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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:

- space-filling
- ball and stick
- secondary structure
- solvent accessible surface

The objects can be coloured conventionally, or to represent some property of interest.

An extension of the same basic method has been used to construct pictures showing the variation of electrical properties on the surface of molecules. For this purpose, instead of using a constant colour for the object, the surface colour at every point is determined by computing the value of the property and mapping this on to a suitable colour range.

The technique of constructive solid geometry will be described, together with examples of its use for displaying molecular properties.

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'Towards fifth generation molecular modelling' **White, D N J and Pearson, J E** Ciba-Geigy, R1046, CH-4002 Basel, Switzerland

The advent of minicomputers of an order of magnitude more powerful than the VAX-11/780, and realtime raster scan displays whose facilities are not possible on calligraphic systems, has made the design of molecular modelling software necessary which uses these new devices.

The software described in this abstract is a preliminary, development version of the COGS (Chemically Oriented Graphics Software) package. It was developed on a VAX-11/750 minicomputer and Whizzard 7295 display but is targeted for a Norsk Data ND-570 minicomputer and a display yet to be announced (both of which will be delivered in July 1984).

In terms of performance the ND-570 relates to an ordinary minicomputer in the same way that a Cray-1 relates to an ordinary mainframe. The ND-570 is a realtime virtual memory machine which executes both scalar and vector instructions with none of the drawbacks of ordinary virtual memory architectures (eg thrashing). In addition to its advanced computational features the ND-570 has an extremely 'user friendly' operating system with features such as multiple window screen editing, built-in scientific word processing software, foolproof command abbreviations and prompts, query language etc.

The display for which COGS was designed is a colour raster scan display with an effective resolution of 3000 × 2000, 4096 colours and the following realtime picture transforms implemented in hardware:

- xyz-axis rotate
- xyz-axis translate
- xyz-axis scale
- xyz-axis clip
- perspective
- depth cueing
- area fill
- backface testing
- Phong shading
- Gouraud shading
- hidden line removal
- hidden surface removal

With all transforms active and all vectors non-trivially clipped the system can draw 100 000 medium length vectors/s. The display list memory can be up to 4.7 Mbytes long and all of this is simultaneously displayable without the flicker or other effects associated with calligraphic displays. Display list datatypes may be 16- or 32-bit integer or 32-bit floating point. The new display generates the following primitives in:

- hardware
- vectors
- polygons
- meshes
- circles
- generalized conics
- circular conic arcs
- splines
- surface patterns

New attributes such as programmable line width are supported as are a range of graphics peripherals and host minicomputer interfaces.

The design philosophy for COGS, with such powerful hardware available, is to provide all molecular modelling features, for both small- and macromolecules on the host minicomputer. In other words calculations such as molecular orbital, large molecule molecular mechanics, and large molecule conformational search are performed on the molecular modelling minicomputer and not on a mainframe. The only exceptions to this strategy are, eg the use of a FPS-164 array processor for quantum chemical and full-matrix molecular mechanics calculations requiring double precision arithmetic, and the use of the indexed sequential file access method of VAX/VMS in conjunction with Dr Murray-Rust's software for accessing the Cambridge crystallographic database. Furthermore, COGS is designed to make maximum use of graphics peripherals. Almost all operations are performed by pointing at atoms, molecules or menus using a puck and graphics tablet. A few options use valuator dials and minimum use is made of the keyboard.

The standard and novel features of COGS are too numerous to mention, but include a full range of 3D model building facilities such as model definition from 2D sketches, amino-acid sequence, and databases of standard internal coordinates. User supplied internal coordinates are also featured along with user-supplied crystal or cartesian coordinates and databases of standard molecular fragments. Easy back and forth swapping between a range of default picture types is provided. Current picture types include coloured stick models, red/green stereo pairs, Pearl/Honnegger molecular surfaces and molecular mesh surfaces. Other representations such as space-filling models may be drawn but are not used as picture types because of the difficulty of pointing at individual atoms in these types of pictures. Hydrogen atoms may be added to medium weight atoms automatically. Bond lengths, angles, and torsion angles may be measured by pointing, and may be dynamically altered in realtime. Single or collections of atoms or molecules may be removed from the screen without individual specification, bonds may be made