecular structure. The programs use a mapping algorithm, calculating the shading parameters only once, to reduce computation time. A simple linear approximation is used for antialiasing of atomic edges, shadows and surface intersections. I have implemented two major advances: depth cueing using an opaque "fog" and z-clipping to show detailed interactions in the interior of molecules. Spherical atoms and cylindrical bonds are also available.

Keywords: molecular surface, antialiasing, depth cueing, cast shadows, clipping

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INTRODUCTION

Computer graphics is a powerful tool for both analyzing and presenting molecular structure. Macromolecular structures pose an interesting representational problem: The large number of atoms in proteins and DNA make for complicated images. During the analysis of a new structure, interactive computer graphics hardware is the solution to this complexity. The molecule is imaged with software such as GRANNY[1] and GRAMPS.[2] Real-time rotation, polarized viewing of stereo pairs, and movable clipping planes increase the comprehensibility of the structure, and the researcher can jump to any point in the molecule, examining any part at will.

Unfortunately, all these advantages disappear when the images are published. Even the clarity provided by stereo pairs is not available to a large sector of the journal-reading audience, especially those outside the field of crystallography. All the tricks of three-dimensional (3D) modeling — shadows, depth cueing, color, and so on — are needed to create images that convey the structural information in an obvious way. A carefully constructed mono image should be able to convey all of the information, with stereo viewing as an added bonus.

RMS (Raster Molecular Surfaces) is a package of programs created to give the researcher a number of imaging options for presenting a macromolecular structure. It is best used after a thorough analysis of the structure. With RMS, the user can create a series of pictures highlighting the interesting aspects of the molecule. Calculating the images requires a moderate amount of time (up to several minutes on a VAX 11-780), so for analyzing a structure, the faster interactive programs are preferable.

Two molecular model representations are available with RMS: spherical atoms and cylindrical bonds. A number of modeling techniques make these images more interpretable. These include antialiasing, depth cueing, cast shadows, Phong shading and z-clipping. Color is added through the use of color separations to allow use of the full 256-step gray scale for smooth shading.

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PROGRAM DETAILS

Mapping algorithm

A mapping algorithm is used to reduce the computing time. A shaded sphere centered at the origin is calculated for eight atom types at the beginning of the run. This template is mapped into a z-buffer, centered at the position of each atom in the molecule. The two highest atoms at each pixel are saved during the mapping operation. This yields a viewer-visible shell, which is processed for depth cuing, shadows and antialiasing of intersections. Only the visible segments are processed in these computationally expensive tasks.

RMS stores several large frame buffers covering the entire image, typically 400 by 600 pixels, containing intensities, z-levels and so on. Arrays of this size are acceptable in the current implementation on a VAX 11-780 and VAX 8800. The programs would be fairly simple to convert to a scan-line algorithm for use on hardware with less dynamic memory, with some loss in computational efficiency.

Antialiasing

Aliasing occurs when a continuous object is sampled at discrete intervals. Unless some technique of antialiasing is performed, distracting "jaggies" appear, especially at edges with slopes nearly horizontal or vertical. Figure 1 shows an image with aliasing artifacts and the same image with antialiasing. Exact analytical or subdivision algorithms typically have been used to calculate how much of the pixel is covered by the object.[3] RMS uses a simpler linear approximation, with lower computational cost.

Calculating the antialiasing percentages at the edge of an atom is performed before the mapping operation.

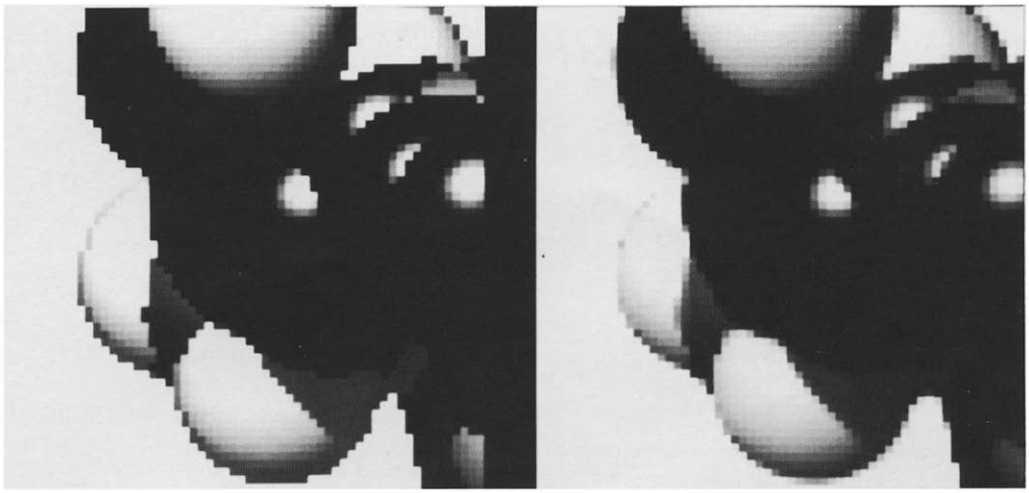

Figure 1. The effect of antialiasing. A small section of Figure 3 is enlarged, so individual pixels are visible. The left image shows aliasing: an abrupt change from foreground to background at the edges, resulting in "jaggies" around the outside of the atoms. In the right antialiased image, the foreground is shaded slowly into the background, over the width of a pixel, resulting in a smooth circular edge. You can also see antialiasing at the edges of the shadows and at the intersections of surfaces

A percentage template is created, with values of 0.0 outside the atom, 1.0 inside the atom and intermediate values near the edge. This template is mapped into a z-buffer, along with the intensity and z-level of the atom. The distances from the center of the atom to the pixel being tested (R_{pix}) and the radius of the atomic sphere (R_s) are used to calculate the antialiasing percentage:

$$\begin{aligned} R_{p.x} < R_s - 0.5 &: P_{\text{antialiasing}} = 1.0 \\ R_s - 0.5 < R_{pix} < R_s + 0.5 &: P_{\text{antialiasing}} = R_s - R_{pix} + 0.5 \\ R_s + 0.5 < R_{p.x} &: P_{\text{antialiasing}} = 0.0 \end{aligned}$$

This calculation is performed only for the eight spherical templates, not for every atom in the molecule. Antialiasing of the cylindrical bonds is calculated similarly, using the perpendicular distance from the center of the bond in place of the distance from the center of the atom.

The pixels in which two atoms intersect also need to be antialiased. The calculation is performed after the mapping operation, using the two highest atoms at each pixel. If the distance between the surfaces of these two atoms is less than three pixel widths in the z direction, the pixel is tested for intersection. Otherwise, the pixel is assumed to be totally covered by the upper atom. The distance, in the xy plane, from the center of the pixel to the intersection of the two surfaces (D_{int}), is used to calculate the percentage of each atom in the pixel:

$$\begin{aligned} 0.0 < D_{int} < 0.5: \quad P_{\text{upper atom}} &= 0.5 + D_{int} \\ P_{\text{lower atom}} &= 1.0 - P_{\text{upper atom}} \end{aligned}$$

The distance D_{int} can be approximately calculated from the z-levels of the two surfaces at the center of the pixel and their surface normals. Both quantities are available from the shading templates. The difference in z-level of the two surfaces was used at first to approximate the antialiasing percentages, but unacceptable artifacts appeared when the surface normals of the two atoms were different. The current process has trouble only when one surface is nearly edge-on to the viewer. Only the viewer-visible segments are processed, not all the atoms, to reduce the computation time of this expensive task.

The intensity of the pixel (I_{pix}) is a sum of intensities of the two highest atoms ($I_{\text{upper atom}}$ and $I_{\text{lower atom}}$) and the background (I_{back}), modified by the antialiasing percentages:

$$\begin{aligned} I_{pix} = (P_{\text{upper atom}} \times I_{\text{upper atom}}) + (P_{\text{lower atom}} \times I_{\text{lower atom}}) \\ + (1.0 - P_{\text{upper atom}} - P_{\text{lower atom}}) \times I_{back} \end{aligned}$$

The shading intensities are calculated by the method of Phong[4] and stored in the shading templates before the mapping operation.

Depth cueing

A "fog" is used to simulate depth: Atoms far from the viewer are attenuated by an amount proportional to their depth. Three parameters define the amount of attenuation, the upper and lower fog percentage ($P_{\text{fog upper}}$ and $P_{\text{fog lower}}$) and the fog intensity (I_{fog}). When the percentages are set to 1.0, no attenuation is performed. If the lower fog percentage is set to 0.0, the molecule will gradually fade out, and very distant surfaces will have the intensity of the fog. A typical application is to set the upper percentage to 1.0, the lower percentage to 0.1–0.2, and the intensity to 255 (white), with the background of the image also set to 255. Figure 2 was calculated this way. The molecule appears to gradually disappear into a white haze. With a black background and the fog intensity set to zero, the molecule will gradually fade to black in the distance, similar to images from interactive vector hardware. Images with different background and fog intensities can yield some strange results.

Depth cueing is implemented in the post-processing stage by a simple linear interpolation using the depth of the pixel. The percent of attenuation of the pixel (P_{fog}) is calculated as follows:

$$P_{fog} = P_{\text{fog upper}} - (P_{\text{fog upper}} - P_{\text{fog lower}})$$

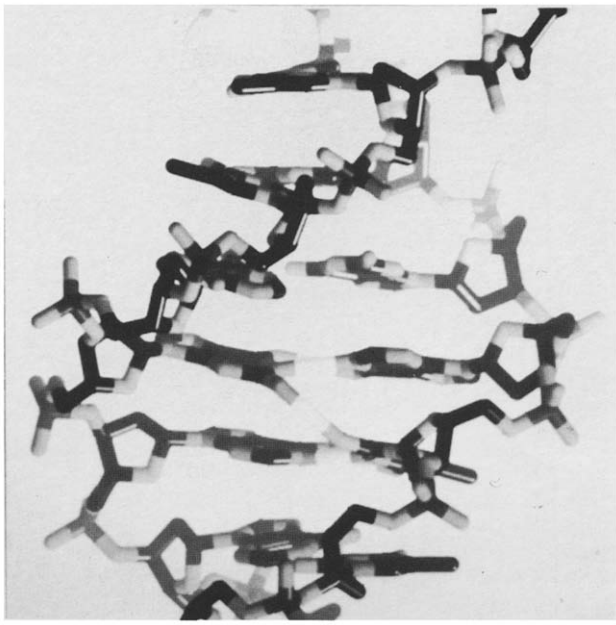

Figure 2. Molecular bond representation. The decamer CCAAGATTGG is shown as a set of molecular bonds. A unique hydrogen bond, bridging between two base pairs, is shown as a light bond. Depth cueing has been added, causing the distant parts of the molecule to fade gradually into a haze

$$\text{x } (Z_{max} - Z_{pix})/(Z_{max} - Z_{min})$$

where Z_{max} and Z_{min} are depths of the highest and lowest atoms in the molecule and Z_{pix} is the depth of the pixel. The depth cued intensity of the pixel (I_{pix}^{d}) is calculated using P_{fog} to modify the intensity of the pixel (I_{pix}):

$$I_{pix}^{d} = P_{fog} \text{ x } I_{fog} + (1.0 - P_{fog}) \text{ x } I_{pix}$$

Cast shadows

Shadows have been implemented for the spherical surfaces. For each pixel, a line is drawn from the pixel to the light source, and the perpendicular distance from this line to the center of shadowing atoms (D_{shadow}) is calculated. D_{shadow} is calculated from the unit light vector (**L**), the unit vector pointing from the pixel to the center of the shadowing atom ($\mathbf{V}_{pix\text{-}atom}$) and the distance from pixel to shadowing atom ($D_{pix\text{-}atom}$):

$$D_{shadow} = D_{pix\text{-}atom} \text{ x } \text{sqrt}(1.0 - \mathbf{L} \cdot \mathbf{V}_{pix\text{-}atom})$$

The shadowing percentage is calculated using D_{shadow} and the radius of the shadowing sphere (R_s). If D_{shadow} is greater than the radius of the shadowing atom, no shading occurs; if less, total shadowing occurs. Antialiasing is performed at values of D_{shadow} approximately equal to R_s:

$$\begin{aligned} D_{shadow} < R_s - 0.5 &: P_{shadow} = 0.0 \\ R_s - 0.5 < D_{shadow} < R_s + 0.5 &: P_{shadow} = D_{shadow} - R_s + 0.5 \\ R_s + 0.5 < D_{shadow} &: P_{shadow} = 1.0 \end{aligned}$$

The shadowing percentage is used to diminish the specular and reflective components of the Phong illumination. The diffuse illumination is not affected by shadowing. The shadows do not appear uniformly black; detail can be seen if different atom types are given different values of diffuse illumination.

Z-clipping

A powerful imaging option of this package is the ability to clip the molecule in the z direction and see the detailed molecular interactions in the exposed surface. Clipping the atomic surface is very simple with the z-buffer algorithm: Merely ignore all pixels above the clipping plane during the mapping operation. The details of the cross sectional plane are overlayed on the final image of the surface. For atoms within one radius of the clipping plane (i.e., those that are actually clipped), a new atom is generated at the clipping plane, with radius equal to radius of the cross section of the atom. These spheres are given a flat, unshaded color, to make them appear planar. When they are processed for intersections, a representation of the overlap inside of atoms and molecules is obtained.

Implementation

RMS is composed of three programs in the implementation at UCLA. RMSCLIP and BONDS calculate images from atomic coordinates, producing binary files of pixel intensities. IMAGE is used to display these images on a particular raster graphics device. Two types of picture file may be calculated: a file containing one black and white image or a larger file containing three color separations, which are combined photographically to produce colored images. The figures in this paper were calculated on a VAX 11-780 and photographed from a VAX GPX workstation. At a resolution of 400 by 600 pixels, these images required from 2 cpu min (Figure 2) to 15 cpu min (Figure 4) for calculation.

APPLICATIONS

I have used RMS in the final analyses and presentation of several local crystallographic projects. Each figure presented here focuses on one interesting structural feature of the molecule. The DNA decamer CCAAGATTGG[5] contains GA mismatches at the center two base pairs, and these guanines form unusual hydrogen bonds with neighboring thymines. Figure 2 shows a bond representation of this structure, highlighting these two unusual structures. Figure 3 shows a space-filling representation of the complex of 4′-6-diamidine-2-phenyl indole with a DNA dodecamer.[6] The images are diverging stereo pairs, for viewing with stereo glasses. The drug fits snugly in the minor groove, causing the amidine group at the upper end of the drug to twist, following the helical course of the groove.

To explain the asymmetrical drug binding behavior of DAPI, netropsin and Hoechst 33258, an analysis of the packing constraints in crystals of the dodecamer CGCGAATTCGCG was performed.[7] Figure 4 is a cross section showing four unit cells of the crystal. The lightest molecule is very constrained, with contacts on two sides, whereas the other two molecules have one side facing a solvent channel. In the three drug complex structures solved in this crystal form, the region of DNA seen in the white molecule is free of drug binding; the drugs prefer to bind in the region seen in the darkly shaded molecules, where the DNA is free to open up and accommodate the drug.

Color Plate 1 contains cross sections of two different

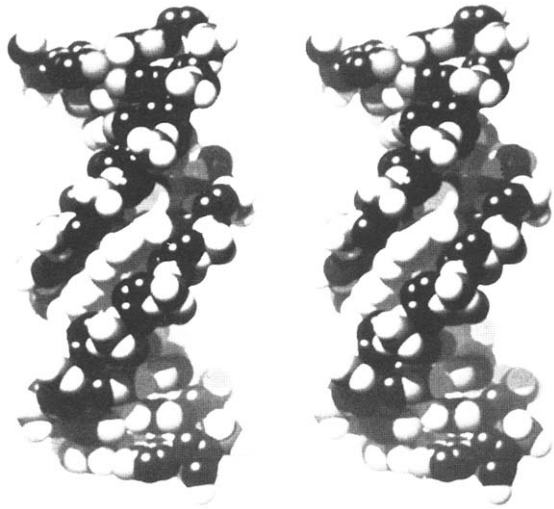

Figure 3. Space-filling representation. The complex of DAPI with the DNA dodecamer CGCGAATTCGCG is shown as a van der Waals surface, in a stereo pair. Cast shadows and depth cueing help create an illusion of depth, even without stereo viewing. Shading and highlights create a believable image of the model

sequences of DNA, showing the flexibility of B-DNA. CGCGAATTCGCG has a narrow minor groove, wide enough for only one water molecule.[8] CCAAGATTGG has a wider minor groove, more typical of DNA with general sequence, with two rows of water molecules lining the sides of the minor groove.

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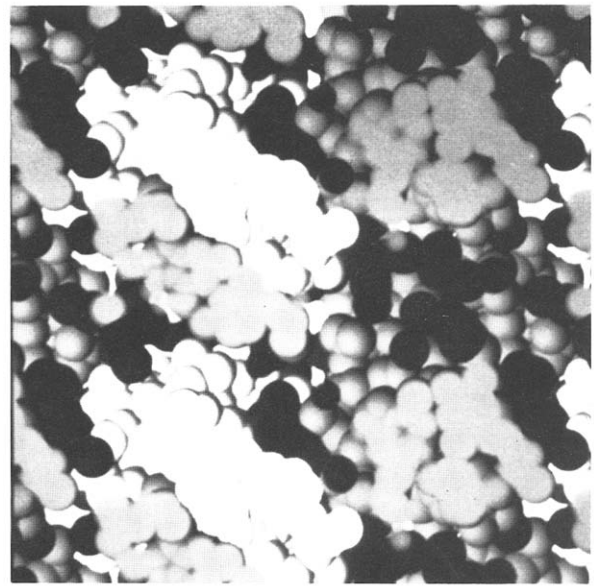

Figure 4. Cross section through a crystal. The packing constraints of the dodecamer crystal lattice are seen in a cross section. Three different molecules are seen in this slice: The white molecule is sectioned at the upper end of the helix, the darker molecule below it is sectioned at the bottom of the helix and the darker helix to the right is sectioned near its center. Solvent molecules are shown in black. The white molecule is pinched between the two other molecules, whereas the darker molecules are free to solvent on one side

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