

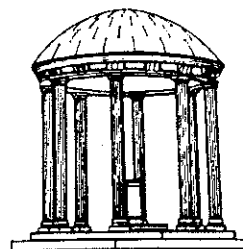
Sixteenth Annual Progress Report-Interactive
Graphics for Molecular Studies

TR90-007

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Progress Report Summary

RR 02170-07

Frederick P. Brooks, Jr
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 Interactive Graphics for Molecular Studies

From May 1, 1989 To April 30, 1990

1. Plans

Our 1988 competing renewal proposal for years 06-10 defined an ambitious program of work on nine subprojects, and set priorities. We were funded for years 06-08. We will discuss plans for year 07 in terms of changes from the renewal proposal.

1.1 Collaborative Research, Service, and Training

No change in plans.

1.2 Dissemination

In addition to the means of dissemination set forth in 1988, we plan to host a one-day workshop, the **Chapel Hill Workshop on Geometry for Molecular Visualization and Characterization**, on March 3, 1990. Some 40 persons are expected, with 14 from across the nation. NSF and the North Carolina Center for Biotechnology are also providing funding. We find such small workshops to be very effective as a medium for idea exchange.

1.3 Technological Research and Development

Priorities

In the proposal we listed our top six subprojects for the initial period. They were indeed the ones on which we concentrated last year, and the ones on which we shall concentrate this year:

Subproject	1990-91 Rank	1989-90 Rank	Proposal Rank
Visualization Impromptu Evaluation Workbench(VIEW)	1	1	1
New graphics engines: evaluation and installation	2	6	5
Protein sculpting	3	4	6
Docking studies, especially with force display (GROPE)	4	2	3
Head-mounted display	5	3	4
Volume visualization	6	5	2

The changes are occasioned by new opportunities and needs. In 1990 we shall have three new high-performance engines in our laboratory, and we shall need to port our software to two of them. Protein sculpting has risen much higher on our list because our collaborators on this subproject, the Richardsons, have raised it higher on their list and committed their time to working with us. Head-mounted display surged way ahead of plan in 1989-90 because of our good fortune in attracting Warren Robinett, who has much experience in the field, to our team. It drops off in 1990-91 not because we think it less important, but because it has become important enough to attract its own funding.

We discuss the subproject plans in the order of their priorities for the coming year.

1.3.1 Visualizations

VIEW – The Visualization Impromptu Evaluation Workbench. Our 1982 videotape, *What Does a Protein Look Like?*, applied some 40 different visualizations to one dataset, that for superoxide dismutase. It convinced us that different visualizations yield different kinds of insight.

Hence one wants a "workbench" on which an investigator can explore data by fashioning new visualizations as fast as the imagination conceives them. If colleagues show me their visualizations, I see at most what they saw in the data. If they share data and computational results with me, and I have a VIEW system, I can hope to see insights never before seen by anyone.

We began sketching such a tool in 1986, assigned three-persons to it in 1987, and increased the team to six in 1988. It now gets more than half of the project's effort. Graduate student Larry Bergman is team leader. Doubling the team demanded, and provided the manpower for, adopting a better software engineering environment, more formal version control, and better documentation procedures.

Our first prototype is running on the Sun 3, Sun4, DEC 3100, and producing pictures on the Adage Ikonas, the PS-300, the Macintosh II, and Pixel-Planes 4. It seems too limited in function and too awkward in use to be a contribution beyond what commercial vendors are providing. So we are engaged in a major rebuild, with special emphasis on a flexible and natural interface. We plan to begin user-testing of our prototype this fall

Ad Hoc Pictures for Users. A steady stream of requests for the construction of particular visualizations of particular molecules came to our Resource; we were able to fill most of them. Each one requires iteration to get an insight-communicating view; the first conception is rarely adequate.

Use of Dynamic Color Mapping in Visualizations. Color perception has many illusions, and these threaten the usefulness of color in scientific visualization for the exact conveying of quantitative variables. Ph.D. student Penny Rheingans is researching the power of dynamic color mappings, under interactive user control, as a general technique for avoiding perceptual distortions and producing extra insights in color-borne visualizations.

1.3.2 Evaluating and Exploiting New Graphics Engines for Molecular Studies

Custom VLSI chips enable many manufacturers to offer specialized computers, and many are aimed especially at high-performance graphics. The market is seeing a veritable explosion of new entries; the pace will not slacken soon.

We therefore believe we can be of service to the molecular graphics community by performing and publishing qualitative and quantitative evaluations of new machines as applied to the molecular field. This work will be part of our collaboration with Scripps Research Institute.

Benchmark Studies. Our first objective for 1990-91 is to bring to publication the careful study, done by Mike Pique of Scripps and Matt Fitzgibbon of this Resource, which undertook to define a representative benchmark of graphics tasks especially appropriate for molecular studies, and to apply it to several of today's engines. The benchmark is ready for publication. The results of the application are being vetted by the vendors of the engines studied.

Pixel-Planes 5. Professors Henry Fuchs, John Poulton, John Eyles, and team are building a new high-performance graphics engine, Pixel-Planes 5. It is expected to be at least ten times faster than the 1986

PixelPlanes 4, which is faster than any general-purpose graphics machine yet delivered. We expect to install this in the Graphics and Image Laboratory in 1990, and to use and evaluate it as we have Pixel-Planes 4. Its graphics speed, and its processing speed, will enable us to attempt whole new kinds of tasks. A high-priority 1990-1991 objective is to port all our present PxPI 4 software to PxPI 5.

Silicon Graphics Power Iris 4D/240GTX Acquisition and Evaluation. After three years of study, we have chosen an off-the-shelf graphics engine on which to field our exportable software. The Silicon Graphics Iris family is very popular in the molecular studies community, and all significant commercial molecular packages run on it. Our 1990-91 objective is to install this system, bring up Sybyl and Mendyl on it, and port VIEW to it.

The system is being acquired in two parts. In year 06, we have purchased the presently-available machine. In year 07 we propose to add the new graphics back end that SGI has just announced. They claim an eight-fold improvement in graphics performance; we can see at least a four-fold improvement. In a year 08 we would expect to run our molecular benchmark on it.

Cray YMP Exploitation. The North Carolina Supercomputing Center has installed a Cray YMP for use by the North Carolina university and industrial research communities. A separate project in our department is pursuing a fiber-optic link from it to our building, which will allow the Cray to be used interactively with PxPI 5. Our Resource's 1990-91 hope is to test this machine on one application, protein sculpting or volume visualization.

MasPar Multiprocessor. Our department has installed a MasPar 2000-processor mesh-connected fine-grained SIMD multiprocessor, a machine very similar to Thinking Machines Corp.'s Connection Machine, available at no cost to the Resource. Duke Ph.D. student Russ Tuck has built a language and compiler system allowing code to be compiled for either PxPI or the Connection machine. We probably won't do anything with this interesting machine in 1990-91, although it appears promising for volume visualization.

1.3.3 Protein Sculpting

The Richardsons are engaged in the design of proteins *de novo*. They need tools with which they can twist alpha helices, dock them, warp beta sheet, etc. We have been exploring mathematics for such graphics tools. The new constraint-based modeling techniques appear to be directly applicable.

The specific objective is to design a graphics tool which shows the biochemist what he is doing as it allows him to do naturally specified and chemically valid gross manipulations of secondary structures. The object is to think and operate in terms of the helices and sheets, rather than upon atom positions, or even backbone ribbon positions. In mathematical terms, our objective is real-time continuous idealization of protein structures as they are deformed by the user. That is, after a set of tugs, pushes, and couples is applied to a structure, we aim to find the new local minimum of its energy in a fraction of a second.

Ph.D. student Mark Surles has chosen this as a dissertation topic. Profs. Brooks and D. Richardson, Prof. R.A. Cohen of the UNC Math department, a specialist in numerical methods for minimization, and Prof. Al Barr of Caltech, a specialist in constrained motion, are serving as guides for his research. We expect to have a prototype system during 1990-91.

1.3.4 Docking

GROPE – Force Display. Even if one had magical technology, it is hard to imagine what one would like to see in order to perceive molecular docking. One really wants to **feel** the hard-surface and the subtler electrostatic forces.

Ph.D. student Ming Ouh-Young built and evaluated such a system, using a master station from an Argonne Remote Manipulator. The forces and torques to be applied to the user's hand are calculated in real time, using the grid method of Pattabiraman and Langridge. The force image is only a supplement to a stereo visual image on a PS-300.

Graduate student Russ Taylor has picked up where Ming left off and is documenting the entire GROPE system. We plan in 1990-91 to offer it for serious use to local drug designers and seek their comments and experiences.

Visual docker. Ming showed that users of his system could effectively, though more slowly, dock inhibitors into dihydrofolate reductase without force feedback, using just his rich visual displays. Undergraduate Andrew Certain will undertake to port the visual docking system to the Silicon Graphics Iris, in hopes of making an effective exportable tool.

1.3.5 Head-Mounted Display

Virtual-Worlds Research. Computer graphics work at UNC concentrates on 3-D model worlds, and on real-time interaction. Appendix C sketches the virtual-worlds systems our teams have built over the years. The problem of the manipulation interface for virtual worlds is especially challenging – how shall one most naturally push, pull, twist, and connect virtual objects? In the molecular graphics Resource, our virtual world is that of molecular structures.

Head-Mounted Display. For some years we have envisioned the ultimate macro-molecule display to be a head-mounted one, with which one could move about inside a room-filling molecule, twisting bonds and testing docking. We generate right- and left-eye images on Pixel-Planes 4. The virtual molecules are superimposed on the real world. Our hypothesis is that the familiar objects in the room will help one become spatially familiar with the molecule.

We have built such a display and begun testing it with molecular structures. When this work was entirely in the Resource, we could invest only one graduate student plus technician time in it. It has attracted favor with our department's ONR contract sponsors, so we were able to triple the size of the team in 1988 – three half-time graduate students. We expect to spin the team off as a separate project with its own funding during 1990-91, so the Resource will be using the HMD, rather than developing it.

Future work of the HMD project will concentrate on the update lag problem until that is solved. The tracking problem is by far the most serious of our technical problems. We have prototyped an optical tracker, as an alternate or supplement to the magnetic tracking used today.

The narrow angle of view is a serious image problem. Post-doc Jannick Roland, Ph.D. from the University of Arizona in optical engineering, will join the head-mounted display project in April, 1990, and undertake to design see-through wide-angle optics for that application.

1.3.6 Volume Studies

Direct Rendering – Westover. Contour lines and ridge lines both fit discontinuous artifacts to the continuous density function. How the density volume looks is a strong function of how these artifacts are fit. Ph.D. student Lee Westover has been exploring the possibility of rendering volume data directly visible, by treating each volume element (voxel) as luminous.

We do not yet know whether Westover's approach will prove fruitful. It has the attraction that one sees the raw density data barely interpreted. In the coming year he should complete his Ph.D. work, including some evaluation of his techniques.

Direct Rendering – Levoy. Marc Levoy has pursued a different approach, in which one or two threshold surfaces in the density are defined and then rendered as shells of specified opacity. Light from one or more external directions is traced through the volume. Levoy has applied his method both to density maps and to CT-scan medical images, completing his Ph.D. work in 1989.

The Levoy studies thus far have used very good quality ($R=0.17-0.19$) maps of 1.8-1.9 Å resolution. Spectacular pictures result. An acid test, for which we are just now preparing, is to see how robust these techniques are on low-resolution or noise-degraded maps.

Direct Map Interpretation. Levoy's work, in particular, suggests that volume visualizations might be better than ridge-lines in a GRINCH-like direct interpretation system. This is on our work queue, but we do not expect to address it in 1990-91.

San Diego Workshop on Volume Visualization. As a result of the unexpected degree of success of the Chapel Hill Workshop, the participants decided that the meeting should be made a recurring event. A team from the San Diego Supercomputer Center and Scripps Clinic will host the second workshop. We have copied all our files to them and met with the committee. During this coming year we shall continue to help as we can.

1.3.7 Surface Studies

Objective for 1989-94: Dynamic Motion of Solvent-Accessible Surfaces. Whereas today's engines let us move CPK models dynamically, we cannot yet do that for solvent-accessible surfaces unless they are approximated by polygons or spheres. We intend to accomplish dynamic motion for such surfaces. In 1990-91 we shall address this objective only as part of our work in exploiting PixelPlanes 5.

Levoy Technique Extended for Solvent-Accessible Surfaces. Levoy's technique involves independent classification and shading procedures. Instead of doing threshold classification in a density function, one can calculate a solvent-accessible surface by Connolly's techniques, and then use Levoy's shading method to render the surface as semi-transparent. No effort is planned on this in 1990-91

Smart Points. Mike Pique has proposed a new graphic primitive for rendering molecular studies – a point having no dimension, but having color, specularity, and a defined surface normal, so that its brightness is a function of illumination direction. Such a primitive seems to us to offer real promise for the visualization of solvent-accessible surfaces. We hope to try it on PxPI 5.

2. Progress

2.1 Collaborative Research

David C. and Jane Richardson – Molecule Sculpting. This project got off the ground in 1989. Prof. David Richardson decided to take his sabbatical year at UNC, and joined us as our project biochemist in September, 1989. Ph.D. student Mark Surles decided to take the protein sculpting problem as his dissertation topic and began to meet weekly with Profs. Richardson and Brooks. He also found committee members with specialized knowledge of his subject.

Scripps Research Institute – Equipment Evaluation. Mike Pique of Scripps and Matt Fitzgibbon of our Resource developed a benchmark for evaluating graphics computers for their suitability for molecular studies and tested it on the Stellar and Ardent computers. Because we feel it only fair to give the vendors a chance to vet the results and agree or disagree, this work has not yet been published.

2.2 Service

Because we were essentially in building mode during 1989-90, we had no new users come to our laboratory. Our users from UNC, Duke, and Burroughs-Wellcome continued.

2.3 Training

Computer Science Students. During 1989-90 we graduated three Ph.D. students who had worked in the Resource. Eleven students who had at some time been part of the Resource team received the M.S. degree. Some are continuing to study for the Ph.D.

We hosted MIT Ph.D. student Margaret Minsky, who spent 1988-89 in our laboratory working on force display research. The costs were partly borne by a grant from Apple. Minsky came here because of our force display work. Brooks is serving on her Ph.D. committee at MIT.

Laboratory for Molecular Modelling and Medicinal Chemistry Course. The UNC School of Pharmacy has established, with major industry support, an educational Laboratory for Molecular Modelling. Professor J. Phillip Bowen is the Director. Dr. Brooks is a Co-Principal Investigator. Dr. Brooks also participated as a lecturer in the graduate course, Medicinal Chemistry 275, Molecular Modelling. About 25 students were enrolled for the offering in Spring 1989.

2.4 Dissemination

Chapel Hill Workshop on Volume Visualization . Our Resource organized and hosted the first workshop on techniques for visualization of data defined on volumes, May 18-19, 1989. The workshop was immensely successful. Some 175 people came; we had expected 125. The program of thirteen papers was selected from worldwide submissions. The Proceedings were prepared and in the hands of the participants. Resource funds for dissemination paid for editing and color separations. Copy printing costs were recouped by sales. We printed more copies than the number needed for the workshop, some 1000, and the Association for Computing Machinery took over their distribution at cost

Participants were invited to submit volume datasets to define a benchmark. Two such datasets were submitted.

These were distributed ahead of time to workshop participants, who were invited to use their volume rendering techniques on those standard sets, and to bring the results on videotape or as live demonstrations. Many did so. All the vendors of high-performance graphics equipment set up demonstrators, so participants could show their work on their native machines.

We have arranged with our department's SoftLab to continue to disseminate the volume datasets at cost, and they have had a slow but continuing demand for them.

In cooperation with the workshop, Pacific Interface/DuPont produced a one-hour long broadcast-quality videotape on volume visualization techniques, including examples and interviews with the key technical contributors to the field. This has been published as Volume 44 of the *SIGGRAPH Video Review*.

2.5 Technological Research and Development

We will discuss R & D progress for year 06 in the order of the priority for that year, as shown on page 6.

2.5.1 Visualizations and the VIEW System

R-Space. Mark Harris of the Resource, working with Prof. C. Carter and Frank Hage of the UNC Biochemistry Department, built R-Space, an interactive system designed to help crystallographers plan data-collection strategies for diffractometers with area detectors. RSpace has been distributed widely.

This year we transferred field distribution and support of the RSpace program to our department's SoftLab, which is permanently staffed for exactly such functions. Our Resource provides the technical support in the form of bug fixes and answers to hard new questions, but SoftLab provides documentation, phone answering, normal question handling, and distribution.

Scientific Visualization. As the only computer scientist on the National Science Board, Brooks has been especially concerned with the operation of the National Supercomputer Centers and their efforts at incorporating visualization in their work. We are concerned that the emphasis on scientific visualization so far has been on the **communication of insights** already grasped by the investigator. The much more promising use of scientific visualization is in the **production of new insights** from data.

This year Brooks did the hour-long scientific presentation for one of the National Science Board's regular monthly meetings on our work on scientific visualization.

VIEW - The Visualization Impromptu Evaluation Workbench. One wants a "workbench" on which an investigator can explore data by fashioning new visualizations as fast as the imagination conceives them. Our first prototype is running on the Sun 3, Sun4, DEC 3100, and producing pictures on the Adage Ikonas, the PS-300, the Macintosh II, and on Pixel-Planes 4.

Our experience with this prototype showed that the interface was too unfriendly and inflexible. More seriously, the function, novel when first planned, now offers little more than commercially available molecular software systems. We therefore undertook a major redirection and redesign, making the system into a collection of building blocks that can readily be assembled for particular visualization tasks, rather than a monolith. Parts of this are now running. A whole new interface has been designed and is being built. We shall see how this next prototype stands up to serious use by chemists.

2.5.2 Molecular Docking and the GROPE System

GROPE – Force Display. The most important accomplishment of our year 06 has been the completion and testing of the GROPE III force-feedback molecular docking system. GROPE III uses the master station of an Argonne Remote Manipulator, (ARM), which Argonne gave us. Kilpatrick [1977] built a force feedback system with it and tested it with users, using as his world model a table and seven toy blocks. He found force feedback to be an effective cue in enabling the viewer to form an accurate mental world model – more effective than stereoscopic vision, in fact. At that time we concluded we would need 100 x our available compute power in order to model molecular docking, so we mothballed the ARM. After a decade, we had the 100 x compute speed, so we reactivated it and attached it to the Masscomp. It has since been moved to a Sun4, which is fast enough.

Ming Ouh-Young completed his Ph.D. work this year, building new electronics for the ARM, building all new software, devising new visual displays, studying the impedance of the human arm, devising critical damping for the arm-ARM system, and measuring the effectiveness of force display for molecular docking with a performance experiment using 12 biochemist subjects and 12 inhibitors for dihydrofolate reductase. He found that human dockers working interactively can find the known docking conformations for the inhibitors in about 25 minutes, whereas pure batch computation would take years. Augmenting the visual display with a force display improves performance by a factor not greater than two.

Minsky's Force Display. Margaret Minsky, a Ph.D. student at MIT, spent 1988-89 at our laboratory working on a 2-D force display as part of her dissertation research. Her pilot studies showed that a two-dimensional force display can effectively simulate textures. Her controlled experiments are now under way.

2.5.3 Head-Mounted Display

Optical tracker. The major accomplishment this year has been Ph.D. student Jih-Fang Wang's design of an optical head-tracker, and his construction and testing of a bench prototype. The design uses a head-mounted CCD camera with a holographic lens to image infra-red LED beacons placed on the ceiling and walls.

Because of the outward-looking geometry, great accuracy can be achieved: total system simulation using the actual parameters measured on the prototype promise translational accuracy of ± 1 cm. rotational accuracy of $\pm 0.8^\circ$. As important, the wearer is not constrained to the 1 m radius sphere of the present magnetic tracker, but can roam about an entire room, if the ceiling has been instrumented with beacons. Most important of all, the prototype, driven by a DEC 3100, will achieve 1000 updates/second, with a lag of one millisecond.

Lag problem. The illusion suffers from a perceptible lag between when the head is moved and when the image is updated. This makes virtual objects swim about in space when they should appear to stay still. Even in this condition, the display appears to be useful. Much effort in 1989 was devoted to careful measurement and accounting for the lag. Most of the lag to the settling time of the Polhemus tracker, some 125-250 milliseconds. The tracking problem is by far our most serious technical problem, hence our effort on the optical tracker.

Display headgear. Since our last report, we have built our third display headgear, a see-through model. We also entered a collaboration with Major Phil Amburn of the Air Force Institute of Technology in Dayton. We gave them our present hardware designs and software, so they could make copies of our HMD system. In return, they gave us another display headgear, fashioned in their machine shop. It is a blind model. VPL Inc. also gave us one of their commercial display headgears, also a blind model. A new board was built to allow PxlPI 4 to generate stereo, and that has been interfaced with the VPL headgear and calibrated for it. The narrow angle of view is a serious image problem. We installed wide-angle optics, although to do so we had to give up see-through capability, which we value.

Sound. The system has been augmented to provide sound cues under program control, to simulate the noises made when virtual objects collide, etc. The system software has been extensively rewritten.

2.5.4 Protein Sculpting.

See Section 2.1 on Collaborative Research for progress on this subproject.

2.3.5.Volumes–Electron Density Maps

Direct Rendering – Westover. Lee Westover has been exploring the possibility of rendering volume data directly visible, by treating each volume element (voxel) as luminous. He continued work on this project as his Ph.D. dissertation this year, while working for a local company. He was not paid by the Resource, but it provided his computer access and data. He is using the Sun4 with a TAAC accelerator board to allow him to manipulate his volumes in real time.

Direct Rendering – Levoy. Marc Levoy has pursued a different approach, in which one or two threshold surfaces in the density are defined and then rendered as shells of specified opacity. This year Levoy completed his Ph.D. dissertation on this work and published some papers from it. Most recently, he has been investigating techniques of texture-mapping grids onto his density shells in order to make their shapes more apparent.

2.5.6 Evaluating and Exploiting New Engines

See Section 2.1 on Collaborative Research for the main progress on this objective.

2.5.7 Small Systems and MOLIX

The important happening in computers in the past five years has been the advent of workstations at \$10K to \$25K. Hence we have been studying how to field our new systems on cheap computers. During 1989-90 we augmented the VIEW system prototype so that it generates pictures for the Macintosh II. We also installed Unix on a Macintosh II and began to port the VIEW system, using a C++ compiler ported by graduate student Jonathan Leech.

2.6 Other

Dr. Brooks received the 1989 Harry Goode Memorial Award, the highest given by the American Federation of Information Processing Societies, "For lasting contributions to computer science education, to 3-D interactive computer graphics, and to hardware and software architecture...."

3. Publications

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- Conn, C., panel chair, "Virtual environments and interactivity, windows to the future." *SIGGRAPH 89 Panel Proceedings*. Boston, MA (August 1989). Jaron Lanier, Margaret Minsky, Scott Fisher, Allison Druin, panelists.
- Levoy, M., "Design for a real-time high-quality volume rendering workstation." *Proceedings of Chapel Hill Workshop on Volume Visualization*. Chapel Hill, NC (May 18-19, 1989): 85-92.
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- Ouh-Young, M., *Force display in molecular docking*. Ph.D. dissertation, University of North Carolina-Chapel Hill, 1990.
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- Wang, J.-F., R. Azuma, V. Chi, H. Fuchs, G. Bishop and J. Eyles, "6D tracking in a large environment." *Proceedings of SPIE 1990 Symposium on Helmet-Mounted Displays II*, City:
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