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Realtime interactive computer graphic visualization of the interactions between molecules uses various geometric representations such as solvent-accessible and resulting van der Waals surfaces. In most molecular modelling methods, however, the main focus is on the 'lock and key' idea, ie is purely steric. We have developed a realtime docking method in which the energy of interaction between drug and receptor is displayed on a high performance 3D colour graphics system as the drug is moved in the receptor site. In our method, the atoms in the receptor are enclosed in a 3D cartesian grid and the electrostatic, repulsive and attractive potentials due to the receptor atoms are stored at the grid points. As the drug molecule is moved inside the receptor, the total energy of interaction is calculated from these grid points and updated on the screen in real time. A simplex method is used to minimize the energy of interaction while docking. Supported by research grant NIH RR-1081 and a Guggenheim Fellowship (RL).

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'Real time rotation of space-filled molecular models'
Pearson, J E Ciba/Geigy, Switzerland

With the development of advanced raster-scan terminals which have more and more local computing capabilities it is now possible to do realtime rotation of true 3D space-filled molecular models.

After a brief review of some of the methods already in use for the display of static space-filled models, the new method will be described in detail. The method relies on an extension to polygon filling known as 'Back face testing'. Polygons described by lines drawn clockwise are shown on the screen whereas polygons drawn anticlockwise are not displayed. When a solid, each of whose faces have been drawn clockwise in turn, is viewed from the front, the back face will be described in a counter-clockwise fashion and will not be displayed.

Although the initial generation of the picture is fairly time-consuming (about 45 s for 100 atoms) the outstanding advantage of this method is that once the picture has been drawn, the host computer is no longer required for picture drawing and is merely required to amend the rotation matrix, if the solid is to be rotated. This means that the movement of a solid can be extremely fast and in practice it has been found necessary to up-date the rotation matrix every third of a degree in order to slow the rotation down to a useable speed.

The new method readily lends itself to software clipping of the surface so that it can be used to describe just part of a larger molecule. This means that the surface can be cut away to reveal a skeletal model inside.

With the latest generation of intelligent raster-scan displays it is possible to request that a surface be displayed as transparent. This would mean that it is possible to see an enclosed skeletal model and be able to differentiate readily between these and skeletal models

which are outside the surface. Such models would be moveable in relation to each other in realtime.

Although the method uses a lot of display memory (~1/4 Mbyte/60 atoms) it can still be used to simplify complex pictures such as drugs in the active sites of enzymes, since only a limited number of atoms on the enzyme need be enveloped by a surface at any one time.

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'Work in progress at UNC Chapel Hill NIH Research Resource'
Pique, M University of North Carolina, Chapel Hill, NC, USA

The University of North Carolina at Chapel Hill operates a research resource supported by the United States government's National Institutes of Health.

Three current computer graphics projects for molecular studies are:

- Evaluating and exploiting the scientific potential of our GRINCH system, which combines Carroll Johnson's ridge line representation of electron density maps with appropriate interactive tools. GRINCH users may trace the main chain, register the sequence, and roughly place side-chain atoms. GRINCH thus bridges mini-map interpretation and the contour-based, atomic-level fitting systems such as GRIP-75, FRODO, and BILDER.
- Developing multiple visual representations of molecules, including skeletal, surface, volume, and non-geometric views.
- Producing smoothly rotating CPK molecular models. We can now draw eight shaded raster images/s of a 50 atom molecule using our coupled DEC VAX-11/780 and Adage Ikonas RDS-3000.

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'The use of constructive solid geometry for molecular graphics'
Quarendon, P IBM UK Scientific Centre, St Clement Street, Winchester, Hampshire, UK

A method of producing realistic representations of objects on a raster graphic terminal is described as is its application to molecular graphics. The basis is a general program which draws simple geometric primitives, such as spheres, cylinders and planes. These can be combined by Boolean operations to build more complex shapes. This method is becoming popular in CAD.

The program input consists of a text file which describes the objects to be drawn as an expression in this Constructive Solid Geometry. It can also specify the colour and surface appearance of the objects and the position and characteristics of the sources of light to be assumed.

The algorithm used to construct pictures is developed from one by Woodwark and Quinlan. It continually subdivides the space in which the objects lie until it finds regions which are either empty, uniformly filled, or are too small to subdivide further.

Relatively simple application programs are then used to generate a variety of representations from molecular data held in a relational database. Examples of the type of pictures which can be produced are: