1991 Research Progress and 1992 Research Plans

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Interactive Graphics for Molecular Studies

From **May 1, 1991** To **April 30,1992**

1. NanoManipulator – Interactive Scanning Tunneling Microscope

1.1 New Collaboration: Real-time Display and Control of STM. The most exciting news is that we have entered into a collaboration with Professor Stanley Williams of the UCLA Department of Chemistry to develop a real-time graphic interface for scanning tunneling microscopes, atomic force microscopes, etc. Prof. Williams and his group have developed ultra-stable STM's 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. Since successive scans are not widely displaced, the drift can in principle be compensated for, so that the scanned surface can be treated as a virtual world for viewing, and for manipulation.

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 can use our GROPE force display arm to allow the user to probe the surface shape, feeling the shape as well as seeing it.

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.

1.2 Progress. Prof. Williams has built two STM's, so he agreed to install one in our laboratory for a trial period. UCLA graduate research assistant Eric Snyder came to Chapel Hill with a microscope in January, 1992, and by the end of his ten-day visit, it was up and running, yielding pictures of barely atomic resolution. Previously UNC graduate research assistant Russ Taylor had written the necessary software, journeyed to UCLA, installed his software on their machine, and convinced himself and Snyder that it could view and control the STM.

Initially Taylor and Snyder operated the STM in imaging mode, gathering data by scanning the sample (initially freshly cleaved graphite and ion bombarded graphite), reconstructing the landscape, and allowing interactive viewing of it. More recently Taylor has implemented a probe mode in which an operator uses our manipulator ARM to position a cursor over the image of the surface he is studying. Thus, in this mode two axes of the ARM are used for input. The system controls the position of the ARM along the third axis to correspond to the local height of the surface. Using this mode the operator can "feel" the contours of the surface. This mode works both with data collected from a previously scanned surface and for real-time investigation of a real surface. In the latter case, the ARM is controlling the x and y coordinates of the STM tip, the servo mechanism of the STM is causing the tip to track the sample surface, and the system is controlling the third axis of the ARM to represent the local height of the sample.

Since installation, Taylor and Mr. Vern Chi of the UNC CS Microelectronic Systems Laboratory have upgraded the STM to provide a stepping motor to bring the tip into tunneling distance from the surface. Even though Snyder trained Taylor in STM operation, the tip distancing proved to be not only tedious but quite exacting, and broken tips were not uncommon. The motor drive makes tip distancing simple and rapid.

1.3 Near-term Plan. Over the next year we plan a variety of experiments and interface development activities:

- Studies of new samples with the existing configuration will be undertaken.
- We shall attempt atomic manipulation in some form or another.
- Drift compensation will be attempted 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 to permit easy and 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 4000-processor MasPar MP-1 installed in our department.
- We shall attempt to reduce thermal drift, the largest apparent drift cause, 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.

1.4 Dream: Atomic Manipulation. According to the physical theory, it should be possible to cause one or a few atoms to attach to the tip by increasing tip voltage about five fold over the imaging level, and to redeposit them by a pulse of the same magnitude and reverse polarity. So one can contemplate picking atoms up, moving them, and setting them down, allowing construction of surface features by both additive and subtractive processes. While atoms are being transported on the tip, imaging is not possible, so navigation has to be by dead reckoning and depends upon having a stable world model.

In one scenario we envision, the user would:

1) survey the surface of a sample within reach of the STM.
2) identify a site suitable for his purpose.
3) position the STM tip.
4) carry out some operation on the surface.
5) re-scan the surface to evaluate the results.

To carry out a complex operation, it might be necessary to repeat this sequence several times. Time is of the essence because thermal drift will eventually carry the selected site out of reach of the STM. We believe the tools we propose to develop for visualization of the surface and manipulation of the STM tip may make a whole range of otherwise impossible experiments feasible.

1.5 Action: Grand Challenges Proposal. We and Dr. Williams have jointly submitted a letter of intent under the NSF Application Groups for Grand Challenges parallel computing research initiative. That initiative specifically calls for application groups made up of collaborations between computer scientists as natural scientists in the field of the Grand Challenge. Dr. Williams works on surface science, specifically for semiconductors, so his work falls under this rubric. The general strategy for the GRIP project is to spawn and incubate new research projects, and then see them grow into self-supporting status, and this fits that plan.

2. SCULPT – Interactive Manipulation with Updated Energy Minimization

2.1 System Concept. The SCULPT system, which was conceived by David Richardson, enables a molecular scientist to view a bond model of a protein, attach one or more springs to specific atoms, and apply tugs to fold, conform, dock, or otherwise manipulate the model. A near-real-time energy minimizer runs repeatedly, updating the conformation of the molecule. Our objective is full real-time operation

2.2 Progress. Research Assistant Mark Surles has the prototype SCULPT system running, and at a rate rather better than once per second for middle-sized proteins. Bond lengths, angles, and peptide planarity are treated as rigid constraints, van der Waal forces are accurately modeled, and hydrogen bonding is approximated. Perhaps Surles's most important contribution is a minimizer which, for backbone-appendage structures, runs in a time provably linear in the number of atoms. SCULPT runs on our four-processor Silicon Graphics Iris 4D/240 GTX.

Most recently, Mark has added a rigid-body feature, whereby whole alpha helices, etc. can be treated as single rigid bodies with relatively few degrees of freedom. This both facilitates the manual specification of molecule manipulation and, since it radically reduces the number of variables, speeds up the operation of the system. The system promises to be useful to the Richardsons for protein design, especially for designing side chains so as to give the desired protein interiors and inter-member bonding and packing.

2.3 Near-Term Plan. Surles will finish his dissertation and defend it this spring. The Richardsons are trying to raise money to fund him as a postdoctoral fellow in their laboratory next year, to continue the work along with graduate students on the GRIP team here. The immediate next steps are obvious:

- electrostatics
- solvent forces
- an easier to use data interface for loading data in and getting structures out for other computations
- further development of the rigid body features.
- more testing on real problems with a variety of users.

2.4 Action: Grand Challenges Proposal. Brooks and Wright have joined the Richardsons and two new colleagues at Duke, Lorena Beese and Homme Heillinga, in making a proposal for a second Application Group addressing a Grand Challenge, this time, protein and drug design.

2.5 Unified Minimizer Concept. Parallel computing makes it conceivable that we can do interactively, in real time, computations that formerly could only be done in batch, over minutes or hours. The overall thrust of our proposal is to prototype, and then to develop into production tools, parallel computing, graphics, and algorithms to enable real-time interactive minimization of complex cost functions, subject to both hard constraints and weighted elastic restraints, as we now do in SCULPT. We envision a sort of scientific pinball machine, in which the user governs global and gross motions aimed at jumping from the domain of one local minimum to another, and the minimizer finds local minima automatically and continually. This basic mathematical approach will be used for several different kinds of cost functions, different constraint sets, and a variety of design spaces. All of these systems require, at their hearts, the very rapid evaluation of atomic force models.

2.6 Spaces. We expect to move structures and search for minima in continuous spaces, such as initially conformation space, and perhaps phase spaces of density maps. We shall also search in discrete spaces, such as sequence spaces, and in combined sequence and conformation spaces.

2.7 Cost functions. We now minimize free energy of a folded molecule and binding energy of complexes. We will extend this minimization to correlation (R) with crystallographic structure factors, and custom cost functions specified for specific active sites.

2.8 Constraints. We now constrain sequences, bond lengths and angles, peptide planarity, other conformer restrictions, In the extended minimizations we will also at various times constrain packing and binding properties. For each, our objective will be real-time performance with the computation actively followed and actively guided by the biochemist researcher.

3. GROPE – Interaction Using Force Display and Visual Display

3.1 System Concept. The GROPE system supplements the visual display of docking molecules with a force display so that the user can feel, as well as see, the forces and torques experienced by the smaller molecule. We have previously shown that this significantly improves the performance of biochemists in arriving at the proper docking position of a drug inhibitor in the active site of an enzyme, in our first case, DHFR. We use a 1960's technology Argonne Remote Manipulator (ARM) master station for the force display, and calculate the binding energy, forces, and torques fast enough to achieve 15 to 20 updates per second.

3.2 SARCOS Master Arm. The big news is that DARPA found $ 235 K to fund our acquisition of a new force display master arm. SARCOS Engineering Company of Salt Lake City is the developer of the high-performance high-realism hydraulic technology. Our arm is under construction there now, and should be delivered this fall. It uses an exoskeleton so arranged that each of the virtual joints are positioned where the users real joints are. A single hydraulic supply furnishes power via 3000 psi fluid, and miniaturized local electro-hydraulic actuators control each degree of freedom.

Our arm will have ten degrees of freedom: 3 shoulder, 1 elbow, 3 wrist, and 3 in the thumb and fingers. This means we shall have to develop the mathematics to resolve our 6-degree-of-freedom molecular forces into the most natural combination of the 10 degrees of freedom available. SARCOS will provide gravity-compensation software so that the user will not have to support the weight of the arm.

3.3 Progress. On the present GROPE system, the principal thrust this year has been put our system on a sounder scientific basis and to explore new modes of use with new users. The system was consolidated so that model maintenance, generation of visual displays, and ARM control now all run on the Silicon Graphics Iris 4D/240 GTX, rather than being divided between a Sun for arm control and model maintenance and a separate graphics engine for visual display generation. If we choose to operate with the Pattabiraman force approximation, the system is self-contained on the Iris. If we choose to use the evaluation of the Leonard-Jones/Coulomb model, we do force and torque calculation on the 4000-processor MasPar MP-1, controlling it from the Iris.

A main effort this year with our present Argonne Remote Manipulator has been to determine the accelerations of the ARM in response to the applied voltages, for each degree of freedom. This has been hindered by the noise levels in the arm sensors, which precluded numerical differentiation of position data. Our attack on this has been to devise electronics and software enabling us to read and to use the velocity data that has always potentially been available from the tachometers built into the ARM in the 1960's. That work is still in progress.

3.4 Plan. The performance of the present system for molecular docking is far from ideal. The sensation of atomic contacts is mushy and with the force gain set for system stability with complex structures the longer range forces are too subtle to convey useful information. We plan to address these problems by constructing several simple systems using our arm to simulate for example: contact with a hard surface, constrained motion such as rotation about an axis, and motion in a viscous medium. The lessons learned will then be applied to the docking application. Our goal is a system that is stable, displays van der Waals contacts as crisp surfaces and enables to user to feel the long range forces when molecules are not in contact.

Toward this goal we are studying the application of digital control theory including Kalman filtering to our system. We plan to add routines to anticipate position of arm so that the displayed forces better represent the current state of the system, to apply calculated force to slow motion and improve stability, and to apply well timed impulses to stop the arm on contact with a surface.

The method we currently use for determining the position of the arm, peak detection of the a/c signal from synchro control transformers, is proving inadequate. Furthermore, we have experienced a significant increase in the signal noise generated by the twenty-five year old synchros we are using. We are exploring several alternative technologies for sensing the position of the arm.

To implement some of the algorithms we are developing for control of the arm, we need to measure its velocity as well as position. Numeric differentiation of the position data has proved inadequate and will probably remain so even with improved technology for measuring position. Therefore, we are activating tachometers that were incorporated into our arm by Argonne but have not been used here. We are currently calibrating the outputs from these devices.

In the next year we plan to prepare for delivery of our new SARCOS arm by developing software for its control. This will include routines for transforming data on the angles of its joints into the position and orientation of the hand grip in Cartesian coordinates and routines for determining what torques must be applied at each joint to display a given force and torque to the user. Delivery and installation of the new arm is currently scheduled for November 1992. The lessons in control theory we learn from our current arm will be applied to the new arm.

3.5 GROPE Usage and Experience. Dr. Ruth Pachter of the Materials Laboratory at Wright-Patterson Air Force Base brought us the atomic coordinates for a family of cyclic siloxane-based molecules. She used our docking system to study the interdigitation of linear sections of these molecules to form liquid crystals. Eleven different combinations of structures were studied, each was maneuvered into several trial conformations using our force-feedback arm, and the binding energy between the molecules was then minimized for each conformation using a command built into our system. Atomic coordinates were recorded for more than sixty stable conformations and sent back to Dr. Pachter's laboratory for further analysis.

In the course of this work we modified our system to allow rotation of the many flexible bonds in the long side chains of Dr. Pachter's molecules. We also found the Patabiraman approximation used to dock small drug molecules did not work because the moveable and fixed structures were about the same size. We were able to proceed, however, using the implementation of our system that calculates the full Leonard-Jones model using our Maspar MP-1 computer. This work pointed up the need to extend our system to work with structures containing more than two separate molecules, the need for a more efficient minimizer algorithm, and the need to generate output coordinates in a standard format.

Dr. Williams' STM project also makes another new kind of use of GROPE capabilities. This is described above in the section on NanoManipulators.

3.6 Docker System in ß-Test. Since we do not expect force-display equipment to become readily and economically available in the next five years, we have a small project to make a GROPE-like system in which forces are explicitly and intuitively displayed on the screen as one attempts to dock two molecules. Undergraduate Andrew Certain has developed this system, using ideas from, among others, our former graduate student Ming Ouh-Young. We simulate force display by a technique developed by Dr. Jeff Blaney of our Advisory Committee. As one attempts to move a molecule with the mouse, the rate of response varies inversely with the force one must overcome. This works remarkably well.

Our Docker program for the SGI Iris is complete and has been released to a small number of people for ß-test, with no reference manual but a videotaped tutorial. A written tutorial has been prepared by Mrs. Fay Ward and Dr. Wright.

4. GROVE – Interactive Volume Visualization of Electron Density Maps

4.1 System Concept. The GROVE system uses the power of the UNC Pixel-Planes 5 MIMD/SIMD graphics processor to enable real-time viewing of electron density maps, with user-specified viewing direction, lighting and shading, slicing, and, we aim, density level for contouring.

4.2 Progress and Evolution of Concept. Because of extensive surgery and recovery of Graduate Research Assistant Stephen Hench, progress, though surprising under the circumstances, has not been as much as we might have hoped. Hench has developed algorithms for calculating the Fourier transform using the Pixel-Planes 5 hardware which was designed for a very different task, rendering of pictures. He has begun coding, and we hope to start testing and measuring performance by the end of the spring term.

An exciting thing has happened in the project, however. Volume visualization technology has depended upon using rather small voxels and tri-linear interpolation within these. Real-time volume visualization has permitted only fairly coarse resolution, with large voxels. Rather than increase the resolution, we set out to investigate higher-order interpolation. This course of action recommended itself the more because Pixel-Planes 5 can rapidly evaluation quadratic functions in an SIMD fashion.

Prof. Wright, thinking about interpolation, realized first that a density map is calculated by Fourier transforms, so sinusoidal interpolants might work better than polynomial ones. Then he reflected that the density map is a derived object, calculated from structure factors and phases. Rather than interpolate at all, why not recalculate the needed map intra-voxel point density values afresh from the structure factors and phases? Investigation of this showed it to be conceivable on a computing engine of the power of Pixel-Planes 5. That in turn led to the realization that we are in striking distance of being able to do real-time direct and inverse Fourier transforms on maps and the data sets from which they come. This has become an objective of the GROVE subproject.

In a related project, another Graduate Research Assistant Xialin Yuan is exploring the implementation of Lorensen and Cline's marching cubes algorithm for displaying isodensity surfaces using our Pixel-Planes 5 engine. He has this running and for a small map of about 8000 voxels the density level displayed can be changed in a fraction of a second.

4.3 Near-Term Plan for Volume Visualization. Hench plans initially to implement his algorithm using a single general purpose processor and a single renderer board of our Pixel-Planes 5 system. The first implementation will also be limited to displaying the electron density on a user selected plane cut through the map. He will then extend his system to use all of the hardware available and to composite many parallel sheets of density into a unified display. Controls will be provided enabling the user to specify the viewing parameters, the density level displayed, the number of structure factors used, and the set of phases or mixture of phase sets used. Experiments will be conducted to determine the effect on performance of all these options. Hench also proposes to explore a second approach in which the Fourier transform is implemented on the general-purpose processors of Pixel-Planes 5 instead of the renderers.

Yuan plans to determine the performance achievable and maximum size map that can be displayed using the marching cubes algorithm with our hardware. He will also implement user specification of density level by means of an analog input device.

4.4 Real-Time Reciprocal Space. We envision a system in which multiple views of a density map are simultaneously maintained, one of which will be the electron density in real space, and another the structure factors and phases in reciprocal space. The user will be able to do local or large-scale changes of, for example, the phases, and see the sensitivity of the density map to the changes. One could similarly examine the effects of omitting or scaling anomalous structure factors if one had reason to suspect their accuracy.

We assume that the user would be able to manipulate a model of the molecule into the density as part of interpretation and fitting. Then yet another simultaneous view might be of the density differences between the map as calculated from structure factors and that calculated from the molecular model. This capability would let us build an immensely more powerful map interpretation system than either GRIP75 or GRINCH, our two previous accomplishments.

Building the real-time reciprocal space capability will be a high priority for the coming project year.

4.5 Unified Minimizer. Prof. David Richardson recognized that the minimizer used in SCULPT for the constrained-restrained energy minimization could be used in density map fitting to give near-real-time optimization of a model fit against the structure factors themselves, enabling a user to perform interactive model fitting while being guided around both fitting and phasing errors. If manpower permits, we shall also tackle this in the coming year.

5. VIEW – Interactive Exploration of new Visualization Paradigms

5.1 System Concept. There are many different ways to visualize a molecule, both in real space and in abstract spaces. Each of many visualizations reveals or highlights a different aspect of molecular structure or function. In contrast to graphical depictions of the macroscopic world, there is no "realistic" visualization; one wants to make as many revealing ones as possible. The VIEW system (Visualization Impromptu Evaluation Workbench) is designed to make it easy for a biochemist to explore an immense variety of novel visualizations rapidly, so that each can readily be evaluated for its informing power. The concept is to furnish the user a toolkit of many simple visualization primitives, each defined by a menu item, and a scripting language that makes it easy to combine these into more sophisticated and powerful menu items.

5.2 Progress. Graduate Research Assistant Larry Bergman has had a prototype running for all of this project year. Dan Aliaga joined him in September. For the first part of the year, the emphasis was on debugging and making the system robust. After this robustness was achieved for a useful elementary set of functions, extensive user tests were made, mostly with Prof. Jane Richardson. Based on this actual use for real visualization tasks, a new package of additional function was designed and built in the last half of the project year. The emphasis of the new function has been on a powerful new set of database searching and handling capabilities. As usual, the new function comes at the cost of new bugs. User testing of the system, especially of the new function, has continued. The VIEW system has been given to a few other laboratories for exploratory use.

5.3 Plans. The immediate goal is to fully debug the system and make it robust. Then the team will write a separate manual for programming-incapable users who want just to use the extensive built-in library of visualization primitives. We anticipate that this system will be very useful to many chemists. The team will then write a manual for users who desire to use the scripting capability and its fairly extensive programming environment to create their own visualization scripts and primitive visualization tools. We hope to enlist a respectable-sized user community from whom we can learn both how VIEW is useful and what its shortcomings are.

We do not foresee extending the present VIEW system over a period of years. Instead, we believe the first fielded version will be useful in itself, and that it will provide us user experience with this new kind of function. This experience should enable us to learn how to make a more powerful and useful VIEW-type system. We do not now plan to build such a system as a free-standing tool, however, but to combine its capabilities with those of SCULPT, GROPE, and GROVE into a unified next-generation molecular graphics system, which we have called *Trailblazer.*

6. Trailblazer – Next-Generation Molecular Graphics System

6.1 System Concept. Our four-year objective is to build a next-generation molecular graphics system that fully exploits the computing power newly available and the graphics power newly available, to give many innovative functions in a fully integrated system. We do not expect this system to be readily fieldable, nor economically within range of the average laboratory. We do expect the costs of computing and graphics technologies to continue to fall, and we see our function as pioneering the development and testing of molecular graphics function, so that the many developers of commercial systems can evaluate the new ideas for use in their systems when hardware costs come within range.

The system we envision is shown in the attached figure. It incorporates

- a novel visual interface that hangs the image of the molecule in the user's hand space,
- the new SARCOS arm that gives the user the capability to feel synthetic forces, torques, and objects, essentially an extension of today's GROPE system,
- the SCULPT real-time energy minimization capability, as it evolves,
- the GROVE volume-visualization and multi-view real-time reciprocal space capability,
- VIEW's novel visualization tools.

6.2 Progress. We built last spring a simple prototype that had the new visual interface we plan for Trailblazer, and the SCULPT function as it stood then. The user grasps a tabletop molecule hung in his hand space with a pair of tweezers. With these he can attach springs between particular atoms and stationary "pushpins" in 3-space, or he can pick an atom and tug it, with the rest of the molecule moving so as to maintain a minimum system energy.. The molecule is displayed as a stereo, colored bond graph on a horizontal monitor screen mounted overhead. A front-surface (fully silvered) mirror in front of the user's face places the virtual image in the space centered about 16 inches from the user's eyes, and superimposes it on his active hand space, with his elbows resting on the table.

The tweezers have a 6-D position- and orientation-sensing device attached, and the image of the tweezers is continually drawn on the monitor, in the space of the molecule. Once one has successfully picked an atom, it is easy to tug it around and watch the whole molecule deform realistically. Most users have trouble picking individual atoms using just stereo and hiding cues for depth perception.

6.3 Plans. Each of today's SCULPT, GROPE, GROVE, and VIEW systems is free-standing, with incompatible data formats and structures, inconsistent control structures, unmatched user interface philosophies, and even different programming languages. As each system reaches field test, we shall define what the proper and useful functions of its successor should be. Meanwhile we shall be thinking about a unified data structure and representation that will support each of these subsystem functions. That is as far as we expect to get in the coming project year. We dream of combining the present GROPE system, using the present ARM, in the Trailblazer viewing configuration, driving the SCULPT system.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: T

TITLE: GROPE -- Force Display

KEYWORDS: force feedback, molecular docking, remote manipulation

AXIS I: 2

AXIS II: 42 50

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Wright, William V.
DEGREE2: Ph.D
DEPT2: Computer Science
NONHOST2:

% BRTP $:

ABSTRACT: Development of force-display technology and testing it in the context of molecular research.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: T

TITLE: Docker -- Molecular docking system for desktop display

KEYWORDS: pseudo force display

AXIS I: 2

AXIS II: 42 50

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Wright, William V.
DEGREE2: Ph.D
DEPT2: Computer Science
NONHOST2:

% BRTP $:

ABSTRACT: Development of a molecular docking system implemented on a standard SGI Personal Iris desktop display. Developing substitutes for force feedback.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: T

TITLE: GROVE -- Interactive Volume Visualization of Electron Density Maps

KEYWORDS: Fourier transform, structure factors, marching cubes algorithm

AXIS I: 2

AXIS II: 42

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Wright, William V.
DEGREE2: Ph.D
DEPT2: Computer Science
NONHOST2:

% BRTP $:

ABSTRACT: Development of techniques for rendering electron density maps and for calculation of Fourier transforms in real time.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: T

TITLE: Trailblazer -- Next-generation Molecular Graphics System

KEYWORDS: integrated system

AXIS I: 2

AXIS II: 42 70

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Wright, William V.
DEGREE2: Ph.D
DEPT2: Computer Science
NONHOST2:

% BRTP $:

ABSTRACT: Integration of results of other subprojects. Pioneering and testing new technologies.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: NanoManipulator -- Interactive Scanning Tunneling Microscope

KEYWORDS: surface studies, head-mounted display, remote manipulation

AXIS I: 2

AXIS II: 42 70

INVEST1: Wright, William V.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Williams, R. Stanley
DEGREE2: Ph.D
DEPT2: Chemistry
NONHOST2: University of California at Los Angeles

% BRTP $:

ABSTRACT: Development and testing of a system for controlling a scanning tunneling microscope via a remote manipulator arm and for displaying its output using a head-mounted display.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: SCULPT -- Interactive Manipulation with Updated Energy Minimization

KEYWORDS: molecular conformation, real-time constrained energy minimization

AXIS I: 2

AXIS II: 42 50

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Richardson, Jane S.
DEGREE2: Ph.D
DEPT2: Biochemistry
NONHOST2: Duke University

INVEST3: Richardson, David C.
DEGREE3: Ph.D
DEPT3: Biochemistry
NONHOST3: Duke University

% BRTP $:

ABSTRACT: Development and testing of an interactive computer graphic system to allow chemists to deform molecular models in real-time while the bond geometry is constrained to canonical values and the free-energy is minimized.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: VIEW -- Visualization Impromptu Evaluation Workbench

KEYWORDS: data base, molecular geometry, computer graphics, script language

AXIS I: 2

AXIS II: 42 50

INVEST1: Brooks, Frederick P.
DEGREE1: Ph.D
DEPT1: Computer Science
NONHOST1:

INVEST2: Richardson, Jane S.
DEGREE2: Ph.D
DEPT2: Biochemistry
NONHOST2: Duke University

INVEST3: Richardson, David C.
DEGREE3: Ph.D
DEPT3: Biochemistry
NONHOST3: Duke University

% BRTP $:

ABSTRACT: Development of visual tools enabling chemists to make new molecular visualizations very rapidly, using data from the Brookhaven database, and mapping data variables to a wide variety of geometries and colorings.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: Cyclic siloxane-based liquid crystals

KEYWORDS: molecular packing

AXIS I: 2

AXIS II: 42 92 (materials science)

INVEST1: Pachter, Ruth
DEGREE1: Ph.D
DEPT1: Materials Laboratory
NONHOST1: Wright-Patterson Air Force Base

I% BRTP $:

ABSTRACT: Investigated the interdigitation of two types of pendant mesogens on a cyclic siloxane-based molecular system using the GRIP force feedback arm. About 60 conformations were generated and algorithmically modified to minimize inter-molecular potential energy.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: Cytidine deaminase

KEYWORDS: cytidine, uridine

AXIS I: 2

AXIS II: 42 50

INVEST1: Carter, Charles W.
DEGREE1: Ph.D
DEPT1: Biochemistry
NONHOST1:

INVEST2: Betts, Laurie
DEGREE2: Ph.D
DEPT2: Chemistry
NONHOST2:

I% BRTP $:

ABSTRACT: Used VIEW system to generate pictures of this molecule for publication.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: Polymer dynamics visualization

KEYWORDS:

AXIS I: 2

AXIS II: 42

INVEST1: Parnas, Richard
DEGREE1: Ph.D
DEPT1:
NONHOST1: National Institute for Standards and Technology

I% BRTP $:

ABSTRACT: Used head-mounted display to help user visualize the dynamics of polymer threads attached to a surface at one end and set in motion by a passing fluid.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: Molecular binding function

KEYWORDS: hydrophobic, polar, coulombic, entropic, hydrogen bonding, solvent

AXIS I: 2

AXIS II: 42

INVEST1: Kellogg, Glen
DEGREE1: Ph.D
DEPT1: Medicinal Chemistry
NONHOST1: Virginia Commonwealth University

INVEST2: Semus, Simon F.
DEGREE2: Ph.D
DEPT2:
NONHOST2: Medical College of Virginia

I% BRTP $:

ABSTRACT: We are planning to modify our system for molecular docking to allow the user to choose a model of the force between atoms proposed by Drs. Kellogg and Semus that incorporates many of the longer range electrostatic effects.

SCIENTIFIC SUBPROJECT

GRANT NUMBER: P41RR02170-08
REPORT PD: 5/1/91-4/30/92

BRTP UNIT: C

TITLE: Binding of peptide fragments to human leucocyte antigen

KEYWORDS: major histocompatible complex

AXIS I: 2

AXIS II: 42 64

INVEST1: Frelinger, Jeffrey A.
DEGREE1: Ph.D
DEPT1: Microbiology
NONHOST1:

I% BRTP $:

ABSTRACT: Dr. Frelinger and his co-workers will use our molecular docking system to study the binding of several peptide fragments to human leucocyte antigen.