

1992 Research Highlights

1. NanoManipulator—A Virtual Reality Interface for Interactive Control of a Scanning Tunneling Microscope

The UNC Molecular Graphics Research Resource, in collaboration with Prof. Stanley Williams of the UCLA Department of Chemistry, has developed a real-time graphics and force-feedback interface for scanning tunneling microscopes, atomic force microscopes, etc. The chemist uses a head-mounted display, flying and viewing controls, and head position sensing, so that he can scale himself down to near-atomic scale and see the surface features as if he were walking or flying over it. We use our GROPE force-display arm to allow the user to probe the surface shape, feeling the shape as well as seeing it. The scanned surface is treated as a virtual world for viewing, and for manipulation. The user can change the lighting, especially the lighting angle, on the surface. The effect is to scale the chemist down by about 10^8 , put him on the surface, and let him move about in real-time, viewing, feeling by probing, and firing pulses of energy at spots he selects on the surface.

We have succeeded in making location-controlled surface modifications to gold samples using gold tips. These humps appear to be deposits from the tip to the sample. They anneal away under repeated imaging. A new result concerns pulse length. Taylor finds that pulses of about 20 ns. duration are necessary for surface modification, with shorter pulses having no effect and longer pulses not moving significantly more material. Most previous work seems to have used substantially longer pulses. This work is an important step towards human-controlled fabrication of quantum-scale devices.

2. SCULPT—Interactive Constrained Manipulation with Concurrent Energy Minimization

The SCULPT system is designed to let a chemist deform virtual protein molecules interactively, while the molecules continue to obey the physical constraints on bond length, bond angle, and dihedral angles, and while they maintain a conformational energy minimum. Ph.D. student Mark Surles built the first prototype of SCULPT, completing and demonstrating it this year. He showed that the running time of his continual energy minimizer is linear in the number of atoms in the molecular system being manipulated. For Felix, a protein designed by the Richardsons at Duke, the system updates the position of all atoms in the deforming molecule, taking one step toward the Lennard-Jones energy minimum, about 3 times a second, running on a Silicon Graphics Iris 4D/240 system, using all four 25 Mhz. processors.

The UNC team has ported the SCULPT interface from the Silicon Graphics monitor and mouse to our large-screen videoprojector and the Argonne ARM. Chemists can now operate SCULPT while viewing the molecule in stereo on the 4'x6' screen, and feeling the deformation forces they are applying. This tool radically speeds up the exploration of possible folding patterns for proteins.

3. VIEW—Interactive Exploration of New Visualization Paradigms

The UNC Resource has just completed the building of a new kind of scientific visualization system, a Visualization Impromptu Exploration Workbench (VIEW), a system designed especially to help scientists understand their own data. The VIEW system is built on a new model of visualization, one which encourages extemporaneous sketching that is data-constrained, but which allows almost infinite flexibility in the geometric, color, surface-treatment, etc. representations used for data features. The use model assumes that many visualizations will be attempted for every one that turns out to be insight-producing, so the system provides backtracking and gives the user easy capabilities to script new tools for visualization as well as new visualizations themselves. The elements of the visualization remain closely coupled to the database, an important new feature. The VIEW approach is especially suited for studying structures such as molecules, cells, and man-made structures, but it appears extensible to continuous data as well.

β-test versions started distribution in January, and some dozen copies are in field-test. The source code, User Manual, and internal documentation will be available for general distribution in May.

1992 Research Progress and 1993 Research Plans

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1.0 NanoManipulator—Interactive Scanning Tunneling Microscope

1.1 Concept: Virtual Reality Interface for Real-time Display and Control of STM.

We have developed a real-time graphics and force-feedback interface for scanning tunneling microscopes, atomic force microscopes, etc. Our approach is to provide the user with a head-mounted display, flying and viewing controls, and head position sensing, so that he can scale himself down to near-atomic scale and see the surface features as if he were walking or flying over it. We use our GROPE force-display arm to allow the user to probe the surface shape, feeling the shape as well as seeing it. The scanned surface is treated as a virtual landscape for viewing, and for manipulation. The user can change the lighting, most usefully the lighting angle, on the surface. This interactive viewing system we call the *microscope*.

1.2 Collaboration. We are collaborating with Prof. Stanley Williams of the UCLA Department of Chemistry, a surface scientist. Prof. Williams and his group have developed ultra-stable STMs that operate with a drift on the order of 1 Å per minute, at room temperature, in atmosphere. This stability means that interactive viewing of the scanned surface makes sense. Prof. Williams has built two STMs, so he agreed to install one in our laboratory. Williams' Research Assistant Eric Snyder and our Research Assistant Russ Taylor installed it and got it operational in two modes: imaging mode, where the sample is scanned, and probe mode, where the user moves the STM tip itself to the desired x,y coordinates using the GROPE arm, and the system forces the arm to a z coordinate representing the height of the sample surface.

1.3 Goal: User-guided atomic manipulation. Prof. Williams believes that suitable voltage pulse controls will enable a user to pick up and put down small chunks of atoms. We aim to use our viewing apparatus and our manipulator arm to control this process, so as to create a *nanomanipulator*.

1.4 Progress: Microscope in full operation. We are now routinely operating in two modes. In the first, Prof. Williams has made two extended visits to Chapel Hill to work with the STM using our interface. In the second, our team, consisting of Research Assistant Russ Taylor and Visiting Scholar Warren Robinett, does experiments using samples and often tips prepared at UCLA and expressed to us. The results, both data and viewing videotape, are then expressed back to the UCLA team.

1.5 Progress: Improvements to the STM. We have made various improvements to the STM to improve its operation and to prepare it for use as a nanomanipulator.

Motorized tip positioning. Since installation, Taylor and Mr. Vern Chi of the UNC CS Microelectronics Systems Laboratory have upgraded the STM to provide a computer-controlled stepping motor to bring the tip into tunneling distance. Manual positioning was tedious and often broke tips.

Shielding. The leads to the tip and to the sample have been replaced with coaxial cable to give a controlled-impedance path for all except the tip proper. This is necessary to reduce noise during imaging, and to preserve pulse shape during pulsing.

Electronics for pulsing. We have tested several pulse generators for providing pulses of controllable height, bias, and width for surface modification experiments. Most instruments seem to have considerable noise on the bias. We are still looking.

New control computer for the STM. Originally we interfaced the STM into a workstation for which we had A-D and D-A cards. This year we installed a dedicated PC, located close to the STM, to enable shorter analog runs and more direct control, and to free up the more powerful and costly Sun.

1.6 Progress: Surface deformation experiments. We have succeeded in making surface modifications to gold samples using gold tips. These humps appear to be deposits from the tip to the sample. They anneal away under repeated imaging. We have also tried other materials for both sample and tip, with mixed results.

A new result concerns pulse length. Taylor finds that pulses of about 20 ns. duration are necessary for surface modification, with shorter pulses having no effect and longer pulses not moving significantly more material. Most previous work seems to have used substantially longer pulses.

NanoManipulator paper accepted by SIGGRAPH'93. A technical paper describing the virtual-reality interface to the STM has been accepted for the SIGGRAPH'93 conference, the premier place for publishing computer graphics work. (The Proceedings publish color pictures, and one can show one's videotape.) We have negotiated a publication emphasizing the materials science aspects in *Science* the same week in August, 1993.

Nanomanipulator Grand Challenges Proposal—not even close. Our proposal for funding the STM work as a separate project via the NSF Grand Challenges program lost out in the competition. The referees felt that this research had too little to do with high-performance computing to qualify, in spite of the necessity for a high-performance parallel computer to create real-time images.

1.7 Nanomanipulator Plan:

Experiments toward building a quantum transistor as first effort. Most of our current effort is going into a series of weekly experiments all aimed at developing our surface modification capability to the point that we can fabricate a quantum transistor. Each weekend Williams sends new samples and/or tips. Each Tuesday Taylor and Robinett do the experiment of the week. All scan data is captured, so we can not only view it interactively during the experiment, but can play it back for closer study of promising scans. A videotape of the visualizations and a data record is expressed to Williams, and then the next week's experiment is planned and preparations made.

New electronics for stability, speed. We believe that we can image much faster, up to the limitation imposed by the piezo crystal resonance frequency, by re-doing the motion electronics. We have to achieve a new level of stability, so as to avoid oscillations induced by the faster motion.

Stage drive for larger range. Although the STM movement is sufficient for fabricating quantum-scale devices, it is too limited for fabricating the pads to which leads can be attached. We are investigating inchworm drives for translating the tip over larger working areas.

Drift. We shall attempt to reduce the thermal drift by developing a closed-loop system that measures the temperature of the apparatus and shines an infrared light on it to hold it at constant temperature.

If drift continues to be a big problem, we shall attempt to compensate for it by correlating the surface features of successive scans, determining the inter-scan drift, and extrapolating it to the next frame. This may prove to be difficult, either because the drift velocity is itself insufficiently stable in magnitude or direction, or because the surfaces are too self-similar for unambiguous correlation. In any case, performing such a correlation in real time will require the use of a very fast computer. We plan to use the 8000-processor MasPar MP-1 installed in our department.

Get supplementary funding for this project. As we discuss later, the GRIP Molecular Graphics Research Resource acts as an incubator for new projects. Many of these mature to the point that they both warrant larger-scale effort that the Resource can provide, and can attract independent funding. We believe the STM is at the point that we should be able to get it funded in its own right this year.

2.0 SCULPT—Interactive Molecular Model Manipulation with Concurrent Energy Minimization

2.1 Concept: The SCULPT system is designed to let a chemist deform virtual protein molecules interactively, while the molecules continue to obey the physical constraints on bond lengths, bond angles, and dihedral angles, and while they maintain a conformation with minimum Lennard-Jones energy. The requirements for such a system was specified to us by professors David and Jane Richardson of the Duke University Department of Biochemistry, who collaborated in its testing and refining.

The chemist specifies deformations by attaching springs to particular atoms or groups of atoms and then specifying the amount and direction of spring pull. Multiple springs can be attached to a molecule, and springs can have their free ends tacked to points in 3-space. Each update time, the system performs a step toward the Lennard-Jones energy minimum of the molecule-spring system and displays the new atom and bond positions (essentially a Kendrew model).

2.2 Progress: SCULPT works at 3 updates/second and in time linear in atom number. Research Assistant Mark Surles built the first prototype of SCULPT, completing and demonstrating it this year. He showed that the running time of his continual energy minimizer is linear in the number of atoms

in the molecular system being manipulated, and proportional to the band width of the band-diagonal matrix of interatomic interactions. For Felix, a protein designed by the Richardsons at Duke, the system updates the position of the deforming molecule, including doing an energy minimization step, about 3 times a second, running on a Silicon Graphics Iris 4D/240 system, using all four 25 Mhz. processors.

Surles gets Ph.D., goes to San Diego Supercomputer Center. Surles defended his Ph.D. dissertation this year. He has gone as a post-doctoral fellow to the San Diego Supercomputer Center, where he is continuing work on SCULPT, particularly highly-parallel implementations.

SIGGRAPH'92 SCULPT paper, video. Surles's paper describing SCULPT, and his video showing it in action, were accepted for SIGGRAPH'92, the premier publication medium for computer graphics research.

SCULPT now operating with ARM, providing force cues to users. Since Surles's departure, Research Assistant Yunshan Zhu of the GRIP team has ported the SCULPT interface from the Silicon Graphics monitor and mouse to our large-screen videoprojector and the Argonne ARM. Users can now operate SCULPT viewing the molecule in stereo on the 4'x6' screen, and feeling the spring forces they are applying.

SCULPT Grand Challenges Proposal—close, but no cigar. Our joint proposal with the Richardsons and other colleagues at Duke University received strong reviews in the NSF High-Performance Computing Grand Challenges competition, but did not get funded. (Eight proposals of 114 did.) The referees offered various useful suggestions for our joint work.

2.3 SCULPT Plan

New, faster Silicon Graphics Onyx display computer arrives in April. Both to achieve true real-time performance and to handle electrostatic forces at the present near-real-time rate, SCULPT needs more compute power. We have ordered a next-generation commercial graphics display system to serve as a base for our own next-generation molecular graphics Trailblazer configuration. Its arrival is expected in April, 1993. Although we have an older system, and we have access to the the UNC Pixel-Planes5 which is about three times faster than current commercial systems, we need a current-generation commercial machine so that the work we do will be readily exported to chemists' laboratories.

In 1992, Silicon Graphics, the largest-volume supplier of molecular graphics workstations, announced its Crimson line of new systems, with processors up to 100 MIPS, and a new, incompatible backplane capable of handling processor-memory communication for such fast machines. The Crimson are, however, all single-processor machines. We feel that a trailblazing molecular graphics installation must incorporate multiple processors, each very fast, so we waited. In January, 1993, SGI announced its Onyx family, which provides the backplane and configuration capacity for multiple processors of the new speeds.

We ordered a minimum system, consisting of a single two-processor card, a graphics engine, and the power supplies, rack, and backplanes to support a much larger configuration. Essentially we spent this year's money on the computer infrastructure. We need to grow a highly capable system over the next few years by adding processors, memory, and graphics accessories.

Incorporate electrostatic forces into the SCULPT model. The prototype SCULPT system does not include electrostatic forces, but only strong forces. The electrostatic forces are difficult because they are long-range, and widen the band width of the minimization matrix substantially. As soon as we can get another research assistant interested in the SCULPT problem, we shall explore two or three possible algorithmic attacks on this problem. The Greengard algorithm proves existence of sub- n^2 algorithms, although that algorithm itself only becomes advantageous for values of n much larger than we encounter.

Possibly port to KSR at NC Supercomputer Center, with interface here. It appears likely that the North Carolina Supercomputer Center will keep the KSR highly parallel computer that is currently installed on a trial basis. If so, we may well port SCULPT to it using Surles' current work on parallelization. UNC's participation in the VISTANET gigabit network testbed should make it possible for us to operate the interface and display from our laboratory in Chapel Hill while the minimization is done at Research Triangle Park.

Unified Minimizer concept. David Richardson has observed that the SCULPT system, almost as it stands, can be used for other user-driven constrained minimization problems of interest in protein science. Besides protein folding, its first use, the energy minimization can be used for interactive docking of flexible molecules.

By changing the cost function from energy to crystallographic R-factor, the same system can provide a powerful tool for fitting molecular models into electron density maps. Local minimization would be algorithmic, global manipulation from one configuration to another would be user-driven in this style of operation. The fitter could see dynamically which global manipulations are improving the quality of the fit, and which are not.

Still other cost functions would allow exploration of tentative rephasings of crystallographic data, and even substitutions in sequence when attempting to design ligand sites.

3.0 VIEW—Visualization Impromptu Exploration Workbench

3.1 Concept. Most scientific visualization systems are designed for the production of publication graphics, high-quality images that show a scientist's work to his colleagues, students, funders, and the public. We believe an interactive visualization system designed to help the scientist explore his data for his own understanding can potentially make a major contribution. The VIEW system is built on a new model of visualization, one which encourages extemporaneous sketching that is data-constrained, but which allows almost infinite flexibility in the geometric, color, surface-treatment, etc. representations used for

data features. The elements of the visualization remain closely coupled to the database, an important new system feature. The use model assumes that many visualizations will be attempted for every one that turns out to be insight-producing, so the system provides backtracking and gives users easy capabilities to script new tools for visualization as well as new visualizations themselves. The VIEW approach is especially suited for studying structures such as molecules, cells, and man-made structures, but it appears extensible to continuous data as well.

3.2 VIEW Progress

System, User Manual, and internal documentation complete. Ph.D. student Larry Bergman has built a VIEW system. The program itself is application independent. He has furnished a language processor for scripting visualization tools, and a standard library of geometric tools and tools particularized to molecular structures. The system is in C++ and runs on Silicon Graphics workstations.

Distribution of β -test version begun in January. Source code and documentation are available from the UNC Resource by anonymous FTP. Some dozen copies have been fielded, and the reported bugs handled. Experience and evaluation from several users is described in Bergman's dissertation.

Bergman's dissertation draft is complete. He will defend it on April 12, and the final version should be ready for distribution by May. He expects to graduate this Commencement.

VIEW paper accepted for SIGGRAPH'93. A paper describing the VIEW system and its new concepts was one of the 42 papers accepted for the very competitive SIGGRAPH'93 conference.

3.2 VIEW Plan

Advertising, distribution, and support. We are almost ready to announce the general availability of the system. We will need to train a research assistant in the support of VIEW users when Bergman has departed.

Next version—not near-term, and integrated into Trailblazer when it comes. We believe that a VIEW capability should be incorporated in our forthcoming Trailblazer integrated molecular structure software system. We expect to use the concepts and the scripting language, and maybe some of the C++ code. Meanwhile we will not be working on further extensions or versions of VIEW proper, but will wait until it can be integrated with fitting, folding, and docking capabilities into a unified system.

Design space map and trek record. Visualizations are objects that have to be designed. Designing visualizations involves a lot of both independent and correlated design decisions. The obvious need in an exploratory workbench is the provision of some kind of computer-maintained map of the visualization design space, at least that part that has been explored so far, so that the visualizer can systematically explore the space. The GIBBS system built at the Microelectronic and Computing Corporation laboratories in Austin provides such a function in generalized form. A possible research subproject, should a research assistant get excited about it, is to study and try that system and build such a subsystem for our Trailblazer facility, testing it first with VIEW users.

4.0 GROVE—Interactive Volume Visualization of Electron Density Maps

4.1 Concept. Computer power now makes it possible to use volume visualization techniques in real time, so that one can show an electron density map with dynamic clipping of electron density levels. This is the modern analog of the real-time contouring that was possible with the MMS systems built a decade ago by Washington University (St. Louis). It appears almost feasible to provide near-real-time (interactive) evaluation of the Fourier transformations by which electron density maps are calculated from structure factors, and vice versa.

4.2 Progress—Real-time contour surfaces. Research Assistant Xialin Yuan has built an electron map visualization system that uses the marching-cubes algorithm to construct a contour surface in an electron density map. The surface is lighted and rendered in real-time on UNC's Pixel-Planes5 graphics supercomputer. The chemist can vary the electron density contouring level dynamically, using a slider, and can view the surface from various viewpoints using a pair of joysticks or our Argonne Remote Manipulator.

If the model of the underlying molecule is known or postulated, it can be displayed embedded in the density map, using semi-transparent surfaces to show the embedding. At present the system does not provide for interactive modification of the model.

4.3 GROVE Plan

GRIP-like fitting capabilities for Trailblazer. Our Resource's first product, GRIP-75, provided very powerful capabilities for fitting a molecular model into an electron density map. The first proteins ever solved on a graphics system without the aid of a physical model were solved on the GRIP-75 system. It served the national community for over a decade before it became obsolete. We should like to combine Yuan's volume visualization and dynamic map contouring capabilities and GRIP-like model manipulation capabilities to provide a modern fitting system. We propose to integrate these capabilities in our forthcoming trailblazer system.

Real-time reciprocal space exploration tool. Research Assistant Stephen Hench is building an implementation of the Fourier transform using our Pixel-Planes5 hardware. If this implementation runs fast enough, we plan to use it to provide for interactive manipulation of either an electron density map or a set of structure factor amplitudes and phases, with quick display of the results in the reciprocal space. A specific application would be the near-real-time update of a $2F_0-F_C$ map while the user manipulates the molecular model he is fitting to it.

Unified Minimizer. Once we have a fitting system, we are eager to try the SCULPT minimizer as a part of it, minimizing R factor locally, while the user makes the large conformational changes.

5.0 Richards' Smooth Molecular Surface

5.1 Concept. Algorithms for both numeric and analytic calculation of the Richards' surface of a molecule are well known. These algorithms require time n^2 . Now that parallel processors are common, one wants a parallel algorithm, preferably one with low overhead.

5.2 Progress. Research Assistant Amitabh Varshney has developed an algorithm which is of linear time in n , the number of atoms in the molecule, with the constant coefficient depending upon k , the number of atoms that a probe sphere can touch while in contact with any selected atom, given the known bounds on atom radii for the elements. Moreover, the algorithm can be distributed over up to n processors, with modest overhead.

Running test cases on Pixel-Planes5 with up to 26 processors, Varshney has achieved times on the order of 0.3 seconds for small proteins. This allows the chemist to interactively change the probe radius used to define the surface and see the result almost instantaneously. Joysticks give dynamic control of viewpoint and lighting.

5.3 Plan. Work will continue on both the speed of the algorithm and testing the resulting surface against other calculations of the same thing. We see Varshney's tool as another of the tools to be incorporated within the Trailblazer system.

6.0 GROPE—Interaction Using Force Display and Visual Display

6.1 Argonne ARM Progress

New control computer and electronics. The Argonne Remote Manipulator originally had 1960s vacuum-tube electronics. When we acquired it in 1972, we replaced them with discrete transistor electronics, which were in turn later replaced during the 1980s. This year we just completed another change of control for this trusty workhorse mechanism. (No substantial mechanical problems over 20 years of use.) It is now interfaced to a dedicated PC, placed very close to the analog electronics so as to reduce noise and line losses. This in turn ties to the ethernet. The synchros that originally measured joint angles have been replaced with potentiometers to reduce the measurement noise and to make it possible to read the ARM position at any time, instead of just twice per power cycle.

ARM velocity. In the past, all our applications of the ARM have used only information about its current position. We have now begun work to determine and to make use of the ARM velocity as well. We hope to use this additional information to dampen spurious oscillations of the ARM, to compensate for its inertia, and to try to compensate for the inherent computational lag in our applications by predicting the position of the ARM a short time ahead. We believe this will enable us to make better simulations of hard surfaces which has proved difficult. We have added circuits for differentiating our position measurements to obtain velocity information.

Kalman filter predictor work. We have this year experimented with Kalman filters which reduce the noise in our measurements of the ARM position and yield values for velocity as well.

Tachometers. The ARM was originally equipped with tachometers, which we have not used in any of our control schemes to date. We have reactivated these and are using the data obtained to validate our work with Kalman filters and electronic differentiators.

6.2 Argonne ARM Plan: Peg-in-Hole Studies. We expect to continue using the ARM as a force-display device even after the SARCOS arm is operational. Our research plan is to attempt to simulate very well defined physical situations, where we can build the real thing and then accurately judge how closely our simulation feels like it. Putting a slender cone into a torus, with varying coefficients of friction, is a good example.

6.3 SARCOS Arm Progress. We have on order, since last spring, a 1990s technology successor to our ARM, a hydraulic teleoperator master station developed by SARCOS Corporation of Salt Lake City. Its precision, reproducibility, strength, sensitivity, and frequency response specifications are impressive. It was promised for August 1992 delivery. We were able to go there and perform an acceptance test in February, 1993, which it passed. The mechanism has arrived in Chapel Hill; we are still awaiting the last bits of software and documentation, which we expect by the end of March.

Meanwhile the university is, at its own slow pace, installing the hydraulic pump and the ultra-clean, high-pressure plumbing that brings the hydraulic fluid from the basement up to our graphics laboratory. We do not yet have a promised date for this installation.

6.4 SARCOS Arm Plan: When the plumbing is installed, we shall install the new arm, co-locating it with a visual display monitor driven by the new SGI Onyx computer, and arranged in the Trailblazer configuration, so that the viewspace and the manipulation space of the arm coincide.

Then we shall test the arm with its own software and diagnostics. Then we shall port the molecular applications which we now run on the ARM, namely SCULPT and Docker. We anticipate that most of the 1993 year will be required to make the new arm really useful.

6.5 Docker. The molecule docking application built by Ming Ouh-young continues to be useful for an occasional chemist. We have not worked on further development of this system this year, and intend none for the coming year. Our basic plan is to incorporate this function, with the new arm and the new display computer, into our Trailblazer system as part of its incremental build, in due course.

7.0 Trailblazer—Next-generation Molecular Graphics System

7.1 Trailblazer Concept: A single unified molecular graphics workbench, for viewing, fitting, docking, folding. Over the years we have built a variety of molecular graphics tools, including the widely used GRIP-75, GRINCH, and R-Space systems, in addition to those mentioned above. Each of these has been built as an independent system, with its own data structures and its own subroutine libraries. We have also developed a variety of graphics techniques and technologies, including force display, and we have experimented with all the technologies offered for stereo viewing.

Our vision now is to build a single unified graphics workbench, implemented on a commercially available family of graphics computers, that will incorporate all of our technology advances and tool capabilities. We do not see this as a software product, for we are not sufficiently funded to build, field, and support robust, documented, major software products. We instead see it as a prototype system, to be field-tested, and aimed to show the way for the next generation of commercial molecular software. We call this system *Trailblazer*. We will build it modularly and incrementally, testing with real users at each stage.

Besides its usefulness to others, we see Trailblazer as a unified support base that will radically reduce the effort at building new prototype visualization tools, for each tool will have data structures and many classes of graphics, interaction, molecular computation, and geometric functions already built, tested, and available. This should make it possible for efforts such as those reported here by Surles, Bergman, Varshney, etc., to achieve more powerful demonstrations of each student's new system concepts.

We plan to develop this software system so that it will support a rich display environment, as well as simpler ones. Our initial Trailblazer hardware configuration will use the SGI Onyx computer, stereo glasses, tracking and force feedback to the right hand using the SARCOS arm, and tracking of the left hand using a magnetic tracker. We will use a front-surface mirror and an overhead-mounted monitor to superimpose the visual 3-D display space on the manipulation space of the hands.

7.2 Trailblazer Progress. We have been fortunate this year to have as our visiting staff scientist Professor Ron Poet of the University of Glasgow, a computer scientist who has been collaborating on molecular graphics with Prof. James White of Glasgow for some years. Prof. Poet is especially interested in data structures for molecular graphics, and he has led our effort to define and build the data structures for Trailblazer. We are building this system in C++, an object-oriented language designed to make modular maintenance and upgrading easy, and designed to maximize code sharing and reuse. Many of the basic classes have been defined and coded. As one goes, of course, one redefines and rebuilds iteratively, and the process is well under way.

In order to make as much progress as possible during Dr. Poet's stay with us, we have assigned experienced Research Assistant James Begley, and new research assistants Juraj Horacek and Yue Li to work on the Trailblazer project. Dr. Wright has been working closely with this group.

7.2 Trailblazer Plan. We shall continue to devote a substantial effort on this new software base during the coming year.

Papers

Bergman, L. "VIEW—A System for Prototyping Molecular Visualizations." Ph.D. dissertation submitted to the University of North Carolina at Chapel Hill (1993).

Bergman, L. "VIEW—An Exploratory Molecular Visualization System with User-definable Interaction Sequences." Accepted for publication in *Computer Graphics: Proceedings of SIGGRAPH'93*, 27:2.

Richardson, D.C., and J. S. Richardson. "The Kinemage: A Tool for Scientific Communication." *Protein Science*, (1992) 1:3-9.

Surles, M.C. "Techniques for Interactive Manipulation of Graphical Protein Models." Ph.D. dissertation. UNC Computer Science Technical Report TR 92-016 (1992).

Surles, M.C. "An Algorithm with Linear Complexity for Interactive, Physically-based Modeling of Large Proteins." *Computer Graphics: Proceedings of SIGGRAPH'92*, 26:2.

Taylor, R.M., W. Robinett, V. L. Chi, F. P. Brooks, Jr., W. V. Wright, R. S. Williams, E. J. Snyder. "The Nanomanipulator: A Virtual-Reality Interface for a Scanning Tunneling Microscope." Accepted for publication in *Computer Graphics Proceedings of SIGGRAPH'93*, 27:2.

Varshney, A., and F. P. Brooks, Jr. "Fast Analytical Computation of Richards's Smooth Molecular Surface." UNC Computer Science Technical Report TR 93-002, also submitted for presentation at IEEE Visualization '93 Conference.