

**Tenth Annual Report
Final Technical Report
Interactive Graphics for
Molecular Studies
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Grant RR-00898
National Institutes of Health**

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B. Highlights - 1983-84

1. GRINCH System Transported to PS-300

Our team converted the UNC GRINCH system to run on the VAX and our new Evans and Sutherland PS-300 color vector display system, and reworked it to get usable response time. 16 biochemists from 7 laboratories used the new system to attack uninterpreted maps.

GRINCH is the Chapel Hill system for *ab initio* interpretation of macromolecule density maps. It uses color and a novel ridge-line representation of maps to make the structure of an entire macromolecule (1) displayable, and (2) comprehensible on the screen.

Originally the GRINCH system used an Ikonas raster scan system for color display of a few lines at a time, and a Vector-General 3303 for monochrome display of all lines at once.

2. GRINCH system Transported to Lower-Cost Masscomp - PS-300 System

At the end of the project year, we transported the VAX code of GRINCH to a Masscomp 500. The display code still runs on an E. & S. PS-300 system. This gives an acceptable GRINCH performance on a computer-display configuration costing well under \$100,000.

Our software has been exported and is in daily use on a Masscomp-PS-300 configuration at Duke.

III. Narrative Description

A. Summary of Research Progress

1. Objectives and Operation

We have built, and operate as a service resource, an effective interactive computer resource for seeing, manually manipulating, and computationally modifying mathematical models of complex molecules. We believe that our present resource, called GRIP, has been shown to be as complete and useful as any in existence. One impressive measure of the power and the utility of the GRIP-75 system is that at least seven of our scientific collaborators have obtained their own graphics systems as a direct result of their successful work here.

Our resource has dual objectives. We are a service center providing powerful computer graphics facilities and expert computer assistance to chemists studying macromolecular structure. We are also computer scientists dedicated to advancing the art of interactive computation and interactive three-dimensional graphics. The objectives are complementary. Our chemist collaborators provide the essential focus and a real, complex, and interesting driving problem for our computer science research; our computer science research in turn provides our clients with more powerful tools to improve their insight into very complex structures.

Fundamental to our approach are the following principles:

- The GRIP Resource is designed to help chemists get results from their research, and its success is measured only by theirs.
- Our systems are designed to help the chemist visualize his molecules, his density maps, etc., so that he can use his knowledge to guide computational processes. That is, they are an aid to, not a surrogate for, human thinking and manipulation. Hence a strong emphasis is placed on human factors research and on human engineering of the system.
- GRIP is designed to serve many users, not one or two, so it includes an armory of alternative tools and techniques.
- GRIP is designed to interface smoothly with any batch computations its users must do, and to incorporate on-line facilities for all computations that can reasonably be done "while you wait."
- We as computer scientists are interested in GRIP as a test-bed for research in man-machine systems design, in man-machine interaction, and in the design of distributed computing systems.

A corollary of these objectives is that we are heavily dependent on observation of and feedback from real users attempting to solve real problems. Our users are almost exclusively working on the structures of molecules of considerable biochemical interest: proteins and nucleic acids. We advance health-oriented biochemical research by enhancing the productivity of individual researchers through better tools.

Our hardware configuration on the VAX system is

- VAX-11/780 with UNIBUS but no MASSBUS;
- the UNIX operating system (Berkeley 4.2 bad version for the VAX)
- 4 MB memory

- 600 MB disk storage
- 800/1600 bpi dual density tape drive
- Vector General 3303 vector graphics display
- Evans & Sutherland Picture System 300 color vector graphics display
- Adage Ikonas RDS-3000 image processing and display system, with 1024 by 1024 pixels at 6 bits/pixel (or 512 by 512 at 24 bits/pixel), color map, two internal high speed processors, cross-bar switch for remapping pixel values, video digitizer, and write mask.
- several data tablets, mice, joysticks
- 16-channel (expandable to 32) analog to digital converter
- high speed parallel link to department VAX, which has hard copy plotters, printer, and a dial-up connection to the national "USENET" UNIX network
- Masscomp 500 color graphics workstation

2. Overview of Five-Year Progress

Since this Tenth Annual Report is also the Final Technical Report on Grant RR 00898, it is appropriate to review the progress of the past five years.

2.1 GRINCH System

Our major accomplishment has been the development of a new *kind* of molecular graphics tool, one aimed at a heretofore unaddressed part of the crystallographer's problem, initial map presentation.

Our earlier molecular graphics system, GRIP-75, aimed to assist crystallographers with fitting molecular structure rather precisely into electron density maps. It, like its counter-parts from other labs, the St. Louis MMSX system, Robert Diamond's Bilder system, Alwyn Jones's Frodo system, all work best after the chemist has an approximate map interpretation, generally derived from a plastic minimap. All systems of this sort represent electron density by contour maps. All present incomprehensibly complex views of maps when a whole protein is viewed.

The GRINCH system, developed first by Thomas V. Williams in collaboration with biochemist Jane Richardson of Duke, aims to substitute computer graphics for the plastic minimap in the *ab initio* interpretation of density maps. This requires the ability to see and comprehend the map globally as well as locally.

Williams addressed this comprehensibility problem in four ways:

- Electron density is represented by a ridge-line representation originally proposed by Carroll Johnson of Oak Ridge, instead of by contour lines. This representation uses about two orders of magnitude fewer line segments. Hence whole molecule-sized maps can be (1) displayed without flicker, and (2) comprehended.

- Each ridge line is tagged with the density of its midpoint. A dynamic slider allows the viewer to smoothly change the display threshold, showing only lines above that density. So one may glide back and forth between seeing only high peaks and seeing fine detail.
- Since there are fewer lines to be redrawn, the viewer can easily and quickly move between enlarged local views and global views.
- Color is used in an integral way to distinguish interpreted ridge lines from uninterpreted ones, and to mark main chain, side chains, oxygens, disulphide bonds, etc.

The GRINCH System has aroused great interest. 7 teams of chemists have come to Chapel Hill to use it; copies of the software have already been exported to three other labs. Versions have been ported to several different hardware and operating system configurations.

2.2 GRIP Used, Converted

Our original density fitting system, GRIP-75, was widely used, even though its hardware configuration made the software essentially unexportable. Some thirty teams of biochemists have journeyed here to use it; new ones keep coming. Over 35 papers describing work done on GRIP-75 have been published by our collaborators in the chemical literature.

The structures of at least Super-oxide Dismutase and Erabutoxin were determined entirely on GRIP-75, without resort to brass models.

We have converted GRIP-75 from an IBM 360/75 - DEC PDP 11/45 - VG 3 - PL/I configuration to a DEC VAX 11/780 - VG 3303 - C configuration and have begun serving collaborators with the new configuration. That conversion was a lot of work.

2.3 Dynamic Viewing of Space-Filling Models

Michael Pique achieved near-real-time display of colored, shaded intersecting-sphere models of molecules of up to several hundred atoms. These models, the computer-graphics analog of CPK plastic spherical models, represent each atom by its Van der Waal's surface. These of course intersect. The space-filling models are useful for studying crystal packing, active sites, and molecule-molecule docking.

Static pictures of space-filling models have been within the art for some time. (Nelson Max of Livermore produced a dramatic model of DNA.) Such pictures have taken minutes to hours of computer time. Dynamic models give much better comprehensibility, since the kinetic depth effect is one of the most powerful cues for 3-D perception.

Pique's system uses an Adage Ikonas 3000 color raster display and its associated AMD 2900 bit-slice processor. He achieves picture update rates of 2-8 frames/second depending upon picture complexity and size (number of pixels to be rewritten). The techniques used to get this dynamic display include

- careful coding of the display processor
- reducing resolution to 256 x 256, without reducing size

- restricting the illumination point to be the viewpoint, so each sphere's surface is shaded with circular symmetry.

Pique's fast solid-model display system has been published and is commercially sold and supported by Intermetrics Incorporated.

2.4 Multiple Visualizations

Molecules are essentially abstract objects, far smaller than the wave-length of light. They must be visualized by analogy. We are convinced that a computer graphics workbench for chemists should include a large collection of different visualizations, each yielding insight about one or another aspect of molecule structure and function.

We started with the familiar stick-figure Kendrew models for bonds for molecules and parallel-plane contours for density maps. Very early we added 3-D contour baskets.

In the past five years we have begun systematically realizing on the computer graphics screen as many other visualizations as we can find, both by importing programs and by collaborations. Techniques pioneered here include

- dynamic, shaded "solid" CPK models described above
- colored ribbon models of main chains, developed in collaboration with Jane Richardson
- the RAMS "solid" shaded and colored solvent-accessible surfaces developed here by Michael Connolly, then visiting.
- a dynamic "flight-of-bees" visualization derived from the electrostatic field, developed in collaboration with John Tainer and Libby Getzoff of Scripps.
- a thermal coloring representation, developed in collaboration with Professor Stephen Pizer of UNC.

Two visual publications have been used to demonstrate these and other visualization techniques:

"What Does a Protein Look Like?" by Michael Pique, is a 20-minute videotape first presented at the *Science Magazine* 1982 Conference on Science and the Computer. This tape showed some 40 different visualizations of Superoxide Dismutase.

Pique and Lipscomb developed a flight sequence exploring SOD as part of an Omnimax-Imax film first presented at SIGGRAPH 84 and now touring among the nation's planetariums. This technique projects 70-mm film over a full half-sphere dome (Omnimax), or over a very wide-angle big screen (Imax), to give viewers the sensation of immersion in the visual space.

2.5 Man-Machine Interface

In GRIP-75 we demonstrated the effectiveness of a joystick-driven interface for molecular modeling. This system-building work was followed up by a scientific study of the interface, in both its perceptual and its manipulative aspects, by J.S. Lipscomb in his Ph.D. dissertation, *Three-Dimensional Cues for Molecular Graphics Systems*.

Three-dimensional cues we have investigated include:

- kinetic depth effect achieved by smooth viewpoint change
- stereo vision

realized by space-division:

- stereoscopic view of side-by-side images
- Ortony's over-under polarized technique

and by time division:

- Evans and Sutherland Lorgnette (disk shutter)
- Bausch and Lomb cylindrical shutter
- PLZT glasses
- liquid crystal glasses
- liquid crystal Tektronix plate
- intensity depth cueing
- perspective
- hidden-surface representations
- head-motion parallax
- real 3-D display on Varifocal mirror.

Lipscomb's work also included time-and-motion studies of user interactions with the GRIP-75 system, and studies of perception artifacts induced by different refresh and update cycles.

2.6 Advanced Technology

As computer scientists serving the molecular structure community, we see one of our roles to be the application of advanced technology from computer graphics research to the molecular application. Over the past five years this work has included:

- exploration of new stereovision technology enumerated above.
- application of a radically cheaper and faster varifocal mirror 3-D technique developed by Fuchs and Pizer at UNC.
- development of special molecular studies algorithms for Fuchs's special-purpose Pixel-Planes display processor, under development at UNC.
- collaboration with Fuchs and Bishop on head-mounted displays.
- application of speech recognition technology to menu-picking in GRINCH.

2.7 Molecular Dynamics

Professor J.H. Hermans and his associates of UNC Biochemistry have developed a suite of programs for modeling molecular dynamics. We have collaborated by providing computer facilities and some know-how. We have benefitted by access to their programs for model building, energy calculation, and file transformations.

3. Resource Progress During 1983-84

3.1 New Research Program Formulated

As we approached the end of our second five-year period as a Research Resource, major effort was spent of reexamining the fields of molecular studies and of computer graphics. Does a computer graphics group still have a key role to play, or has all the interesting and critical work been done in bringing computer graphics to molecular studies, as some say?

In looking at molecular studies, we see structure determination continuing to be exciting, enhanced by big collectors, better X-ray sources, and increasing use of NMR data. Structure-function studies, including enzyme-substrate docking and analytic design of proteins and drugs is a dramatically growing activity. Molecular dynamics techniques are increasingly being developed, and they generate vast amounts of data. We see a variety of new needs for computer graphics and needs for new computer graphics techniques and tools.

In looking at the computer graphics field we see an explosive development of new technology and concepts, and, most important of all, a continuing radical decline in costs, with no end in sight.

Hence it looks as if there is still a key role for us at the intersection of these two dynamic fields. The new role is different, however. The importance of our Resource as a place chemists come to do work will decline, but not vanish. Our most important function is to explore new technology and to develop molecular graphics application software for export to biochemists, anticipating and riding the waves of advance in commercially available hardware. Since it takes several years to develop, debug, and polish a software system, we need at Chapel Hill to be that far ahead in anticipating the hardware biochemists will install in the future.

For these reasons our new five-year research plan emphasizes Resource-Related Research rather than Resource operation. Figure 1 shows our "Seven-Bubble Research Plan" symbolically.

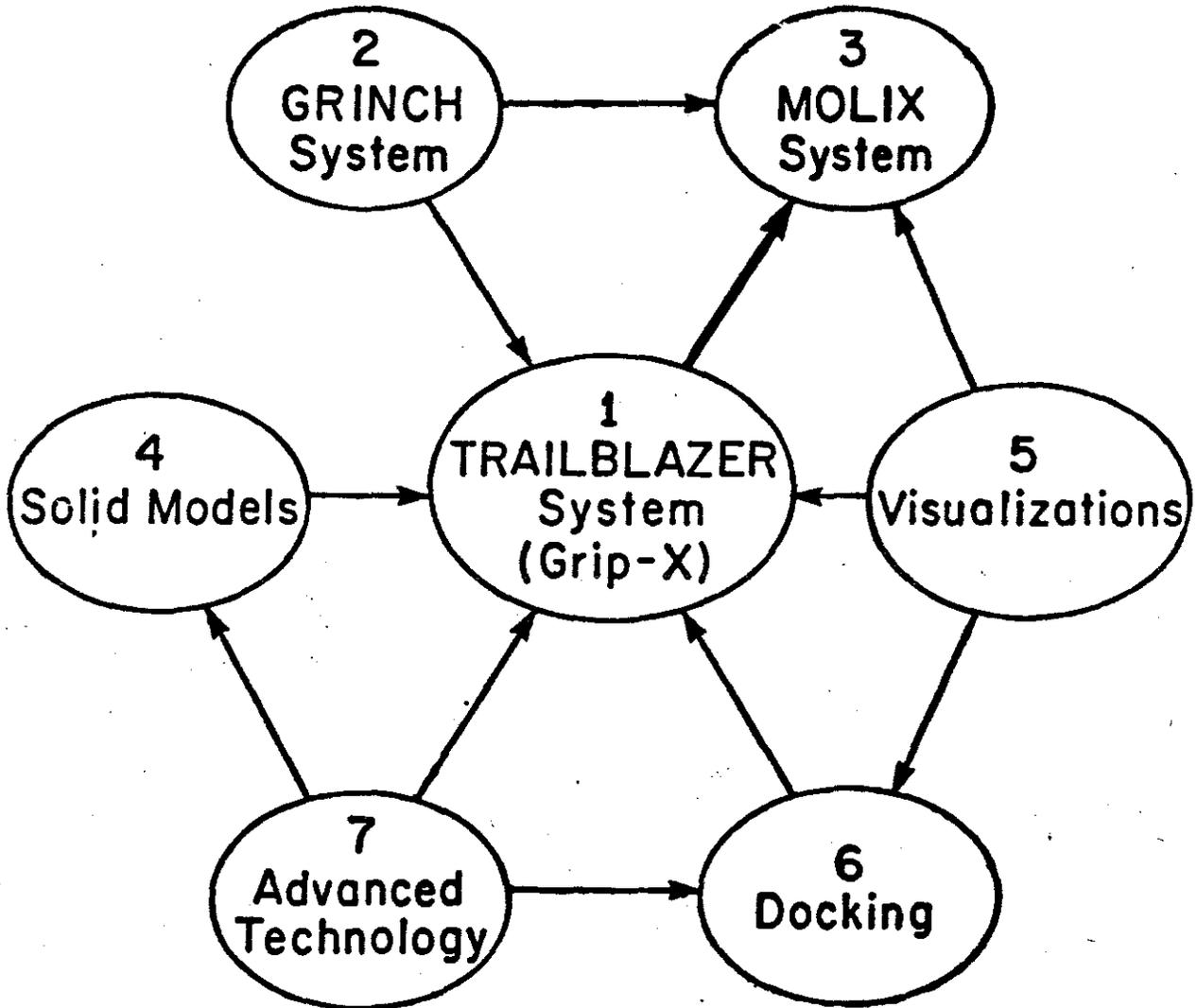


Figure 1 "Seven-Bubble Research Plan"

At the center is the continuing development and operation of the Resource at UNC as a "trailblazing system", where collaborators may come to use the most advanced hardware and software, and to work with us on developing new techniques.

Further polishing, export, and testing of the GRINCH ridge-line interpreting system is our second activity. We plan further exploitation of the economical ridge-line representation and hope to test the hypothesis that a more comprehensible representation may allow lower-resolution maps to be interpreted. A major effort will be to combine GRINCH and GRIP capabilities into a single system.

The MOLIX activity consists of transporting molecular graphics software to 68000-based graphics workstations in the under-\$50,000 price range. We are currently moving GRINCH to a Masscomp 500. We expect to move GRIP or GRIP function.

The Fast Spheres activity is to push both hardware and software art hard to make it possible to rotate pictures of CPK models, intersecting spheres representing Van der Waal's surfaces, smoothly in real time.

The Visualizations activity is a continuation of our exploration of the insight-producing power of unconventional ways of visualizing molecules.

The Docking activity, currently in the early exploration phase, will study effective ways to assist the user in perceiving molecule docking situations — surfaces, close-approach displays, energy modeling, force-displays to the sense of feel.

The Advanced Technology activity will continually adapt and apply latest computer graphics ideas and hardware to molecular studies.

3.2 GRINCH Ported to PS-300

Our major activity in 1983-84 was the upgrade of our E & S PS-300 vector display by addition of a color tube, the porting of our GRINCH system to it, and enhancement of response on it.

The GRINCH system was originally built using an Ikonas color raster display and a VG-3303 black-and-white vector display. It needed color and lots of lines. The Ikonas provided color but couldn't do many lines; the VG provided up to 10,000 short vectors with smooth rotation, but only in black and white.

Evans & Sutherland gave our project a monochrome PS-300 in '82. In '83-'84, we scraped together all available money and bought (at deep discount) a color tube. This offered the possibility of doing GRINCH properly — plenty of colored vectors.

The PS-300 is

- (1) programmed differently from all other displays
- (2) connected to the host by a slow (19.2 kilobaud) channel.

Most of our systems work this year was devoted to the conversion and overcoming these two obstacles. The system is now converted and respectably responsive.

Chemists who have used the PS-300 version are

Jane and David Richardson and Duncan McRee of Duke University, Judith Kelly of the University of Connecticut, Bud Suddath, Howard Einspur, Seguna of the University of Alabama in Birmingham, Chang Park and Rich Blevins of Michigan State University, John Rosenberg and Christine Frederick of the University of Pittsburgh, Rufus Burlingame and Brad Branden of Johns Hopkins University and Roger Fena and Robert Egan of the University of Miami.

Professor Tom Hern, visitor from Bowling Green State University led this effort. Doug Schiff, Isidore Rosenblum, Lee Westover were key contributors.

3.3 MOLIX Project Started — Masscomp Chosen, Acquired

In moving high-performance software to a small machine, many hard questions arise. The first is what machine? We evaluated a variety of graphics workstations built on the Motorola 68000 processor, including those by

Sun Microsystems
Apollo
Masscomp

Apollo was finally ruled out because it doesn't run the Unix operating system, and it became evident that it would not.

We installed a Sun with color graphics attachment. After extensive evaluation, we chose Masscomp, fundamentally because the graphics board is much more usefully designed. It has, for example, double-buffering, essential for animation. Masscomp also offers faster floating point and an array processor option.

After making our selection, we began negotiations with Masscomp. As a result they are furnishing us a fully-loaded development system, to which we have made the first MOLIX and GRINCH transports. We will later do ports to other brands of high-performance workstations. It has been installed and is operating.

3.4. GRIP-75 Converted to VAX-Unix

GRIP-75 was developed for a dedicated PDP11/45 driving a VG-3 vector display and running time-shared on an IBM System/360-75. In 1983-84 we completed the conversion to the C language, the Unix 4.2 bsd operating system, and DEC VAX11/780 computer, and the Vector General 3303 display. The old machinery has been removed and the first visiting collaborators have used the converted GRIP. It still needs stereo and some operating system priority enhancements to improve response.

3.5 Visualizations - Omnimax

As a continuation of our unconventional visualizations work, Mike Pique and Jim Lipscomb made a 90-second sequence of Super-Oxide Dismutase as perceived from a flight into the active site and up the beta-barrel, showing ribbons, surfaces, and animated electrostatic lines of force. This explored the perceptual effects of very wide-angle display. Omnimax film is projected on a

half-sphere planetarium dome and gives the audience, seated as nearly as possible in the sphere center, the effect of total immersion in the scene.

The Pique-Lipscomb sequence pioneered the use of motion-blurring, in which objects are blurred in each frame calculated so that the intermittently- projected frames reproduce the visual sensations of continuous motion. Their experiments showed that the brightness necessary in blurred images of lines could not be calculated by the constant-energy formulas derived theoretically.

The sequence was published as part of the first totally computer-graphics-generated Omnimax film. The film premiered in July at SIGGRAPH, at the St. Paul Museum of Science.

3.6 Prophet

In 1983-84 The Resource applied for its own Prophet membership. Heretofore we had been users through the kindness, and at the expense, of Burroughs-Wellcome. Doris Knecht built tools to access the database, to use Prophet molecule-building tools, and to feed Prophet data into our 3-D display programs.

3.7 Database Studies

Doris Knecht, supported by a Burroughs-Wellcome Research Assistantship, studied the applicability of the Troll general-purpose relational database system to our molecular data. This followed studies by our collaborators at the IBM United Kingdom Scientific Centre, where Stephen Todd showed that the Peterlee Relational Test Vehicle could readily produce a wide and flexible variety of views with waits of only 15-30 seconds for arbitrary requests.

Knecht's studies showed that the use of Troll required about 3 times as much memory/disk space, and about 3 times as much access time, as our special-purpose data structures.

Our net is that a general-purpose database system is a useful adjunct to a molecular graphics system, but that the system itself should have a specialized data handler, into whose formats the general-purpose database translates its outputs.

3.8 Molecular Dynamics

Professor Jan Hermans and Michael Carson made extensive use of the resource for molecular dynamics computations and for the display of the results. Such graphical display proves essential for the assimilation of the immense volumes of data produced by molecular dynamics calculations.

The GRIP team uses Hermans's programs for model-building new molecular structures.

3.9 New Graphics Laboratory Designed

In 1983 the North Carolina General Assembly appropriated \$9.25 million for a new 74,000 square-foot building for the Department of Computer Science. A major effort by Brooks during 1983-84 was the planning of the new building, whose funding was totally unanticipated.

The computer graphics faculty (Professors Henry Fuchs, Stephen Pizer, Turner Whitted, and Brooks) will be clustered together on the third floor. The Graphics Laboratory will be about four times the size of the present one, with a large multi-display shared room, about twice as big as our present lab, plus specialized areas for (1) displays used by visiting chemists, (2) special-purpose displays such as head-mounted, (3) videotape editing, (4) videotape viewing, (5) teleconferencing with Duke collaborators, and (6) offices for visiting chemists. Completion is scheduled for 1986 (and expected in 1987).

3.10 Advanced Technology Projects

Advanced technology projects continued in 1983-84.

Milgram Glasses. New electronic stereo glasses, using liquid crystals for shuttering, were first field tested in our laboratory by inventor Paul Milgram, of Belgium. These glasses switch slightly slower than our PLZT glasses, but the transmissivity is very high (90%). This is a crucial improvement. We made a videotape of test and demonstration 3-D images for Milgram to use with his glasses.

It now appears that a Dutch firm will be manufacturing the glasses and offering them commercially.

Speech Recognition Experiment. All menu-driven computer graphics systems suffer from a need for two cursors, one staying in the data to pick data objects — atoms, bonds, contours — and the other selecting commands from the menu. Using one cursor for both purposes requires hand and eye to flip-flop between the two regions, violating Foley and Wallace's maxims of Tactile Continuity and Visual Continuity.

In 1983-84 we experimented with using off-the-shelf speech recognition equipment to do command recognition in GRINCH.

After considerable investigation, aided by computer scientist Professor Alan Biermann of Duke, an expert in speech recognition, we selected equipment by Votan. This provides state-of-the-art recognition for up to 256 isolated utterances. Recognition is speaker-dependent: the system must be trained by the user.

A student team from our Software Engineering Laboratory course built prototype software to integrate this equipment into GRINCH, and they demonstrated successful operation in May, 1984. The team members were Brad Frecker, Howard Gross, Elizabeth Hookway, Gray Moody, and Janette Dresser.

The prototype is now being modified to product-quality software. The first test by a chemist in real production use is scheduled for November, 1984.

Head-Mounted Display. Professors Fuchs and Brooks continued their collaboration on developing a head-mounted display. Such a system would allow a chemist to move around in a 3-D room-sized molecule, say 20 cm/A, viewing and manipulating.

Gary Bishop, for his Ph.D. dissertation, developed a whole new scheme for tracking the position and orientation of the head. He uses a set of 12 head-mounted sensors that integrate motions of objects in the room. He designed a VLSI chip embodying optical sensors, amplifiers, correlation

circuitry. The chip has been through several fabrication/redesign iterations and operates at a rate of 500-100 images/second!

This is a big project, which will take years, but the sensor work is a major advance.

4. Collaborative Research

4.1 User Collaborators, 1983

The scientific collaborators who used our facility in 1983 are listed in the table. Every member of our team helped our collaborators with their work.

Table I: Resource Users, 1983

M. Schiffer	Argonne National Laboratory
H. C. Taylor	Berkeley Springs Research Consortium
B. Roth	Burroughs-Wellcome
J. Bentley	
M. Cory	
L. Kuyper	
D. C. Richardson	Duke University
J. S. Richardson	
D. McRee	
M. Z. Atassi	Mayo Clinic
C. Wright	Medical College of Virginia, Virginia Commonwealth University, Richmond
F. L. Suddath	University of Alabama in Birmingham
W. Cook	
H. Einspur	
J. Kelly	University of Connecticut
A. Blaurock	University of North Carolina Anatomy Dept.
A. Andersen	
J. Hermans	University of North Carolina Biochemistry Dept.
M. Carson	
L. Pedersen	University of North Carolina Chemistry Dept.
M. Eastman	
G. Long	
P. Singh	University of North Carolina Chemistry Dept.

4.2 Close Collaborations

We continued close collaborations and consultations as to the direction of our facility development with

- Professor Jan Hermans, Biochemistry, UNC
- Professors David and Jane Richardson, Biochemistry, Duke
- Doctors Barbara Roth, Michael Cory, Lee Kuyper, Burroughs-Wellcome
- Messrs. Tom Haywood, Peter Quarendon, Stephen Todd, Dr. Andrew Morffew, Dr. William Wright, IBM UK Scientific Centre, Winchester, England. We have a half-hour telephone conference between their team and ours each week.

4.3 Resource Advisory Committee and Allocation of Resources

Table II lists the members of our Advisory Committee.

We currently offer the facility, and such help as we can give, free of charge to any chemist:

- who has a scientifically interesting problem,
- whose work is at a stage where our facility might be useful,
- who is willing to commit his time, travel money, and effort to a serious use of the facility, and
- who is willing to give us written and oral feedback from his experience.

Table II: Advisory Committee Members

<u>Name</u>	<u>Degree</u>	<u>Title</u>	<u>Department</u>	<u>Institution</u>
F. P. Brooks	Ph.D.	Kenan Professor	Computer Science	UNC-CH
J. Hermans	Ph.D.	Professor	Biochemistry	UNC-CH
D. Richardson	Ph.D.	Professor	Biochemistry	Duke U.
J. Richardson	M.S.	Assistant Professor	Anatomy	Duke U.
W. V. Wright	Ph.D.	Senior Systems Architect	Communications Division	IBM

4.4 Dissemination of Information

The availability of GRIP-75 is widely known among crystallographers. We publicize the facility by announcements and notices at scientific meetings, by demonstrations to all interested parties, and by word of mouth. Demonstrations are perhaps the most effective means.

4.5 GRIP Molecular Computer Graphics System Publications

Compiled by J.S. Lipscomb and M.E. Pique
19 December 1988

Department of Computer Science
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Publications by NIH Facility Users

- Hermans, J., Excluded-volume theory of polymer-protein interactions based on polymer chain statistics, *J. Chem. Phys.* 77, 2193-2203 (1982).
- Knoll, D. and Hermans, J., Polymer-protein interactions: Comparison of experiment and excluded-volume theory, *J. Biol. Chem.*, (accepted).

Publications by GRIP-75 Users

- Beem, K.M., Richardson, D.C., and Rajagopalan, K.V. Metal Site of Cu,Zn Superoxide Dismutase. *Biochemistry*, 16, #9, 1930-1936, (3 May 1977).
- Carter, C.W. X-ray Analysis of High Potential Iron-Sulfur Proteins and Ferredoxins. *Iron-Sulfur Proteins*, Academic Press, Chapter 6, (1977).
- Ferro, D.R., McQueen, J.E., Jr., McCown, J.T., and Hermans, J. Energy Minimizations of Rubredoxin. *Journal of Molecular Biology*, 136, 1-18, (1980).
- Fontecilla-Camps, J.C., Almassy, R.J., Suddath, F.L., Watt, D.D., and Bugg, C.E. Three-dimensional structure of a protein from scorpion venom: A new structural class of neurotoxins. *Proc. National Academy of Sciences USA*, 77, #11, 6496-6500, (November 1980).
- Getzoff, E.D. *The Refined 2Å Structure of Bovine Copper, Zinc Superoxide Dismutase: Implications for Stability and Catalysis*. Ph.D. Dissertation, Department of Biochemistry, Duke University, (1982).
- Getzoff, E.D., Tainer, J.A., Sack, J.S., and Richardson, D.C., Determination of the 4Å Structure of the Root-Effect Hemoglobin from the Fish Spot. *Proc. National Academy of Sciences USA*, (in preparation).
- Getzoff, E.D., Tainer, J.A., Weiner, P.K., Kollman, P.A., Richardson, J.S., and Richardson, D.C., Electrostatic recognition between superoxide and copper, zinc superoxide dismutase. *Nature*, 306, 287-290, (17 November 1983).
- Girling, R.L., Houston, T.E., Schmidt, W.C., Jr., and Amma, E.L. Macromolecular Structure Refinement by Restrained Least Squares and Interactive Graphics as Applied to Sickling Deer Type III Hemoglobin. (Abstract). *ACTA Crystallographica*, A36, 43, (1980).
- Girling, R.L., Houston, T.E., Schmidt, W.C., Jr., and Amma, E.L. Molecular Packing and Intermolecular Context of Sickling Deer Type III Hemoglobin. *Journal of Molecular Biology*, 131, 417-433, (1979).

- Hendrickson, W.A. and Konnert, J.H. Stereochemically Restrained Crystallographic Least-squares Refinement of Macromolecule Structures. *Proc. International Symposium on Biomolecular Structure, Conformation, Function, and Evolution*. Edited by Srinivasan, R. Madras: Pergamon Press. January 1981. 1, 43-57, (1981).
- Hendrickson, W.A. and Smith, J.L. Quaternary and Tertiary Structure of Hemerythrins. *Invertebrate Oxygen-Binding Proteins: Structure, Active Site, and Function*. Edited by Lamy, Jean and Lamy, Josette. New York, Basel: Marcel Dekker, Inc. 343-352, (1981).
- Holbrook, S.R., Sussman, J.L., Warrant, R.W., Church, G.M., and Kim S.H. RNA-ligand Interactions: (I) Magnesium Binding Sites in Yeast tRNA Phe. *Nucleic Acids Research*, 4, #8 (August), 2811-2820, (1977).
- Honzatko, R.B., Crawford, J.L., Monaco, H.L., Ladner, J.E., Edwards, B.F.P., Evans, D.R., Warren, S.G., Wiley, D.C., Ladner, R.C., and Lipscomb, W.N. Crystal and Molecular Structures of Native and CTP-liganded Aspartate Carbamoyltransferase from *Escherichia coli*. *Journal of Molecular Biology*, 160, 219-263, (1982).
- Kim, S.H. and Sussman, J.L. Pi Turn is a Conformational Pattern in RNA Loops and Bends. *Nature*, 260, #5552, 645-646, (15 April 1976).
- Kimball, M.R., Sato, A., Richardson, J.S., Rosen, L.S., and Low, B.W. Molecular Conformation of Erabutoxin b; Atomic Coordinates at 2.5Å Resolution. *Biochemical and Biophysical Research Communications*, 88, #3, 950-959, (13 June 1979).
- Love, W.E., Fitzgerald, P.M.D., Hanson, J.C., and Royer W.E. Intermolecular Interactions in Crystals of Human Deoxy Hemoglobin A, C, F and S. *Proc. The International Meeting on The Development of Therapeutic Agents for Sickle Cell Diseases*. 19-21 July 1978, 65-75, (1979).
- Monaco, H.L., Crawford, J.L., and Lipscomb, W.N. Three-dimensional Structures of Aspartate Carbamoyltransferase from *Escherichia coli* and of its Complex with Cytidine Triphosphate. *Proc. National Academy of Sciences USA*, 75, #11, 5276-5280, (November 1978).
- Richardson, J.S. The Importance of Non-Local Interactions and Non-Repetitive Structures in Protein Folding. Abstracts for USA - Japan Seminar on Self-Organization of Protein Molecules, Cornell Univ., ed. H.A. Scheraga, (1981).
- Richardson, J.S. Chapters on "Interpretation of Electron Density Maps" and "Common Folding Patterns in Protein Domains" for *Methods in Enzymology: Diffraction Methods for Biological Macromolecules*, ed. Wyckoff, Timasheff, (in preparation).
- Richardson, D.C. Three-dimensional Structure of Cu, Zn Superoxide Dismutase. *Superoxide and Superoxide Dismutases*. Edited by A.M. Michelson, J.M. McCord, and I. Fridovich. London, New York: Academic Press. 217-223, (1977).
- Schevitz, R.W., Podjarny, A.D., Krishnamachari, N., Hughes, J.J., Siglar, P.B., and Sussman, J.L. Crystal structure of a eukaryotic initiator tRNA. *Nature*, 278, #5700, 188-190, (8 March 1979).
- Stenkamp, R.E., Sieker, L.C., Jensen, L.H., and McQueen, J.E., Jr. Structure of Methemerythrin at 2.8Å Resolution: Computer Graphics Fit of an Averaged Electron Density Map. *Biochemistry*, 17, #13, 2499-2504, (27 June 1978).
- Sussman, J.L., Holbrook, S.R., Church, G.M., and Kim, S.H. A Structure-factor Least-squares Refinement Procedure for Macromolecular Structures using Constrained and Restrained Parameters. *ACTA Crystallographica*, A33, 800-804, (1977).
- Sussman, J.L., Holbrook, S.R., Warrant, R.W., Church, G.M., and Kim, S.H. Crystal Structure of Yeast Phenylalanine Transfer RNA. I. Crystallographic Refinement. *Journal of Molecular Biology*, 123, #4, 607-630, (25 August 1978).
- Sussman, J.L. and Kim, S.H. Idealized Atomic Coordinates of Yeast Phenylalanine Transfer RNA. *Biochemical and Biophysical Research Communications*, 68, #1, 89-96, (1976).
- Sussman, J.L. and Kim, S.H. Three-Dimensional Structure of a Transfer RNA Common in Two Crystal Forms. *Science*, 192, #4242, 835-838, (28 May 1976).

- Tainer, J.A. *Determination and Analysis of the 2Å Structure of Bovine Copper, Zinc Superoxide Dismutase*. Ph.D. Dissertation, Department of Biochemistry, Duke University, (1982).
- Tainer, J.A., Getzoff, E.D., Beem, K.M., Richardson, J.S., and Richardson, D.C. Determination and Analysis of the 2Å Structure of Copper, Zinc Superoxide Dismutase. *Journal of Molecular Biology*, 160, 181-217, (1982).
- Tainer, J.A., Getzoff, E.D., Richardson, J.S., and Richardson, D.C., Structure and mechanism of copper, zinc superoxide dismutase. *Nature*, 306, 284-287, (17 November 1983).
- Taylor, H.C., Richardson, D.C., Richardson, J.S., Wlodawer, A., Komoriya, A., and Chaiken, I.M. "Active" Conformation of an Inactive Semisynthetic Ribonuclease-S. *Journal of Molecular Biology*, 149, 313-317, (1981).
- Tsernoglou, D. and Petsko, G.A. Three-Dimensional Structure of Neurotoxin a from Venom of the Philippines Sea Snake. *Proc. National Academy of Sciences USA*, 74, #3, 971-974, (March 1977).
- Tsernoglou, D., Petsko, G.A., and Hudson, R.A. Structure and Function of Snake Venom Curarimimetic Neurotoxins. *Molecular Pharmacology*, 14, 710-716, (1978).
- Tsernoglou, D., Petsko, G.A., McQueen, J.E., Jr., and Hermans, J. Molecular Graphics: Application to the Structure Determination of a Snake Venom Neurotoxin. *Science*, 197, #4311, 1378-1381, (30 September 1977).
- Tsernoglou, D., Petsko, G.A., and Tu, A.T. Protein Sequencing by Computer Graphics. *Biochem. and Biophys. ACTA*, 491, 605-608, (1977).
- Warrant, R.W. and Kim, S.H. Alpha Helix-Double Helix Interaction: Structure of a Protamine-Transfer RNA Complex and Nucleoprotamine Model. *Nature*, 271, #5641, 130-135, (12 January 1978).

Unpublished Conference Presentations by Users

- Hermans, J.H. *Excluded-volume theory of polymer-protein interactions based on polymer chain statistics*. Biophysical Society Meeting, Boston, Mass. (February 1982).
- Richardson, J.S. A User's Eulogy of Computer Graphics for Interpreting Protein Structure. *Thrasymachan Conference*, (biochemistry meeting), Memphis, Tenn., (28 March 1981).
- Richardson, J.S. One of two lectures on computer graphics given as "Ethel Mae Wilson Visiting Scholar" at Vanderbilt Univ., Nashville, Tenn., (21 April 1981).
- Tainer, J.A. and Getzoff, E.D. Metal Sites in Cu,Zn Superoxide Dismutase. *Metals in Biology Gordon Conference*, Ventura, Calif., (9 February 1982).
- Wright, H.T., Manor, P.C., Beurling, K., and Fresco, J.R. A Crystal Structure of Yeast tRNA-Gly; Possible Solvent Effects on tRNA Conformation. *Katzer-Katchalsky Symposium*, #7, Israel, (24 February 1980).
- Wright, H.T., Manor, P.C., Beurling, K., and Fresco, J.R. A Structure of tRNA-Gly Differs Markedly from that Determined for tRNA-Phe. *Pittsburgh Diffraction Conference*, (15-16 November 1979).

Publications by Builders

- Britton, E.G. *A Methodology for the Ergonomic Design of Interactive Computer Graphic Systems, and its Application to Crystallography*. Ph.D. Dissertation, University of North Carolina, Chapel Hill, North Carolina, (1977).

- Britton, E.G., Lipscomb, J.S., and Pique, M.E. Making Nested Rotations Convenient for the User. *Proc. 1978 ACM SIGGRAPH Conf., Computer Graphics, 12, #3, 222-227, (August 1978).*
- Brooks, F.P., Jr. The Computer "Scientist" as Toolsmith: Studies in Interactive Computer Graphics. *Proc. 1977 IFIP, 625-634, (1977).*
- Brooks, F.P. Jr. and Pique, M.E., What Does a Protein Look Like: Views of Unseen Worlds, (videotape), *ACM SIGGRAPH Video Review, (in preparation).*
- Foley, J.D. and Wright, W.V. An Interactive Molecular Graphics System with a Satellite Terminal Closely Coupled to its Host. (Panel discussion position paper) *Proc. ACM 1975 Annual Conference, 88-89, (1975).*
- Lipscomb, J.S., Grace Period for Picks. *ACM Transactions on Graphics, (submitted).*
- Lipscomb, J.S., Motion Decomposition, Orthogonality, and Stereo Display in a Molecular Computer Graphics System. *ACM Transactions on Graphics, (accepted).*
- Lipscomb, J.S. Reversed Apparent Movement and Erratic Motion with Many Refreshes per Update. *ACM SIGGRAPH, Computer Graphics, 14, #4, 113-118, (March 1981).*
- Lipscomb, J.S. *Review of Three-dimensional Display Techniques in Molecular Computer Graphics for Crystallography.* M.S. Thesis, University of North Carolina, Chapel Hill, North Carolina, (1979).
- Lipscomb, J.S. *Three-dimensional Cues for a Molecular Computer Graphics System.* Ph.D. Dissertation, University of North Carolina, Chapel Hill, North Carolina, (1981).
- Lipscomb, J.S., Brooks, F.P., Jr., and Pique, M.E. *The GRIP-75 Man-Machine Interface, (videotape), published in ACM SIGGRAPH Video Review, #4, (30 August 1981).*
- Pique, M.E., Fast 3-D Display of Space-filling Molecular Models, (videotape), *SIGGRAPH Video Review, (in preparation).*
- Pique, M.E. *Nested Dynamic Rotations for Computer Graphics.* M.S. Thesis, University of North Carolina, Chapel Hill, North Carolina, (1980).
- TenEyck, L.F., Pique, M.E., and Lipscomb, J.S., *UNC Interactive Raster Graphics Sampler, (videotape, 21 minutes), Published in ACM SIGGRAPH Video Review, #6 (22 October 1982).*
- Williams, T.V. *A Man-machine Interface for Interpreting Electron Density Maps.* Ph.D. Dissertation, University of North Carolina, Chapel Hill, North Carolina, (1982).
- Wright, W.V. *An Interactive Computer Graphic System for Molecular Studies.* Ph.D. Dissertation, University of North Carolina, Chapel Hill, North Carolina, (1972).
- Wright, W.V., *GRIP: An Interactive Computer Graphics System for Molecular Studies.* Computational Crystallography, ed. Sayre, D., Oxford University Press, p. 294, (1982).
- Wright, W.V. The Two-Dimensional Interface of an Interactive System for Molecular Studies. *ACM SIGPLAN notices, 7, #10, 76-85, (October 1972).*

Unpublished Conference Presentations by Builders

- Brooks, F.P., Jr. The GRIP-75 Man-machine Interface, (Invited speaker), Video Panel Session on Interactive Systems, ACM SIGGRAPH Conf., Dallas, Texas, (6 August 1981).
- Brooks, F.P. Jr., *Views of Unseen Worlds*, keynote lecture for *Science Magazine* conference *Computers in Science*, Chicago, (December 1982).
- TenEyck, L.F. *High-performance raster graphics.* United Kingdom Molecular Graphics Group Workshop, Oxford, England. (22-24 March 1982).

Wright, W.V. (Invited speaker), Interactive Computer Graphics in Molecular Structure Analysis. *International Union of Crystallographers, Ottawa, Canada, (22 August 1981).*