Twentieth Annual Progress Report
Interactive Graphics for Molecular Studies

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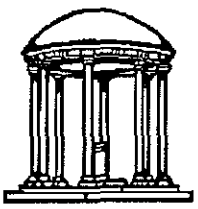

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1993 Research Progress and 1994 Research Plans

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Interactive Graphics for Molecular Studies

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1. Richards' Smooth Molecular Surface—Important New Theoretical and Practical Results

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

1.2 Progress: New linear, parallelizable algorithm. Research assistant Amitabh Varshney has developed an algorithm which is of linear time in n, with the constant coefficient depending upon a function of k, the number of atoms that can conceivably touch another atom, given the known bounds on atom radii for the elements. Moreover, the algorithm can be distributed over up to m processors, with modest overhead and performance nearly m times as fast.

Running test cases on Pixel-Planes5 with up to 18 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. Varshney reported the algorithm and his results at Visualization '93, where it was received with some excitement.

New polygonal simplification algorithm. Once one has calculated a Richards' surface, one needs to tessellate it for display. With a real-time surface-finding algorithm, one wants a tessellation method that allows the surface to be triangulated with a controllable coarseness, so as to speed display. The problem of finding optimal approximants to polygon-tessellated surfaces is known to be NP-complete, essentially impossible for the numbers of polygons we have to treat for molecular surfaces.

Varshney identified this as a problem in set partitioning, found some important results in the operations research literature, and adapted them to develop a new fast algorithm that

1. Uses a subset of the original vertices. (This ensures that there is available for rendering a good set of surface normals.)
2. Preserves the topology of the original surface.
3. Produces an approximating surface guaranteed to be within a pre-specified tolerance of the original surface.
4. Produces a set of triangles that is small and whose difference from the minimum number can be quantitatively estimated.

This result is important for not only molecular graphics, but for a very general set of graphics problems. One often wants to produce multiple representations of objects, containing different levels of detail, so that objects far from the viewer at any point in time can be economically rendered. This problem has received considerable attention in the recent literature. Varshney's polygonal simplification algorithm is an important addition to the known approaches.

Boundary surface between two smooth molecular surfaces. Varshney also has applied his methods to finding and tessellating the boundary surface between two abutted molecules. As two molecules are brought up against each other, motion is stopped after, in the general case, three contacts are made, because the atoms cannot interpenetrate. Varshney's boundary surface algorithm then finds a surface such that the two molecules are partitioned. Obviously the surface goes through the contact points; very little else can be said in general, since there may be protrusions and indentations in each molecule. This provides an excellent means of visualizing and understanding the structure of molecular contacts.

Gap volume between two smooth molecular surfaces. An important question in molecular docking is how one defines goodness of fit. Varshney has begun work on a facility in his system to allow the user to specify a closed curve on the boundary surface between two smooth molecular surfaces. He can then calculate the total volume defined by the enclosed boundary surface and the two molecular surfaces. It appears that this may prove to be a useful goodness-of-fit metric.

1.3 Plan. We will complete documentation and testing this spring and begin distribution by summer. We see Varshney's tool as another of the tools to be incorporated within the Trailblazer system.

2. NanoManipulator – Interactive Scanning Probe Microscopes

2.1 Concept: Virtual reality interface for real-time display and control of scanning probe microscopes.

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-displaying Argonne Remote Manipulator 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 *microscape.*

2.2 Collaborations. We are collaborating with Prof. Stanley Williams of the UCLA Department of Chemistry, a surface scientist; with Prof. Sean Washburn of the UNC Department of Physics, also a surface scientist whose specialty is characterization, and with Prof. Richard Superfine of the UNC department of Physics, who's specialty is atomic force microscopy.

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 installed of his STMs one in our laboratory. It operates 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 while the system controls the z coordinate of the manipulator arm, giving the user the impression that he is feeling the surface.

2.3 Goal: User-guided atomic manipulation. Suitable voltage pulse controls enable a user to pick up and put down small chunks of atoms. We are using our viewing apparatus and our manipulator arm to control this process, so as to operate a *nanomanipulator*.

2.4 Progress: Nanomanipulator experiments toward building a quantum transistor. 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 Prof. Washburn, and Research Assistants Russ Taylor and Mark Finch, does experiments using samples prepared at UCLA and expressed to us, with tips made by Washburn. The results, both data and viewing videotape, are then expressed back to the UCLA team.

We first made 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. The most exciting work involves pitting PtSi which is on an Si base, using W tips. We have in some experiments been able to make decently small and properly located pits in the PtSi, pits that completely remove the conductor down to the Si.

Nanonanipulator results published in *Surface Science Letters*. A technical paper describing a newly discovered phenomenon in which it appears that gold tips spot-weld to gold samples and then are drawn out to the breaking point was published.

2.5 New Thrust—Atomic Force Microscopy

New collaboration. During this year we began a collaboration with Prof. Richard Superfine. Our joint plan is to hook our virtual probe microscope interface up to his atomic force microscope, both to test its utility in another application and to enable the use of our interface with biological molecules. Since an AFM does not depend upon electrical conductivity for its imaging, it can handle macromolecules, even though not necessarily at the same resolution an STM can achieve.

We have acquired the necessary interface computer for his AFM, and tested our software in it. We have installed a fiber optics cable between our building's communication systems and Superfine's laboratory. We expect to attach all the connectors, and, if all goes well, begin AFM operation before the end of the 93-94 grant year.

2.6 Nanomanipulator Plan:

Improvements to the STM. We are in the process of making various improvements to the STM to improve its operation and to prepare it for use as a nanomanipulator.

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. We are rebuilding the feedback circuit.

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.

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 have acquired inchworm drives for translating the tip over larger working areas and are working on the control electronics that interface these drives to the control PC.

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.

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.

Our 1993 proposal for funding the STM work as a separate project from NSF and or ONR did not succeed, due in part to its ambitious nature and magnitude. Reviews ranged from Excellent to Poor. We were asking for a vacuum system to enclose our STM, which made the total proposal over $ 400 K. We shall try again with a more modest proposal that will support one person and pay for the materials.

3. 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

Bergman completes system, User Manual, internal documentation, and Ph.D. 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 begun. Source code and documentation are available from the UNC Resource by anonymous FTP. Some dozen copies have been fielded that we know about, and the reported bugs handled. Experience and evaluation from several users are described in Bergman's dissertation.

Bergman joins IBM Research at Yorktown Heights, N.Y. He will be researching other user interfaces for scientific visualization.

VIEW described at SIGGRAPH '93. Dr. Bergman's paper describing the VIEW system and its new concepts was one of the 42 papers delivered at the very competitive SIGGRAPH '93 conference.

3.2 VIEW Plan

Support, use, and technology transfer. We have trained a research assistant in the support of VIEW users. Two scientists visiting here in January '94 made extensive use of VIEW. Tripos is evaluating VIEW to see if they want to support it as a product.

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. Room-Filling Molecule Viewed with Virtual Reality Technology

4.1 Concept. This year saw the realization of a long-running Resource vision first articulated by David Richardson. The vision is to be able to study complex molecules with the molecule made to fill the space between floor and ceiling of a room, so that details could be visible even as the whole molecular context could be observed. One could walk around and through it, and rotate it by hand as if it were a real (but colored) brass Kendrew model.

4.2 Progress—running system built, and good enough to yield new insights. In 1991, the Virtual Reality project in the department invented and rendered operable a room-sized head-tracker, so that the user could walk around in a 10'x12' room, exploring objects embedded in that space. In 1992, the GRIP team first attempted to realize our room-filling molecule, using this tracker and the best available head-mounted display. The result was stunningly disappointing: the low resolution of the display made all of the detail a blur when one stood far enough away to see the whole molecule.

In 1993, the UNC VR team developed and brought on-line a new higher-resolution HMD using new small CRTs from Tektronix. Whereas then-available commercial HMDs had resolution of 160x240 colored pixels, the new UNC HMD has 480x640 colored pixels, approximately the resolution of NTSC television.

GRIP Research Assistant Yunshan Zhu, working with Research Assistant Ron Azuma of the VR project, brought up superoxide dismutase as a room-filling molecule. At last, one could see the detail! At last, the colors were bright! Even so, when I studied the molecule, it still looked incomprehensible to me, and very hard to wayfind in. We were first able to show this in January, 1994, at the meeting of our Advisory Committee. The chemists were enthusiastic! And they could find their way around in the SOD model.

In February, Advisory Committee member Dr. Vivian Cody of the Medical Foundation of Buffalo visited our lab for a working weekend. She brought with her Dr. Wojtczak of Nicolaus Copernicus University in Torun, Poland, who was visiting her laboratory. Each of them made extensive and enthusiastic use of VIEW, of the real-time Richards's surface system, and of the room-filling molecule. Dr. Wojtczak was able to see that he had fitted a beta strand wrong when he solved the molecule. Each user stayed in the HMD for hours at a stretch, something we had never seen before.

Further tests with the Richardsons and with visiting chemist Dr. Celia Bonaventura of the Duke Marine Laboratory showed us that we needed a new physical configuration and a new display mode. The modes for flying and manipulating multiple objects are awkward for molecule viewing, so a new mode is under design. The chemists do not want to walk around proteins, they want to sit in a chair and to be able to rotate the molecule and bring it nearer or farther easily. We have recently been operating in this fashion.

4.3 Plans for Room-Filling Molecule. Research Assistant Li Yue has chosen this as her application to prototype as part of the Trailblazer subproject. Our first work will be on new interaction modes suited for the molecular application. We also plan to put in aids to wayfinding, such as backbone high-lighting, and the ability for the user to identify residues at will, and to capture views to disk for later study or printing. Indeed, the idea list is rather long.

5. GROVE—Interactive Volume Visualization of Electron Density Maps

5.1 Concept. Computer power now makes it possible 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.

Vision — Real-time reciprocal space exploration tool. Our vision is of a system with two screens on which one sees a graphical representation of the amplitudes and phases of structure factors on one screen and the corresponding electron-density map on the other. Manipulation on either screen would cause the other to be updated in real time. In particular, one could see whether a particular change in the postulated phases of a molecule made the map look more or less like a protein's.

5.2 No progress — Research assistant Stephen Hench dies of brain tumor. Hench, who had been battling brain tumors over the past two years, became mostly incapacitated this summer and died in October. Research assistant James Van Verth, who enrolled in Fall, '93, has picked up the project, and is exploring work on the Silicon Graphics Onyx, as opposed to the Pixel-Planes 5 machine Hench was working on.

5.3 GROVE Plan

GRIP-like crystallographic fitting capabilities for Trailblazer. Our Resource's first product, GRIP-74, 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-74 system. It served the national community for over a decade before it became obsolete. We should like to combine Hench's and Xialin Yuan's volume visualization and dynamic map contouring capabilities, Van Verth's real-time phasing adjustment capability, and GRIP-like model manipulation capabilities to provide a modern fitting system. We propose to integrate these capabilities in our forthcoming trailblazer system.

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.

6. SCULPT – Interactive Molecular Model Manipulation with Concurrent Energy Minimization

6.1 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 length, bond angle, and dihedral angles, and while they maintain a conformational energy minimum. The requirements for such a system was specified to us by professors. David and Jane Richardson of the Duke University Department of Biochemistry, who continue to collaborate in its testing and refining.

The chemist specifies deformations by attaching springs to particular atoms or rigid 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 static energy minimization of the molecule-spring system and displays the new atom and bond positions (essentially a Kendrew model).

6.2 Progress: Surles at San Diego Supercomputer Center continues work on SCULPT. Research assistant Mark Surles built the first prototype of SCULPT here, completing and demonstrating it last 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 a complete static energy minimization, about 3 times a second, running on a Silicon Graphics Iris 4D240 system, using all four 25 Mhz.processors.

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. He has added electrostatics, the most important missing component, and has simplified the input of data. Prof. Jane Richardson is continuing to meet with him and to use the system.

SCULPT now operating here with ARM, providing force cues to users. Since Surles's departure, the GRIP team 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.

Little work on SCULPT here this year. New SGI Onyx installed. 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 installed a next-generation commercial graphics display system to serve as a base for our own next-generation molecular graphics Trailblazer configuration.

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 that 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. During '93-'94, we have spent most of our energies getting this system usable and reliable, which required going through versions of the buggy operating system. We are now doing experiments to determine whether to use this year's equipment money to add processors, raster managers, or memory.

6.3 SCULPT Plan

Plan is student-driven. For the coming year we are attempting to interest one of our pre-dissertation students in SCULPT. If one gets excited, we shall proceed; if not, we rejoice that Surles is still improving it.

Unified Minimizer concept. One possible direction of research is to study the more general applicability of SCULPT. 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 molecular docking.

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 conformation 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.

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 currently installed on a trial basis. If so, we may well port SCULPT to it using Surles's 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.

7. 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-74, 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 in object-oriented technology 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.

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.

7.2 Trailblazer Plan. We shall continue to devote a substantial effort on this new software base during the coming year. Dr. Wright is leading this, our biggest subproject. Each member of the Trailblazer team has some important software classes to define and build. Each also has an individual prototype application to build, both to test the classes and to help us see if the class structure will support the applications we envision.

8. Inverse Kinematics

8.1 Concept. UNC professor Dinesh Manocha, while a doctoral student at Berkeley, produced some important results in inverse kinematics. He showed that a linkage with six degrees of freedom has up to 16 solutions, occurring in pairs. We believe this result can be used in chain-tracing and in detailed molecular

fitting. It appears especially promising for finding the possible locations of the turns linking secondary structures such as alpha helices and beta sheets.

8.2 Progress—Interactive System Built and Running. GRIP Research Assistant Yunshan Zhu, working with Prof. Manocha, has built a real-time interactive graphics system that displays, for user specified positions of the end links positions and directions, all the possible solutions of a chain between them. The chain is made up of links of typical bond length. All of the six degrees of freedom are phi and psi dihedral angles.

User interface. The user controls the chain end-points and end directions with the ARM, viewing the configurations on the big screen with stereo glasses. A button allows him to cycle among the valid solutions for any position. As he moves the end constraints, the system always shows one solution for the chain position, if one exists.

Twelve-degree-of-freedom chains achieved. Zhu and Prof. David Richardson came up with the idea of the user controlling the center point of two subchains, each of six movable dihedral angles. The system then shows the user the (independent) sets of solutions of each of the possible subchain positions.

8.3 Plans for Inverse Kinematics. These results were just achieved in January, so exploration has just begun. Zhu (and Wright and Manocha) are exploring the significance of imaginary solutions, for as one moves the end constraints about, the real solutions become imaginary and vice versa in a continuous way. Zhu is also interested in understanding how the system may be used to show solutions to over-constrained configurations when the solutions just happen to exist, and how it may be used to define solution spaces for under-constrained systems.

9. GROPE – Interaction Using Force Display and Visual Display

9.1 Argonne ARM Progress

Kalman filter predictor work. The accurate simulation of hard-surface contact forces is a difficult problem. Essentially one wants to change the damping coefficient dynamically as one makes contact, so there is no overshoot, and hence no bounce. In any sampled-data control system, the system measurement lag adds to instability and oscillatory behavior. After one has improved physical and computational lag as much as possible, some end-to-end lag remains. Prediction (extrapolation) algorithms can eliminate the effects of this lag much of the time. This year we have followed the work of Research Assistant Ron Azuma on the head-tracking project, who has been developing prediction methods as part of his Ph.D. research. The GRIP team itself has not done any prediction work this year.

9.2 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. Like many others of our plans, this work depends upon a graduate research assistant getting excited about it.

9.3 SARCOS Arm Progress. We have been bringing up, since last spring, a 1990's 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. We installed the new arm co-located with a visual display monitor driven by either of our SGI computers. We plan to arrange the display and SARCOS arm in the Trailblazer configuration, so that the viewspace and the manipulation space of the arm coincide.

Progress has been slow, as anticipated. The SARCOS now passes the tests and diagnostics furnished by the manufacturer, and gravity compensation works. We have ported the Docker application to it. Docker now runs using the arm as an input device, but it does not yet deliver proper forces back to the user.

9.4 SARCOS Arm Plan: We expect to get Docker fully functional this spring, and then to port SCULPT to the SARCOS and test the arm with real users on real applications.

9.5 Docker. The molecule docking application built by Ming Ouh-Young continues to be useful for an occasional chemist. We have begun working with a new user, Professor Wolfenden of UNC-CH Department of Chemistry. 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.

The Cybernet Systems Corporation of Ann Arbor, Michigan, is using a copy of the Docker code to demonstrate and evaluate the PER-Force "Force Reflecting" Handcontroller that they market as suitable for this application. We have provided some help bringing their system up and have agreed to advise them with the evaluation.

10. Miscellaneous Progress and Plans

10.1 Rheingans's dissertation shows power of dynamic color mappings. Penny Rheingans, in a study that may be important for the visualization of electron density maps, showed that color representations of data communicate better when the mapping between data values and color values can be dynamically controlled by the user. In two rather carefully designed experiments, Rheingans also showed that the users have strong preference for the dynamic color mappings. Dr. Rheingans reported her results in a paper at Visualization '93.

10.2 Visualization for Molecular Dynamics. GRIP Research Assistant Jonathan Leech has chosen to work on devising new methods of visualizing and performing real-time analysis on the results of molecular

dynamics calculations. MD calculations are a principal activity of the KSR highly parallel computer at the North Carolina Supercomputer Center in Research Triangle Park. Leech has this year been arranging and debugging a high-speed fiber optic realization of a HIPPI interface between the KSR at NCSC and the PixelPlanes5 high-performance graphics engine at UNC-CH.

Spun-off activity and plans. In the coming year Leech will continue his exploration of new visualization methods that are possible with a high-performance graphics engine. Since NCSC is the center for a new Research Resource in molecular computation, they have picked up Leech's research as one of their activities. He is working with UNC chemistry professor Jan Hermans and UNC computer science professor Jan Prins.

10.3 New ridge-finding methods offer improvement for chain-tracing. Some years ago the GRIP Resource developed GRINCH, an interactive graphics tool for *ab initio* chain tracing. The central concept was that of finding the ridges in the 3-D density map, since the density ridges correspond to bonds. During 1993, David Eberly, a research assistant in the UNC Computer Science medical image project, completed a dissertation in which he invented new, more accurate, and more robust ways of finding such ridges.