

Fourteenth Annual Report  
Interactive Graphics for  
Molecular Studies

*TR88-010*

*March 1988*

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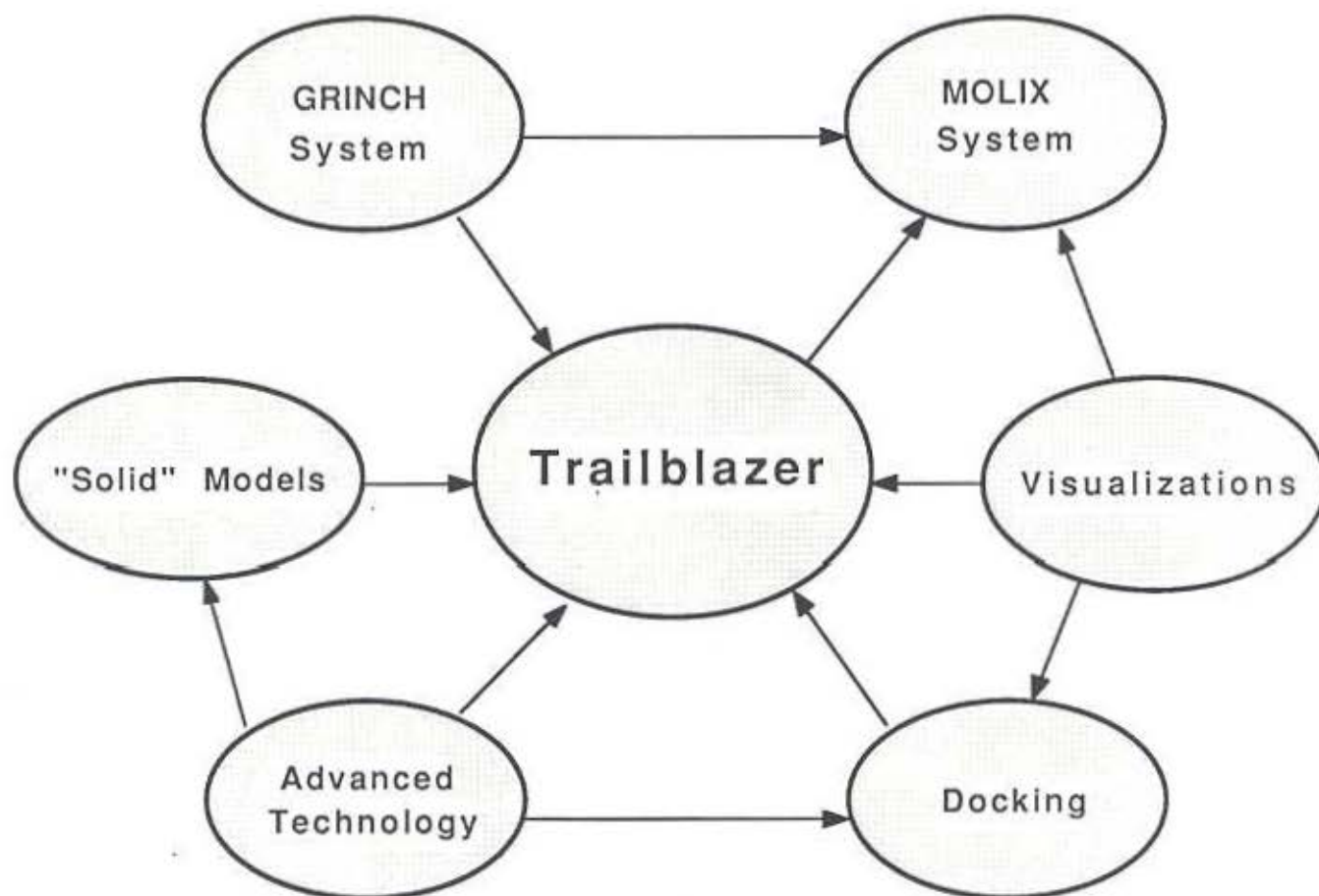
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The Project's research plan for 1984-89 calls for seven sets of activities, shown in the figure below. We report progress and plans during 1987 in each category.



The Seven Projects—Relationships

## 1. RESEARCH PROGRESS IN 1987

### 1.1 Trailblazer – A Frontier Resource for Molecular Graphics

#### New RSpace Tool Helps Planning of Area Collector Sweeps

Mark Harris, helped by Matt Fitzgibbon, has built RSpace, an interactive graphical model of a diffractometer with an area detector. It runs on the PS330. The program enables the crystallographer

to explore various collection strategies while graphically studying the swept volume of the reciprocal space.

We worked with the Biochemistry Department at UNC, who are now beta-testing for us. Users there find that the program has improved the efficiency of collection up to 30%, reduced erroneous scanning, and enabled inexperienced crystallographers to plan their own collections. Use so far:

Charles Carter (with Dr. Charles Zelwer of LURE): Met. tRNA synthetase, 4 datasets to 3 Å

Dr. Francine Smith: Ypsilanti mutant hemoglobin, 2 datasets to 2.5 Å

Laurie Betts: Cytidine deaminase E. Coli, 1 dataset to 2.7 Å

Eric Baldwin: Pseudo catalase, 1 dataset to 3.5 Å

Katherine Crumley: Complexed Trp tRNA synthetase, 1 dataset to 5 Å

Frank Hage: Trp tRNA synthetase type 3, 2 datasets to 4.5 Å

David Coleman: Trp tRNA synthetase type 4, heavy atom screening.

### **Tripod's Mendyl Adopted as Base System for Future Trailblazer Software**

We are using the Mendyl database facility in the VIEW project. The port of Mendyl to the VAX Unix-PS330 configuration is near completion. This required installing an additional megabyte of memory in our PS330. We are currently porting Mendyl to the Masscomp-Unix-PS330 configuration at the Richardsons' lab. We will also port Mendyl to the Sun3-Unix-PS330 configuration.

### **SUN-TAAC and PIXAR Each Installed on One-Year Loan**

Our laboratory is now evaluating a 10 MIPS TAAC accelerator board from Sun Microsystems, and a PIXAR 4-way fast graphics processor from Philips Medical Systems. We are using both in volumetric representation studies.

## **1.2 GRINCH and Volumetric Representation**

### **Powerful New Volumetric Representations Devised for Density Functions**

Density functions, such as electron-density maps, are difficult to visualize in computer graphics. Established methods include the use of single-plane contours and chicken-wire contours.

Marc Levoy and Lee Westover have each invented new methods for the direct volumetric rendering of each voxel datum. In Westover's technique the density value at each voxel is represented as a transparent and luminous object. The result appears as a cloud of glowing particles concentrated at the atomic centers, much as a chemist might imagine electron-density "really" looks. The appearance is not selected by arbitrary thresholds, so all the data is visible simultaneously. This can be overwhelming, and although it gives a useful perspective, at present it is hard to follow the molecular chain unaided.

Levoy's technique displays smooth, reflective, transparent surfaces at user-specified thresholds or gradients of the data. The technique has the advantage that the contour-surface position and normal is calculated at every voxel involved, so a smooth, isotropic surface is drawn. Because this rendering is transparent and reflective, concentric surfaces of large regions of the molecule can be displayed.



simultaneously, without the customary confusion. The clarity of the images suggests that such techniques might allow interpretation of poor quality maps.

Appendix pictures 1 and 2 (Levoy) show one and two levels of density for a part of Cytochrome B5. Pictures 3 and 4 (Levoy) show how the density map can be augmented with a postulated bond structure. Picture 5 (Westover) shows the luminous-element technique.

### **GRINCH Ported to New Systems, Documented, and Distributed More Widely**

Michael Pique at Scripps adapted GRINCH to run on a color Sun 3.

The user's manual is revised and now completely up to date. Separate versions of the manual for the PS330 and the Masscomp are maintained together in one TeX file.

GRINCH has been exported to the following additional users:

Guy Dodson, University of York, England  
N. Isaacs, St. Vincent's Institute of Medical Research, Melbourne, Australia  
Dave Stout, Scripps Clinic, La Jolla  
Howard Einspar, Upjohn  
National Institute of Genetics, Shizuoka, Japan  
Martin Zwick, University of Portland, Oregon  
Tom Palmer, Frederick Cancer Research Facility, Maryland

Reports from some GRINCH users:

Judy Kelly, University of Connecticut. The group used GRINCH for preliminary studies of the map of bacterial beta-lactamase. They plan to start chain tracing soon.  
Duncan McRee, Scripps clinic. The group continues to use GRINCH to interpret the map of the rhodopsin-like bacterial yellow photoactive protein.  
F. Scott Matthews, University of Washington used GRINCH in an attempt to interpret a 3 Å map of Para-cresol methyl hydroxylase, but the data proved to be intractably poor.

### **1.3 MOLIX – Porting Advanced Software to Workstations**

We completed GRINCH on Masscomps. The 6-plane version, the 10-plane version, and the ridge-line calculator all work properly now. We will release these through Masscomp shortly.

Mike Pique sent us a new version of the Porter/Huang/Ferrin CPK program, which we adapted to run on Masscomps. We have a draft user's guide.

We modified the old ZBS program on color Suns and Masscomps to allow user data to be read in, and drafted a user's guide. We have also added x and z rotations.

Workstation versions of ZBS and/or CPK were sent to:

George Drake, Dept of Zoology, UMass  
Akira Komoriya, Meloy Lab Inc, Rockville, Md.  
Mary Beth Litster, Sun Microsystems, Lexington, Mass.  
Edith Jarisch, formerly with Bundesministerium fur Unterreicht, Kunst u. Sport, Vienna.

## 1.4 Real-Time Moving Display of Spheres and Other Solid Models

### Pique's Vibrating Molecule Program, FLEX, Implemented on Pixel-Planes

Two versions of Mike Pique's FLEX were implemented on our Fuchs-Poulton Pixel-planes high-performance graphics processor. The resulting viewing is very powerful.

FLEX1 loads a sequence of atom position snapshots, which are displayed very rapidly in sequence as space-filling models. The viewpoint can be changed dynamically, with joysticks.

FLEX2 reads and loads into Pixel-planes the initial atom positions and normal mode information, calculates the different atom positions, and displays the vibrating space-filling model in real time. The different normal modes can be turned on and off interactively, and the temperature can be changed. As before, the viewpoint can be changed dynamically with joysticks.

### Palmer Implements "Rubber Stamp" Spheres on the Adage Ikonas and on the Sun 3

The program calculates Phong-shaded sphere templates in several sizes. Each includes z values by pixel. Then these are replicated to make up a molecule view. Interpenetrations work properly. Rendering several hundred atoms takes seconds.

## 1.5 New Visualizations of Macromolecules

### Visualization Impromptu Evaluation Workbench (VIEW) Prototype Under Construction

Our largest 1987 effort was in the specification and design of a major new software system, one to enable chemists to devise, rapidly construct, evaluate, and revise new ways of visualizing molecules and density maps. We see this system as an example of a powerful new class of auxiliary programs to help scientists understand the results of large computations.

We decided to implement VIEW first on a Sun 3 workstation, producing final images on any of several different display devices. We are designing the system using the object-oriented approach and therefore implementing in the C++ language. For ease of implementation and portability, we are using standard subsystems where possible. We are using the Mendyl database facility, and the X-windows screen manager for the user interface.

We recently doubled the VIEW team. This demands, and provides the manpower for, adopting a better software engineering environment and more formal version control and documentation procedures.

### Beta-Testing Done on Connolly's New PPMS and TRB Programs

We beta-tested Mike Connolly's new programs PPMS (Piecewise Polynomial Molecular Surface) and TRB (Triangulation by Recursive Bisection). We displayed the triangulated molecular surfaces on the Vector General, PS330, Sun 3, and Pixel-planes.

## 1.6 Docking

### ARM Force-Feedback System Demonstrated for Molecular Docking

Just before we dismantled the system for the move to Sitterson, Ming Ouh-Young demonstrated force-feedback as one attempts to dock Trimethoprim into Dihydrofolate Reductase. The physical move and reinstallation, which required additional steelwork in Sitterson, stopped further work on the ARM itself for six months.

Ming and Neela Srinivasan rewrote our version of the Pattabiraman-Langridge energy evaluator, adding interpolations between grid points. Bump checking was added; an orange vector now appears between two bumping atoms.

Ming did a stereo effectiveness study with a ring-and-wire toy, both real and simulated on the PS330. As a result, stereo was added to the PS330 version of the ARM program.

### Tom Palmer Implements Barry's Docking Algorithm in DOCKTOOL on the Ikonas

In order to get real-time docking on a slower machine, Dave Barry proposed that one move a stick-figure small molecule in real time, against a precalculated stationary double-atomic-radius surface of a large molecule. Tom Palmer built such a system as an M.S. project. The small molecule can dip into the surface, and the user can clip, but not move, the surface. A small red cross shows when and where a bump is detected.

## 1.7 Advanced Technology

### Head-Mounted Display Continues to Progress and Attracts Other Funding

The head-mounted display system has improved in image quality, function, and speed. Image quality was improved by switching to 320 x 220 resolution color screens, and by developing an interface to the Pixel Planes raster graphics system. Installation of toggle switches and of a second Polhemus sensor now enables user interaction with the image.

Update rates were improved by using asynchronous reads operating in continuous-output mode, by looking up rotation cosines on the host rather than calculating them on the Polhemus micro, and by sending transformation matrices to the PS300. Update rate and lag remain our most difficult problems.

With the recent improvements in performance we can at last begin application to molecular structures. The first try will be molecular datasets that can be pointed to with a wand-controlled cursor, drug shaped to simulate docking.

Additional support has been put into the Head-Mounted Display by the Office of Naval Research, enabling us to enlarge the team from one graduate assistant to three.



## **Votan Speech Recognition System Used for GRINCH Menu Commands**

Jih-Fang Wang reattached the Votan segmented-speech recognition device to the GRINCH Masscomp, rewrote the votan code, and made it work reliably. One need not lose one's position in the map by moving the cursor from the data to identify its type, as one formerly had to do by menu picking.

## **1.8 Other**

### **Project and Department Move to Sitterson Hall**

The new 74,000 sq. ft. computer science building was occupied in the summer of 1987, as we moved from seven other sites into one. Delays in structural alterations meant that the video projector was usable only in a lash-up, and the Argonne Remote Manipulator not at all for six months. We now have superb laboratory space (five times larger) and two coherent clusters of offices.

### **Alumni Join Molecular Graphics Groups Elsewhere**

Tom Palmer joined the Frederick Cancer Research Facility in Frederick, Md. He is continuing to collaborate with us on VIEW.

Doug Schiff joined the applications accelerator group of Sun Microsystems in Raleigh. He is their molecular graphics expert.

Neela Srinivasan joined Biosym Technologies in San Diego. She works on Insight, their molecular modeling program.

### **Collaborative Activities**

Prof. William Switzer, Department of Chemistry, North Carolina State University, is a visiting scholar with the project this term, during his sabbatical. He is modeling a complex chromatography diffusion on a supercomputer. We hope to learn more about scientific visualization from his experience.

We ported FRODO to the UNC Biochemistry Masscomp-PS350. UNC Biochemistry are now on the ethernet. We can display on their PS350 from our lab and vice versa.

Mike Pique and Helga Thorvaldsdottir still maintain the international list of molecular graphics installations. We discussed the need for keeping this list with Martha Teeter of Boston College, who maintains a machine-readable directory of crystallographers. There seems to be need for both.

We loaned our monochrome Masscomp graphics head to Duke for the Richardsons' machine.

Prof. Frank Starmer of Duke Cardiology used our Resource and the program SECSTR to search for correlations between the sequences of proteins involved in various biological channels, including Acetyl CoA, Calcium, and Sodium channels, but was unable to find any significant similarity.



### **Brooks Changes Boards**

Fred Brooks completed a four-year term on the Defense Science Board. The Senate confirmed him for a six-year term on the National Science Board.

## 2. RESEARCH PLANS FOR 1988-89

### 2.1. Trailblazer – A Frontier Resource for Molecular Graphics

At any time the computer industry offers new high-performance computers and display engines. Each of these promises some important new capability for molecular studies. They are typically too expensive for the working chemist's laboratory.

We continually monitor new machines as they appear, attempt to choose those most promising for molecular studies, install them in our laboratory, and exploit their capabilities with new software and ports of old software. Because we are a part of a multi-project computer graphics laboratory, with several research groups funded from many sources, we have access to many powerful graphics machines, most of which our molecular studies project pays nothing for. At present, for example, we have available to us and our Resource users, but *not* purchased or maintained by our Resource:

- a Fuchs-Poulton Pixel-Planes IV, the fastest general-purpose graphics engine yet delivered
- a Pixar
- a Sun TAAC applications accelerator, especially suitable for graphics
- a Masscomp array processor
- a varifocal mirror true 3-D display
- two Adage Ikonas 3000 display processors
- a Sun 4 computer server

We also develop entirely new molecular graphics techniques and programs. This year's progress report describes three: two new ways of visualizing density maps and a new kind of tool for planning data-taking.

We invite biochemists from all over the world to come use our Research Resource and its advanced capabilities for tasks they cannot do in their own laboratories. We *help* them use it. We also welcome and assist other people who develop molecular graphics software and who need access to advanced equipment and software environments. Twice, for example, we have hosted Michael Connolly, developer of new surface calculation programs.

The prices for a given level of performance are dropping in half every two years – some industry figures claim every year. This means that by the time we have significant software ready on our Trailblazer installation, the advanced machines on which it was developed have become candidates for affordable fielding. We export our software to anyone who has a suitable configuration. Fielding and user support on workstation-level machines is the business of our Molix subproject.

#### New-Generation Display Engine For the Resource

The most powerful graphics equipment owned by the Resource is the Evans and Sutherland PS-330 and the VAX11/780 that drives it, both acquired in 1983. By choice, we have invested equipment money in the past four years in equipping us with modern raster workstations, so that many people could be developing graphics programs at once. In short, we have gone for breadth rather than higher power in a single machine.

This strategy has been livable because of our access to Pixel-Planes IV, UNC's powerful homegrown

display generator. Although Pixel-Planes has enabled us to get some remarkable results since it became operational in 1986, it is not a commercial machine. We can prototype new techniques on it, but we cannot field software for the biochemistry community on it.

We now have a critical need for one of the new generation of commercial high-performance graphics displays that are suddenly coming over the horizon, after a lull of several years. The first of these, the AT&T Pixel Machine, is only now being delivered; serious competitors will appear this spring and summer from Stellar, Ardent, Silicon Graphics, and perhaps Evans and Sutherland.

A major effort in 1988 will be the evaluation, specification, purchasing, and installation of a new-generation, high-powered graphics system. Then we will port software to it and begin exploiting its capabilities for entirely new functions.

### **New RSpace Tool**

Mark Harris, helped by Matt Fitzgibbon, has built RSpace, an interactive graphical model of a diffractometer with an area detector. It runs on the PS300, attached to a VAX or a Masscomp. The program enables the crystallographer to explore various collection strategies while graphically studying the swept volume of the reciprocal space.

Beta-testing of a first version is underway, as described in the Progress section. This year we plan to export a version for general use.

We will also add function:

- quantification of the swept volume
- quantification of the degree of redundant calculation
- statistical analysis of other parameters.

Work is in progress to port RSpace to VAX/VMS/PS300. We will also port it to stand-alone workstations, including Masscomps and Suns.

## **2.2 GRINCH and Volumetric Representation**

### **New Volumetric Representations for Density Functions**

Marc Levoy and Lee Westover have each invented new methods for the direct volumetric rendering of each voxel datum, as is described in Section 1, Progress.

A major effort in 1988 will be devoted to developing this technique and testing it for robustness with a variety of maps of varying resolutions and qualities. We are just now ready to show it to several of our collaborators and get their evaluations of the results thus far.

Our dream is that the combination of Levoy's technique and the better maps now being routinely produced with area detectors may make most chain-tracing far easier. The clarity of the images produced by the Levoy technique suggests that such techniques might even enable the interpretation of



poor quality maps not now tractable.

Levoy's technique produces flat rendered images only, not models that can be viewed from many angles. We plan to work on ways to combine it with the 3-D models in the GRINCH system, discussed below.

Westover's technique, although not so usable today, has the advantage that the density data speaks for itself – no contouring threshold has been applied, no contouring planes inject anisotropy into the view. The images are much more effective when a set of related views are combined into a rocking sequence. In 1988 we will work on improving the clarity so that their potential can be realized.

## GRINCH

We observe GRINCH users to do three things dynamically and very often:

- They rock the viewpoint, to get kinetic depth effect and to uncover obscured local features.
- They often change the density threshold, seeing fewer ridge lines for better overview or more lines for more detail.
- They zoom often between local looks at details and global views to see how neighborhood and molecular patterns explain local features.

We hypothesize that a few Levoy views from various directions and at various density levels might provide useful global overviews of a new map, obviating many iterations of the last two steps. We will explore this concept.

We also plan to incorporate intensity depth cueing of colored lines into the existing GRINCH, using a new technique sent us by Judy Kelly of Connecticut.

## 2.3 MOLIX – Porting Advanced Software to Workstations

We will release GRINCH, CPK, and ZBS to the public through Masscomp shortly.

We continue to port various programs to the Masscomp, which several of our collaborators have installed, as well as to Suns. The Sun has proved to be the most popular workstation, and Masscomp has essentially withdrawn from the general workstation market, although they continue to be major providers of workstations interfaced to laboratory instruments.

In the future, we will port almost everything to the Sun, with decreasing emphasis on the Masscomp.

The rich variety of application software makes the Macintosh very attractive; many labs have one for general-purpose use. The Macintosh II is a sufficiently powerful machine that it is increasingly being installed in workstation environments. If molecular software were available for it, the same machine could serve many chemists as a small molecular workstation and as a general-purpose office tool. In 1988 we will install ethernet and Unix on our Mac II and begin porting some of our molecular programs to it.

## 2.4 Real-Time Moving Display of Spheres and Other Solid Models

We can display spherical models of protein complexity and move them in real time on Pixel-Planes. We are already evaluating, both in our docking work and with Pique's FLEX program, the significance of this capability to the understanding of structure. We will continue this evaluation with our collaborators, using new molecular coordinate sets. We will also keep exploring how to realize this capability on commercial display engines.

In 1988 the Pixel-Planes engineers will add a minor hardware change that will enable it to do bump-checking in hardware. We will work with them to make the new capability work for spheres as well as for polygons.

The next challenge is to achieve yet other visualizations in fully dynamic form. The most useful, and hard, is the Richards solvent-accessible surface, which requires convex and concave spherical patches, and toroidal patches. Our 1988 objective is to separate Connolly's program into the part that calculates the surface and the part that renders the surface. We will program a new renderer that allows later binding of the colors of surface pixels.

## 2.5 New Visualizations of Macromolecules

### Visualization Impromptu Evaluation Workbench (VIEW)

Our largest 1987 effort was in the specification and design of a major new software system, one to enable chemists to devise, rapidly construct, evaluate, and revise new ways of visualizing molecules and density maps. We see this system as an example of a powerful new class of auxiliary programs to help scientists understand the results of large computations and to study large databases.

VIEW is a workbench on which the chemist can build visualizations from molecular data. The construction can be done interactively, with the user choosing components and modeling styles each in an impromptu fashion.

A visualization is built in two steps. First one builds a *model* of a molecule. A model is a three-dimensional entity that represents the molecule. Brass stick-figure or plastic CPK models are familiar example, realized in brass or plastic. VIEW models are realized in the computer's memory only, but they have all the other attributes of real 3-D models.

Once one has a model, the viewer can look at it from any direction, at any zoom, and under a variety of lightings, just as he could with a real model. This viewing can be done interactively or dynamically, depending upon the power of the display machine.

One can save views on film or tape. One can also save all or part of the model parameters, so one can easily make other variants. And one can save a models itself, with the most recent viewing parameters. From this one can quickly reconstruct this view or any other view of the same model.

We plan to have a proto-prototype of the VIEW system running by June, and a prototype ready for chemist beta-testing by the end of 1988.



## 2.6 Docking

### Argonne Remote Manipulator (ARM) Force-Feedback System

The most serious problem with the force illusion today is the lag between user motion and the consequent visual change and force change. Work in 1988 will concentrate on measuring that lag, identifying its component causes, and attacking each separately. The first to be attacked will be the energy-model evaluator that calculates the forces and torques. We newly have access to a Sun 4, a 10 MIPS computer server. We shall undertake to run the energy model on that, rather than on the 1 MIPS Masscomp that controls the ARM.

The system is now good enough that we are ready to start some user studies with our collaborators. A first calibration experiment will be to simulate the docking of two 8 inch magnets, and to compare the force sensation with that experienced when real magnets of that sort are attached to the ARM and to a target.

Studies in 1987 showed the importance of stereo vision for the 3-D simulated docking task. In 1988 we plan to work with the Pixel-Planes engineers to get a modification that will make stereo generation simple and fast. We are also working with Tektronix to get stereoplates custom-made for our Barcodata video projector, an essential component of the whole ARM illusion.

A minor change to be incorporated will be an audible signal, as well as the present visible one, when the docker molecule bumps the dockee.

## 2.7 Advanced Technology

### Head-Mounted Display

Our long-term goal is to incorporate the system into a molecular-modeling package, so that the chemist can grasp a piece of molecule with a data-glove and manipulate the virtual structure just as if it were a solid model. This will require specification of how much of the structure has been grasped, and of control points for the manipulation.

With the recent improvements in performance, we can at last begin application to molecular structures. Our first try will be virtual molecules, hung in space, that can be pointed to with a wand-controlled cursor. The cursor will be drug-shaped to simulate docking.

Update rate and lag remain the most difficult problems with the fidelity of the virtual-object illusion. In order to reduce the update lag we need to identify the bottlenecks in the loop by controlled timing experiments, including end-to-end delay measurements using interrupted light beams and photocells. We will continue to look for alternative tracking mechanisms that do not have the lag and range limitations of the Polhemus.

Image richness and quality will be improved in 1988 by feeding the HMD's TV's directly from Pixel-Planes, obviating the intermediate cameras used today with the PS330. This will enable us also to



take advantage of the new stereoscopic hardware to be developed for Pixel-Planes. We plan to acquire, if possible, the LEEP wide-angle optics.

Interaction will be improved by the use of a data-glove sensor with its gesture libraries, and by harnessing our Votan spoken-command recognition system.

Our work is similar to that of the NASA-Ames group, in that we both use Polhemus trackers and miniature TV's, but our system is directed towards doing useful work rather than concept proving, and our update rate and lag time are slightly superior. Their system has a much wider field of view and already incorporates the VPL data-glove.

The NASA-Ames system encloses the wearer's head so that he cannot see the real world. We feel that superimposing the virtual image on the real world makes using the device much less claustrophobic. As important, it provides a real frame of reference for the virtual molecules. (It might also be valuable to the oncologist superimposing virtual tomographic data and virtual treatment beams on a real patient.) We might be wrong as to the best method, however, so in 1988 we plan to try some tests each way.

#### **Votan Speech Recognition System for GRINCH Menu Commands**

Now that the system is working, we need to evaluate its effectiveness. This requires a crystallographer with a map to interpret who is willing to come here. We have been looking for a suitable experimenter, and we will keep looking in 1988.

## **2.8 Collaborative Activities**

We are collaborators. We have to be if we are to be useful; for we build tools for molecular studies, a craft we do not know. Hence we seize every reasonable opportunity to collaborate with people who need our expertise or resources for scientifically interesting problems. We plan to continue this next year, both with our ongoing collaborators and with new ones as they may appear. Currently active collaborations include the following persons and their colleagues and students:

- David and Jane Richardson, Biochemistry, Duke
- Jan Hermans, Biochemistry, UNC
- Charles Carter, Biochemistry, UNC
- Michael Pique, Scripps Research Institute
- Michael Cory, James Bentley, Burroughs-Wellcome
- Phil Bowen, Medicinal Chemistry, Pharmacy School, UNC
- William Switzer, Chemistry, North Carolina State University
- Tom Palmer, Frederick Cancer Research Center
- Application Accelerator Division, Sun Microsystems
- Tripos Division, Evans & Sutherland

Prof. Switzer is modeling a complex chromatography diffusion on a supercomputer. This year we will help him visualize his results in various ways.

We expect to formalize our collaboration with Scripps Research Institute with an agreement, continuing the working visits of 1986 and 1987 and formalizing a summer intern program.

The Richardsons are designing artificial proteins. They need a convenient way for an interactive user to specify the warping and shaping of beta sheet and alpha helix. We have been trying to enlist a graduate research assistant with the appropriate mathematical skills and interests, for the problem is important and general. We will keep trying in 1988.

We will in 1988 assist in the teaching of a new graduate class in molecular modeling and molecular graphics, organized by Prof. Bowen in the School of Pharmacy.

### 3. Publications

Brooks F.P., "No Silver Bullet," *IEEE Computer*, 20(4), pp.10-19, April 1987. (Reprinted).

Brooks F.P., chairman, et al. *Report of the Defense Science Board Task Force on Military Software*. Office of the Under Secretary of Defense for Acquisition, Washington D.C., 1987.

Brooks F.P., "Grasping Reality Through Illusion," Proceedings *CHI '88*, Washington D.C., May 1988. (Keynote speech, submitted for publication).

Glassner A.S., "Supporting Animation in Rendering Systems," Proceedings *CHI+GI '87 Workshop on Rendering Algorithms and Systems*, Canadian Information Processing Society, Toronto, April 1987. (Workshop participation by invitation only).

Holloway R.L., *Head-Mounted Display Technical Report*, UNC Dept of Computer Science Technical Report TR87-15, June 1987.

Levoy M., "Rendering Surfaces from Volume Data," *IEEE Computer Graphics and Applications*. (Accepted).

Levoy M., "Direct Visualization of Surfaces from Computed Tomography Data," *SPIE/Medical Imaging II*, Newport Beach, Feb. 1988.

Lipscomb J.S., "Comparison of Stereoscopic Display Devices at the University of North Carolina at Chapel Hill," *Chemical Design Automation News*, 2(5), pp.3-6, May 1987. (Invited paper).

Ouh-young M., Pique M.E., Hughes J., Srinivasan N. and Brooks F.P., "Using a Manipulator for Force Display in Molecular Docking," *International Robotics and Automation Conference*, Philadelphia, April 1988. (Accepted).

Palmer T.C., *Docktool: A Dynamically Interactive Raster Graphics Visualization for the Molecular Docking Problem*, Master's thesis, Dept of Computer Science, UNC at Chapel Hill, May 1987.

Thorvaldsdottir H., "Computer graphics model of an ATP molecule," cover picture, *Chemistry and Life* by J.W. Hill and D.M. Feigl, 3rd edition. Macmillan Publishing Company, 1987.

#### Unpublished Conference Presentations

Thorvaldsdottir H. and Pique M.E., "Scouting Expeditions in Molecular Graphics," *Shell Conference on Computer Aided Molecular Modeling*, Hoenderloo, The Netherlands, Oct. 1987. (Invited talk).