Sixth Annual Report
Interactive Graphics for
Molecular Graphics System

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PART I. NARRATIVE DESCRIPTION

A. SUMMARY OF ACCOMPLISHMENTS

Objectives and Operating Policies

We have built, and operate as a service resource, an effective interactive computer resource for seeing, manually manipulating, and computationally modifying mathematical models of complex molecules. We believe that our present resource, called GRIP-75, has been shown to be as complete and useful as any in existence; we are aware of many inadequacies and needs.

We are building a second-generation version of this system, now called GRIP-X, designed to be more comprehensive in the biochemical problems that can be attacked, more powerful in the mathematical tools available, smoother in the user interface, and constructed as product-quality, documented, exportable software.

Fundamental to our approach are the following objectives:

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

A corollary of these objectives is that we are heavily dependent on observation of and feedback from real users attempting to solve real problems.

Our users are almost exclusively working on the structures of molecules of considerable biochemical interest: proteins and nucleic acids. We aim to advance health-oriented biochemical research by enhancing the productivity of individual reseachers through better tools.

Changes in Resource Direction and Problems

1979 has been for the GRIP Molecular Graphics Project a year of transition, and in some sense, frustration. Early in the year came word of the Council recommendation of five-year renewal funding for the project and of provision for the first time of funds for equipment to be dedicated to GRIP Service and Development. Budgetary difficulties at DRR, however, forced the deferral of any equipment acquisitions until almost the end of the calendar year. Procurement processing time means that installations will take place in the spring and summer of 1980. The same budget difficulties meant that we could not proceed to the new budget levels for personnel, but instead operated for most of 1979 at the same level of funding as was originally authorized for the 05 year. Due to substantial inflation in all our costs, it was necessary for us to in fact lower the number of personnel on the project in order to operate within this budget.

As a consequence, we cut back the service to visiting chemists. We suspended advertising or promoting the availability of the facility, but we continued to serve our existing client base, both local clients and visitors who returned for repeated work sessions. We also took new clients who sought us out.

The other major event during the year was the mitosis of the project, originally a UNC-IBM collaboration at Chapel Hill, into two separate projects continuing to cooperate but at much greater distance. Dr. William V. Wright, who had been the IBM collaborator and other senior investigator on the project, had his work recognized by IBM, was given a project with a total staff of three and separate equipment of his own, and will be operating in the IBM United Kingdom Scientific Centre at Winchester and serving a clientele of British biochemists. He will continue, with his staff, to

collaborate with us in the design and in the construction of GRIP-X.

The collaborative contributions of Dr. W. V. Wright here during the past years have been made without charge to the project under a joint study agreement with the International Business Machines Corporation. We are in the process of formalizing a new joint study agreement for the new collaboration.

Dr. Wright's departure in June brought to an end some of the active development underway on our campus; due to the difficulties of transition, staffing, and equipping his laboratory and ours, the development work, in fact, only began again at the end of the year. The first joint session between the two projects was held on November 26-27, and many matters of technical decision were discussed. The next joint session will be held in March 1980 at Winchester.

Mr. John E. Leonarz, who had been serving as Acting Director of the resource's service operation also left the project during the year. Following the recommendation of the Special Study Section, we shall fill that post with a trained and experienced biochemist, since our team has no one with such knowledge. Mr. Leonarz made valuable and valued contributions, both in keeping our facility operating smoothly in the vicissitudes of hardware troubles and staff turnover, and in providing a caring personal interface to our clients.

Our five-year renewal and prospect of a new facility has occasioned much excitement on the project. Much effort has gone into planning the new equipment and the layout of the new facility. All major items of equipment funded for this year except the vector-drawing graphics subsystem have been ordered, and that will be out on bid within the month.

Accomplishments in Service to Biochemists

The use of GRIP by our clients exceeded 1100 hours during 1979, up about 7 per cent over the previous year. We had six new user groups during 1979, and eight returning groups.

Form 11 identifies the fourteen service projects which made use of the GRIP system during 1979.

Table I summarizes the use of the GRIP system for all purposes since we began demonstrations and productive operation on July 15, 1975. We have not tried to estimate the system time spent on development before the beginning of productive operation but know it to be many hundreds of hours. Because we changed from manual to machine logging of GRIP sessions in mid-1976, we believe the true buildup of system usage to be substantially greater than suggested by these data. We have observed that users tend to overestimate the time they spend using GRIP.

Table I. GRIP Use by Year (Hours)

	1975	1976	1977	1978	1979	Totals
Production	329	581	781	1034	1108	3833
Demonstrations	12	50	161	137	43	403
Development	297*	186	198	213	345	1239
Totals	638	817	1140	1384	1496	5475

* System development July 15, 1975 through December 31, 1975.

Table II gives the use of the GRIP system by year for each team of biochemists. These teams are identified by their principal investigators.

TABLE II. -- GRIP PRODUCTION TIME (hours)

User	1975	1976	1977	1978	1979	Total
Hermans	7	29	42	13	11	102
Kim	200	321	105	24	49	699
Richardson	83	79	91	188	384	825
Lipscomb	12			102	-	114
Carter	27	21		4	5	57
Jensen		46	62		-	108
Tsernoglou		85	11		-	96
James			19		-	19
Low			55	191	65	311
Davies			85	92	-	177
Schiffer			35	28	26	89
Amma			163	35	-	198
Wright			41		96	137
Hendrickson			72	80	34	186
Schevitz				74	-	74
Love				94	-	94
Kartha				109	-	109
Taylor					89	89
Rich					78	78
Sarma					188	188
Olson					20	20
Bugg					39	39
Premilat					24	24
Total Hours	329	581	781	1034	1108	3833

Table III is a list of the biochemists whose research teams have used the GRIP system and their institutions. These are listed in the order of their first use of GRIP. For groups sending more than one biochemist to use our system, the principal investigator is given first and the names of his colleagues follow indented. The institutions of these colleagues are given only where they differ from the principal investigator's. In four cases, Sarma, Rich, Love and Sigler, the principal investigator has made little or no direct use of GRIP himself.

TABLE III. -- GRIP USERS (1975-1978)

J. Hermans	University of North Carolina
D. R. Ferro	Istituto di Chimica delle Macromolecole
J. E. McQueen	
T. Kuntz	University of California School of Pharmacy, San Francisco
M. Vacatello	Institute of Chemistry, University of Naples, Italy
S. H. Kim	Duke University
J. L. Sussman	
R. W. Warrent	
S. R. Holbrook	
G. M. Church	
W. Shin	
C. J. Alden	
D. E. Richardson	Duke University
J. S. Richardson	
E. D. Getzoff	
J. A. Tainer	
W. N. Lipscomb	Harvard University
J. L. Crawford	
C. W. Carter	University of North Carolina
R. A. Jones	
L. H. Jensen	University of Washington
K. Watenpaugh	
R. E. Stenkamp	Yale University
D. Tsernoglou	Wayne State University
G. A. Petsko	
M. James	University of Alberta
L. T. J. Delbaere	
G. Brayer	
B. W. Low	Columbia University
A. Sato	
M. Kimball	
D. R. Davies	National Institutes of Health
M. C. Liu	
E. A. Padlan	

M. Schiffer	Argonne National Laboratory
E. L. Amma R. L. Girling R. C. Paslay	University of South Carolina
H. T. Wright	Princeton University
W. Hendrickson	Naval Research Laboratory
P. B. Sigler A. Podjarny R. W. Schevitz	University of Chicago
W. E. Love W. E. Royer	Johns Hopkins University
G. Kartha	Roswell Memorial Institute
H. C. Taylor	Berkeley Springs Research Consortium
A. Rich N. Woo	MIT
R. Sarma A. Laudin	SUNY, Stony Brook
A. Olson	National Resource for Computational Chemistry
C. Bugg R. Almassy J. Fontecilla	University of Alabama
S. Premilat	Universite de Nancy France

Accomplishments in System Development

Subproject 1, Study of Three-Dimensional Cues for Molecular Graphics. James S. Lipscomb has, for his Ph.D. dissertation, investigated the relative power of a variety of cues usable in a molecular graphics system to induce three-dimensional perception. He not only compared cues, he studied the subtleties and non-linearities involved in implementing them in a way most effective for the user.

He found that the kinetic depth effect is the single best depth cue for graphic displays of 3-D objects such as molecules. Surprisingly, it is more powerful perception aid even than stereopsis, the display of different images to each eye.

Lipscomb found that the kinetic depth effect achieves its full power only if the rocking or rotation of the image appears smooth to the viewer. It has been known for some time that this requires very frequent (about 12 times per second) updates to the displayed image. Lipscomb discovered that this is not sufficient: the illusion of smooth motion also requires that image updating and image refreshing be synchronized, and best effects are achieved when there is one update per refresh.

Besides Lipscomb's work, one other pilot project explored the used of a head-mounted display for molecular studies. Such a display was simulated by mounting a miniature TV receiver on our manipulator arm, with its picture generated by the Vector General and fed into a camera. As the arm moves, its position is sensed and the picture on the TV changed to represent what one would see from that position if looking in that direction. One can zoom in, for example, on one residue in a molecule, or even fly through a benzene ring. As technology matures, such a display appears to be likely to become feasible and economical.

Subproject 2, Varifocal Mirror 3-D Display. Jon Cohen investigated, as his master's thesis project, the use of the well-known varifocal mirror for three-dimensional images. Present plotting speeds rule out such a device for molecules, but the reconstruction of 3-D images from slices of a 3-D space should be feasible with present technology. Cohen built a varifocal mirror system in which a microprocessor synchronized the firing of xenon flashbulbs in a set of projectors, one per slice. Each was fired at the proper point in the excursion of the mirror. The several source images were all focussed on a single screen by the use of a mirror-tunnel designed and lent by the Picker X-Ray Corporation.

Cohen's pilot system didn't work very well because the light losses in the optical system were too great for the power of flash available and the light duration tolerable. We plan to try again using a more powerful lights source, shuttered by Kerr-effect shutters.

Subproject 3, Specifying Manipulations by Data Tablet Dragging. Dirk Voss has undertaken as his master's thesis investigating the integration of our Summagraphics data tablet into the GRIP system as the input device for manual manipulation of molecular structures. If successful, this will enable us to replace two joysticks with three input axes each and eight knobs by this single input device, thus improving the tactile continuity of the GRIP man-machine interface. Later we hope to expand the function of the data tablet to replace the light pen, the programmed function keyboard, and the slide potentiometers of the current system.

Other projects aimed at improving the human factors of the manipulation of objects perceived through computer graphics included a pilot system whereby the GRIP user moves the master arm of an electrical remote manipulator to specify the motion of a residue or side chain. The manipulator arm combines three translational degrees of freedom and three rotational degrees of freedom in one device, controlled in a natural way by one hand. GRIP-75 uses two three-degree-of-freedom devices to specify such manipulations, which is not very natural.

The arm project worked after a fashion, but it was only at a pilot stage. We do not plan to integrate it into a production version of GRIP.

Lack of memory on the PDP11/45 really precludes the integration of any of the features of our exploratory systems into the production system. Such will have to wait for the VAX.

Subproject 4, Ridge-line Techniques of Initial Fitting to Densities. Tom Williams has taken as his Ph.D. dissertation project the development and evaluation of a set of ridge-line techniques whereby initial interpretations can be made of electron density maps. Such techniques have previously been explored by Greer, at Columbia, and by Carroll Johnston at Oak Ridge. Williams has imported the Johnston package from Stanford and will be using it as a standard test-bed against which he can compare the techniques he has devised and will devise. His very first results, done on a real but very clean map, are most encouraging. Practical techniques must be not only effective but also robust in the presence of noise.

Subproject 5, New Version of GRIP-75. During 1979 we made few changes to the GRIP-75 program itself, satisfying most user requests by building new commands, or even whole new

menus of commands, by stitching together existing pre-programmed functions. The flexibility of GRIP's multilevel command language developer lets the system's appearance to users be tailored by developers and shepherds with reliablity and speed.

Supplementing the shared standard menus, each user group can have its own menu of selected or customized commands, ones such as "LgCon2Da", which contours a region larger than the current viewing cube from density map set #2, showing the resulting contour lines dashed. We keep menus assembled for out-of-town guests off-line in readiness for their return.

We continue to improve the human factors of GRIP-75 when that can be done without major rebuilding or redesign. During 1979 we reworded many error messages, arranging for the more serious errors to flash the text as an attention drawing warning. To make screen menu items easier to read we use both upper and lower case letters: compare 'CENRESNUM' and 'CenResNum', for example. We added a 'Roll Stack' command so users can inspect command parameters without disturbing them; it is especially useful for editing targets and weights during on-line geometric idealization.

A few other commands have been added or improved to make contouring, fitting, and on-line idealization easier and faster to use. Previously GRIP-75 required a user to load a molecular model even if the user only wished to view a density map; we have lifted this restriction. Dynamic fitting has been enhanced by allowing the user to pick the atom to become the logical center of bond-twisting; the 'dog', so to speak, relative to which wag the various tails of bonded atoms. By default the flying residue pivots about that atom as well. This lets the user keep relatively stationary whatever part of the residue is best defined by the density, twisting the other atoms around to fit them in as well as posible. The number of the knob which will cause turning about each twistable bond is displayed on the bond line, offset toward the more fixed end of the bond. We have eliminated the need for separate 'Fit Protein residue' and 'Fit nucleic acid nucleotide' commands. Users who need only simple geometric idealization to clean up a residue after fitting it have been offered the 'Ref3Res' command. 'Ref3Res' idealizes ["Refines"] the three residues containing and immediately adjacent to the atom most recently picked by the user, saving him the 36 keystrokes and button pushes peviously required to set up this commonly-wanted action.

We have improved the way the GRIP-75 system can display to the user input parameters or results of computations. The GRIP-75 operand stack holds three kinds of data: a number, a direction in space, and an identification of an atom in the molecular model. GRIP displays each of these on the screen in an appropriate way; for example, the atom is circled if it is in view. But some commands interpret these data in other ways not previously displayed: the atom as a bond, and the number-direction pair as a point in space. GRIP now brightens the bond associated with the circled atom and draws a tiny hash-marked box at the specified point in space. While generally helpful, these two enhancements have made on-line idealizaton in particular easier to use. For example, the biochemist can now unambiguously see what bond he is cutting free or making fixed, and can see the points in space to which atoms have been targeted to move.

Dynamic Update Speeded Up. The PDP-11/45 computer has 8K bytes of 500 nanosecond-cycle, MOS storage and 40K bytes of 1200 nanosecond-cycle core storage available for GRIP-75 program execution. By rearranging the order in which parts of GRIP are loaded into the PDP-11, we have placed the most heavily used subroutines into the faster MOS. Measurements show the machine now spends about 80% of its execution time in this 15% of its memory space. This has yielded an update rate improvement of roughly 40%, giving our users smoother, better-perceived motions during viewing and manipulation.

We also tried to improve the Vector General display's refresh rate to increase the number of lines visible without flicker. By rearranging physical memory modules we gave the VG a dedicated memory and controller, hoping it would run faster by no longer sharing a memory controller with the PDP-11. No measurable improvement resulted, however, either because the display was already drawing lines as fast as it could, or because it still must contend with the PDP for the UNIBUS.

Subproject 6, Facilties and Design for GRIP- X. In order to solve a number of architectural and implementation problems inherent in the current system, we plan a complete ground-up redesign of the system to be called GRIP-80. The major design objective for this system are:

Architecture

GRIP-80 will retain all functions which have been proved useful in GRIP-75, but some functions may be provided in a new form.

The mathematical model of a molecule will be an abstract linear graph which corresponds more nearly to the physical structures than the tree data structures used in GRIP-75.

On-line modification of molecular constituents and connectivity will be possible.

If technically feasible, real-time zoom and pan of the view area will be provided.

The display of electron density data by means of contour maps will be supplemented by a technique for marking the peaks and ridges of high electron density.

A facility for displaying the surface of a molecule as an opaque shaded colored object will be provided but not the real-time animation of such pictures.

Many of the input devices of GRIP-75 will be replaced by a single locator device, probably a data tablet. This will improve the tactile continuity of the GRIP man-machine interface.

Commands in GRIP-80 will be specified in prefix order, i.e., operation followed by operands.

The system will be able to prompt the user to guide him through the specification of the operands required by an operation. A description of the function of each verb will also be available to the user at the work station.

The system will distinguish among several types of objects (e.g., atoms, bonds, angles, residues, and peptide units) and will require the user to specify the appropriate type of object for each operand.

The system will store sets of parameters called profiles for controlling display, contouring, manipulation and optimization operations. The user can call these up as needed.

A quick, easy means will be provided for adding new function to the system.

Generalized tools for constrained manipulation will be provided which enable the user to change any aspect of the molecular geometry while holding other features fixed.

The scope of the system will be enlarged by bringing in more types of application data and functions. For example,

structure factors, hydrogen bonds, R-factor calculation and optimization, and minimization of the potential energy associated with a structure.

Implementation

Two implementations of GRIP-80 are planned, one in the Department of Computer Science at UNC and one in the IBM/UK Scientific Center in Winchester, England. These implementations will be based on different hardware configurations thus assuring a degree of hardware independence.

In both these systems more functions will be implemented on the dedicated satellite computer than with GRIP-75. In particular all command interpretation and execution of all trival and frequently invoked functions will be done by the satellite computer. A user's data and his private extensions of the system function will be stored on a private disk pack which will be mounted on a drive near the work station.

The Decade Ahead -- Why Work on Molecular Graphics?

Since Drs. Wright and Brooks have each embarked on a project that assumes that the molecular structure application is an area of vast potential payoff for computer graphics in the decade ahead, it is fair to ask why we think so. Is there indeed a future for molecular graphics research? Why work on molecules instead of any of the other exciting applications of computer graphics? Why should those who support molecular studies support graphics work instead of any of the other exciting developments in data taking and analysis?

From the point of view of the computer graphics researcher, the molecular application has very high potential for many years.

First, the application is important. The structures of proteins and nucleic acids must be understood if the functions are to be understood, and the functions lie at the heart of all life processes.

Second, the molecular structure problem is inherently a visualization problem. Hence computer graphics are inherently promising.

Third, the molecular structure problem is inherently three-dimensional. The structure must be perceived and understood as a geometric object in space. Moreover, molecules have structures that are "completely" three-dimensional, in contrast with most man-made objects that were designed from two-dimensional views. Visualizing such structures will require many and subtle techniques of illusion; only computerized graphics have the logical power such require.

Fourth, both the fitting of molecule models to data and the study of the action of molecules requires models that are flexible and easily moved and changed. Of all graphic media, only computerized graphics offers this flexibility.

Fifth, the molecular structure problem requires mathematical manipulation. Only computer graphics yields representations which can be immediately subjected to algorithmic processes whose results in turn are immediately displayed.

Sixth, the molecular structure problems for biochemical macromolecules are very hard, requiring the powerful pattern-recognition and information-retrieval capabilities of the human brain for the foreseeable future. There is little chance that purely algorithmic methods will get very far. Hence computer graphics will be needed to transduce visualizations into the human head and to transduce manipulations from the human hand back into the mathematical model.

All of these reasons illustrate why the potential usefulness of computer graphics will be great in the molecular structure application for some time to come. The application of graphics is not limited to fitting X-ray density maps. Crystal packing, molecular dynamics, active-site deformation, docking, folding -- all of these are distinct and important applications for computer graphics in molecular studies.

Merely to list those applications answers the last question: Has all the important work already been done? Now that many crystallographic centers have minicomputer-based computer graphics systems for density fitting, why keep working on fancier systems? In fact, the most powerful of today's systems merely begin to address the density-fitting problem. Most of those other applications have hardly been attacked at all. Certainly no system provides an integrated attack on all of the geometric problems of molecule structure and action. So there is

plenty of exciting work to keep us busy for a decade, without beginning to exhaust the molecule structure and action problems.

B. HIGHLIGHTS

1. Superoxide Dismutase Structure Determined

The structure of the active site of the superoxide dismutase molecule was determined by the team of Richardson, Richardson, Getzoff, and Tainer of Duke University.

How it was done. The Richardson team used GRIP-75 to manually fit a model of SOD to an experimentally determined electron density map. Computer graphics enabled them to fit the entire crystal structure of four subunits, totalling about 5000 atoms, to superimpose these four subunits, and then to arbitrate apparent differences among them.

On-line idealization, on-line checking of bond lengths and angles, on-line display of Ramachandran plots all aided the work considerably.

The quality of the map was then improved by refinement at Wayne Hendrickson's lab, using a process that is highly sensitive to the quality of the initial fit. The resulting map is good enough to resolve long-standing questions about how groups of atoms in the active site are associated.

What it means. SOD neutralizes destructive superoxide radicals which arise from normal metabolism, and it converts them to harmless oxygen and peroxide. Some people suffer from anemia when a lack of SOD allows superoxide to build upand attack cell walls. Researchers have tried for years to synthesize molecules that act like SOD. Perhaps now that the structure of the active site is known, its method of action can be deduced well enough to illumine these efforts at synthesis.

2. Smooth Kinetic Motion Found to be the Most Helpful Depth Cue in Molecular Graphics.

James S. Lipscomb of the University of North Carolina Department of Computer Science found that the kinetic depth effect is the single best depth cue for graphic displays of 3-D objects such as molecules. Surprisingly, it is more powerful perception aid even than stereopsis, the display of different images to each eye.

Lipscomb found that the kinetic depth effect achieves its full power only if the rocking or rotation of the image appears smooth to the viewer. It has been known for some time that this requires very frequent (about 12 times per second) updates to the displayed image. Lipscomb discovered that this is not sufficient: the illusion of smooth motion also requires that image updating and image refreshing be synchronized, and best effects are achieved when there is one update per refresh.

These results will be useful not only to computer graphics workers everywhere, but also to the designers of medical image display systems.

3. (In progress) GRIP-75 System Proves Useful for Nucleic Acid Studies

Many computer graphics systems for molecular studies are designed for handling chiefly protein molecules. Some such systems are implemented on minicomputers where memory size or computer speed makes the handling of very large biological macromolecules impractical.

Since GRIP-75 uses a large computer and a large memory region (384 kilobytes), it is capable of handling not only proteins but also the large nucleic acid molecules. For this reason it continues to attract clients studying these large molecules. Sung-Hou Kim, of the UC-San Francisco Medical School and formerly of Duke, completed during 1979 the structure determination of Yeast phenalaninetRNA. His results included the atomic coodinates of about 3000 atoms, deposited in the National Protein Data Bank, and an elucidation of the interaction of the nucleic acid with protamine.

Other researchers who have used the GRIP-75 system for nucleic acid studies include:

1977 H.T. Wright, Princeton; Glycone tRNA
1978 A. Podjarny, R. Scheritz, Chicago; FMET tRNA
1979 A. Rich, N. Woo, MIT; Initiator tRNA
1979 S. Premilat, U. Nancy; DNA
1979 C. Carter, R. Jones, UNC; Supercoiled DNA

These nucleic acid structures carry the genetic blueprint for all of life, or they decode the blueprint and use itsinformation to control body growth processes.

C. ADVISORY COMMITTEE AND ALLOCATION OF RESOURCES

We currently offer the GRIP-75 facility, and such help as we can give, free of charge to any chemist:

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

We have extended this offer publicly on many occasions. So far, we have had as many users as we have been able to handle.

All service projects were health-related, and we charged none of our clients for their use of the system. All local user groups (Duke and UNC), however, paid the UNC Computation Center directly for some batch processing of their data and its storage in our host computer. These direct payments to the Computation Center are not included in the financial data in this report.

Advisory Committee Members

Name	Degree	Title	Department	Institution
F. P. Brooks	Ph.D.	UNC-CH Kenan Professor & Chairman	Computer Science	
J. Hermans	Ph.D.	Professor	Biochemistry	UNC-CH
D. Richardson	Ph.D.	Professor	Biochemistry	Duke U.
J. Richardson	M.S.	Assistant Professor	Anatomy	Duke U.
W. V. Wright	Ph.D.	Senior Systems Architect	UK Science Centre	IBM England

D. DISSEMINATION OF INFORMATION

During 1979 we made no effort at publicizing the resource's availability because of our limited capacity to increase our service level. There was one substantial exception. We demonstrated the system to the biochemists, chemists, and crystallographers attending the Southeastern Crystallography Society Conference at Duke University.

Some 43 hours of resource time were used in demonstrations. During 1979 we also demonstrated GRIP to the following computer scientists, plus a few others.

Dr. Gene Amdahl	Amdahl Corporation
Mr. Peter D. Atkinson	IBM UK Science Centre, England
Dr. William Roy Baker, Jr.	National Institutes of Health
Mr. S. Balasubramanian	Shell Oil Corporation
Mr. Charles Brack	Evans & Sutherland
Prof. Richard Conway	Cornell University
Dr. Bob Englemore	Defense Adv. Res. Proj. Agency
Prof. Edward Feigenbaum	Stanford University
Mr. John Gillett	IBM UK Science Centre, England
Mr. David E. Haynes	University of North Carolina
Dr. P. Jerome Kilpatrick	IBM Office Products Division
Mr. J. Kuehler	IBM Systems Communication Div.
Mr. Lavigna	Bolt, Beranek and Newman
Prof. Eugene Long, Jr.	University of North Carolina

Mr. Kenneth G. Pauwels	University of North Carolina
Dr. Lawrence Sher	Bolt, Beranek & Newman
Prof. Thomas S. Wallsten	University of North Carolina
Dr. Peter Woon	IBM Office Products Division

E. CRITICISMS OR SUGGESTIONS

From the point of view of this resource, we have had much encouragement from the NIH office with whom we work. The chief difficulty we have encountered has been a rather erratic fluctuation in support. This can best be seen by examining the going rate of operating budget (excluding equipment) support for our project over the past six years:

Year	Period	Going Rate (dollars/year)
01	74-75	$ 75 K
02	75-76	$ 75 K
03	76-77	$ 51 K
04	77-78	$ 90 K
05	78-79 May-Nov (7 mo.)	$ 51 K
	Dec-Apr (5 mo.)	$144 K
06	79-80 May-Nov (7 mo.)	$109 K
	Dec-Apr (5 mo.)	$170 K

As one might imagine, this sort of fluctuation in the operating (mostly staffing) budget has meant an alternation between feast and famine. To the extent that we have staffed with graduate assistants, it has caused fluctuation in the number at work. Twice we have had to lay off permanent staff people because of budget fluctuations, only to seek replacements for them in a year or so. Stability and smoothness of funding support would help the project a great deal, and make it possible for the Principal Investigator to spend less time on budgetary worries.

PART II, SECTION A — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative, Research and Service, and Training. Check one of following:

[X] CORE RESEARCH AND DEVELOPMENT [ ] COLLABORATIVE RESEARCH AND SERVICE [ ] TRAINING

1 Descriptive Title (53 characters) Abstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor: Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
1. Three-dimensional cues for molecular display A variety of techniques for enhancing 3-D perception of molecules and density maps displayed on a 2-D screen were studied experimentally. The kinetic depth effect is the best depth cue, stronger than stereopsis.	16a	52	Brooks; J.S. Lipscomb	All: Computer Graphics System	19	1292	12063
2. Varifocal mirror 3-D display A varifocal mirror using multiple projectors was investigated as a technique for 3-D display of image spaces. A running model has been built; a better one will be.	16a	52	Fuchs; J.S. Cohen		28	376	3510
			All: Department of Computer Science, UNC				
SUB-TOTALS: No. of Subprojects							

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

PART II, SECTION A CONTINUED — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative, Research and Service, and Training. Check one of following:

[X] CORE RESEARCH AND DEVELOPMENT [ ] COLLABORATIVE RESEARCH AND SERVICE [ ] TRAINING

1 Descriptive Title (53 characters) Abstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
6. Hardware-software facility for GRIP-X We specified hardware and constructed software tools for the next-generation GRIP-X molecular graphics facility.	-	52	Brooks, Fuchs; M.K. Smotherman, M.T. Cronin, F.L. Brown, Jr. b. All: Dept. of Comp. Sci., UNC	All: Computer Graphics System	34	1167	238047
SUB-TOTALS: No. of Subprojects	6				345	5425	277800

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

PART II, SECTION A CONTINUED — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative Research and Service, and Training. Check one of following:

[X] CORE RESEARCH AND DEVELOPMENT [ ] COLLABORATIVE RESEARCH AND SERVICE [ ] TRAINING

1 Descriptive Title (53 characters) Abstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor: Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
3. Data-tablet as manipulation specifier Biochemists fitting molecules to maps mostly move segments parallel to the plane of the screen. We studied the gains and losses of constraining all manipulations to be parallel to the screen plane.	16	52	Brooks; D. Voss	All: Computer Graphics System	91	548	5116
4. Ridge-line techniques for initial fit to densities Computer graphics have not yet been successfully used for the initial interpretation of density maps. Ridge-line techniques and graph algorithms are being investigated for this purpose.	-	52	Brooks; T.V. Williams		67	750	7001
5. New version of GRIP-75 A new version of GRIP-75, embodying many small improvements and fixes was integrated, tested, and made the production system.	-	52	Brooks; M.E. Pique b. All: Department of Computer Science, UNC		106	1292	12063
SUB-TOTALS: No. of Subprojects							

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

PART II, SECTION A — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr.30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative/Research and Service, and Training. Check one of following:

☐ CORE RESEARCH AND DEVELOPMENT ☒ COLLABORATIVE RESEARCH AND SERVICE ☐ TRAINING

1 Descriptive Title (53 characters) Abstract Abstracts not available for our users' subprojects.	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
1. Scorpion Venom Toxin	5	36c	Charles Bugg; R. Almassy, J. Fontecilla Dental Research Institute University of Alabama-Birmingham	All: Computer Graphics System	39	222	2813
2. High Potention Iron Sulfur Protein	-	36c	Charles W. Carter; R.A. Jones Biochemistry, UNC-CH Sponsor: NIH GM-21991		5	20	299
3. Myohemerythrin	4	36c	Wayne A. Henrickson Structure of Matter Laboratory, Naval Research Laboratory Sponsor: NRL Internal Project		34	133	1987
4. Neurotoxin/Rubredoxin	5	36c	Jan Hermans Biochemistry, UNC-CH Sponsor: PCM 76-22723		11	43	642
SUB-TOTALS: No. of Subprojects							

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used
See Instructions, Page 4-6.

PART II, SECTION A (CONTINUED) — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative/Research and Service, and Training. Check one of following:

☐ CORE RESEARCH AND DEVELOPMENT ☒ COLLABORATIVE RESEARCH AND SERVICE ☐ TRAINING

1 Descriptive Title (53 characters) Abstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor: Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
5. Phenylalanine tRNA	23	36d	Sung-Hou Kim; S.R. Holbrook, W. Shin, C.J. Alden Biochemistry Duke University Sponsor: NIH CA-15802 NSF GB-40814	All: Computer Graphics System	49	192	2868
6. Erabatoxin	5	36c	Barbara Low; M. Kimball Biochemistry Columbia University Sponsor: NIH NS-07747		65	254	3795
7. Tobacco Bushy Stunt Virus	22	36c	M. Olson National Resource for Computational Chemistry University of California-Berkeley Sponsor: NRCC Internal Project		20	114	1444
8. Alternating-coil models for DNA	-	36d	S. Premilat University de Nancy		24	137	1734
SUB-TOTALS: No. of Subprojects							

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

PART II, SECTION A (CONTINUED) — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 INST: UNC

Fill out a separate Subproject Form for Core, Collaborative/Research and Service, and Training. Check one of following:

☐ CORE RESEARCH AND DEVELOPMENT ☐ COLLABORATIVE RESEARCH AND SERVICE ☐ TRAINING

1 Descriptive Title (53 characters) Abstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor: Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
9. E. coli Initiator tRNA	23	36d	Alexander Rich; N. Woo Biology Department M.I.T. Sponsor: NIH CA04186-22		78	444	5627
10. Superoxide Dismutase	-	36c	David C. Richardson; J.S. Richardson, E.D. Getzoff, J.A. Tainer Biochemistry Duke University Sponsor: NIH GM-15000		384	506	14797
11. Immunoglobin Dob	9	36c	Raghupathy Sarma; A. Landin Biochemistry SUNY - Stony Brook Sponsor: NIH 5R01-CA2504807		188	1072	13574
12. Mcg Bence-Jones	-	36c	Marianne Schiffer Biological & Medical Research Argonne National Laboratory Sponsor: Argonne Internal Project		26	148	1875
SUB-TOTALS: No. of Subprojects							

1/ Identify Resource Technology Used

2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

PART II, SECTION A (CONTINUED) — DRR SCIENTIFIC SUBPROJECT FORM

GRANT NUMBER P41RR00898-06 — REPORT PERIOD: May 1, 1979 TO Apr. 30, 1980 — INST: UNC

Fill out a separate Subproject Form for Core, Collaborative/Research and Service, and Training. Check one of following:

☐ CORE RESEARCH AND DEVELOPMENT ☒ COLLABORATIVE RESEARCH AND SERVICE ☐ TRAINING

1 Descriptive Title (53 characters) bstract	2 Science Code Anat.	Path.	3 (a) Investigator(s) (b) Department (c) Non-Host Institution	4 Usage Factor Resource Technologies 1/	Hours Used 2/	Resource Staff Hours	5 BRP Funds Allocated
13. Ribonuclease-S	-	36d	Hope C. Taylor Berkeley Springs Research Consortium Berkeley Springs, West Virginia Sponsor: NIH Contract 263-MD-900751		89	506	6413
14. Glycine tRNA	-	36d	H.T. Wright Frick Laboratory Princeton University Sponsor: NIH GM-23598		96	546	6920
SUB-TOTALS: No. of Subprojects	14				1108	4337	64788

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used

See Instructions, Page 4-6.

RT II, SECTION B GRANT NUMBER P 4 1 R R 0 0 8 9 8 — 0 6

INVESTIGATORS WITH OTHER SOURCES OF SUPPORT DIRECTLY RELATED TO PROJECTS LISTED IN PART II, SECTION A

Fill out a separate form for each of the following categories: Check one

☐ CORE RESEARCH & DEVELOPMENT ☒ COLLABORATIVE RESEARCH & SERVICE ☐ TRAINING

1. Last Name, First Middle 2. Institution ONLY If Non-Host Inst.	3. Sources of Support (Other than this grant) (a) Type	(b) Agency Abrev.	(c) Grant/Contract Number	(d) Funds
BUGG, Charles University of Alabama	FED FED	NIH NIH	CA-13148 DE-02670	
CARTER, Charles W.	FED	NIH	GM-21991	
HENDRICKSON, Wayne A. Naval Research Laboratory	FED	DOD	NRL Internal Project	Not available
HERMANS, Jan	FED	NSF	PCM 76-22723	
KIM, Sung-Hou Duke University	FED FED	NIH NSF	CA-15802 GB-40814	
LOW, Barbara Columbia University	FED	NIH	NS-07747	
OLSON, Arthur National Resource for Computational Chemistry	FED	NSF	NRCC Internal Project	Not available
RICH, Alexander M.I.T.	FED	NIH	CA04186-22	
RICHARDSON, David C. Duke University	FED	NIH	GM-15000	
SARMA, Raghupathy SUNY, Stony Brooks	FED	NIH	5R01-CA2504807	
SCHIFFER, Marianne Argonne National Laboratory	FED	DOE	Argonne Internal Project	Not available
TAYLOR, Hope C. Berkeley Springs Research Consortium	FED	NIH	263-MD-900751	
WRIGHT, H. T.	FED	NIH	GM-23598	

4. Total Number of Investigators	13	5. Total Other Support	
(a) This Page		(a) This Page	
(b) Cumulative Total		(b) Cumulative Total	

See Instructions, Pages 6-9.

RT II, SECTION C	GRANT NUMBER	P	4	1	R	R	0	0	8	9	8	—	0	6
INSTITUTION	REPORT PERIOD						TO							

Fill out a separate form for each of the following categories: Check one

☒ CORE RESEARCH & DEVELOPMENT ☐ COLLABORATIVE RESEARCH & SERVICE ☐ TRAINING

Number Published:	BOOKS	0	PAPERS	2	ABSTRACTS	0	
Number IN Press	BOOKS		PAPERS		ABSTRACTS		

Author(s) — Title of Article, Journal, Volume, Number, Pages (e.g., 44-48), Year Published

* Lipscomb, J. S., "Three-dimensional Display of Molecular Models," M.S. Thesis, University of North Carolina, Chapel Hill, North Carolina, 1979.

* Lipscomb, J. S., Three-dimensional Cues for a Molecular Computer Graphics System, Department of Computer Science Technical Report #TR79-008, University of North Carolina, Chapel Hill, North Carolina, 1979.

Indicate by an asterisk (*) that the resource was given credit.

See Instructions, Page 8.

RT II, SECTION C	GRANT NUMBER	P	4	1	R	R	0	0	8	9	8	—	0	6

INSTITUTION UNC - Chapel Hill REPORT PERIOD May 1, 1979 TO April 30, 1980

Fill out a separate form for each of the following categories: Check one

☐ CORE RESEARCH & DEVELOPMENT ☒ COLLABORATIVE RESEARCH & SERVICE ☐ TRAINING

Number Published:	BOOKS	0	PAPERS	5	ABSTRACTS	1	
Number IN Press	BOOKS		PAPERS		ABSTRACTS		

Author(s) — Title of Article, Journal, Volume, Number, Pages (e.g., 44-48), Year Published

* Ferro, D. R., McQueen, J. E., Jr., McCown, J. T., and Hermans, J., 1980: "Energy Minimizations of Rubredoxin," J. Mol. Biol., 136: 1.

* Girling, R. L., Houston, T. E., Schmidt, W. C., Jr., and Amma, E. L., 1980: "Macromolecular Structure Refinement by Restrained Least Squares and Interactive Graphics as Applied to Sickling Deer Type III Hemoglobin," (abstract), Acta. Cryst., A36: 43.

* Girling, R. L., Houston, T. E., Schmidt, W. C., Jr., and Amma, E. L., 1979: "Molecular Packing and Intermolecular Context of Sickling Deer Type III Hemoglobin," J. Molecular Biology, 131: 417-433.

* Kimball, M. R., Sato, A., Richardson, J. S., Rosen, L. S., and Low, B. W., 1979: "Molecular Conformation of Erabutoxin b; Atomic Coordinates at 2.5 A Resolution," Biochemical and Biophysical Research Communications, 88 (3): 950-959 (13 June).

* Schevitz, R. W., Podjarny, A. D., Krishnamachari, N., Hughes, J. J., Siglar, P. B., and Sussman, J. L., 1979: "Crystal Structure of a Eukaryotic Initiator tRNA," Nature, 278 (5700): 188-190 (8 March).

* Tsernoglou, D., Petsko, G. A., Hudson, R. A., 1977: "Structure and Function of Snake Venom Curarimimetric Neurotoxins," Molecular Pharmacology, 14: 710-716.

Indicate by an asterisk (*) that the resource was given credit.

See Instructions, Page 8.

PART III --- PROGRAM SPECIFIC DATA FOR BIOTECHNOLOGY RESOURCES PROGRAM

GRANT NUMBER P 4 1 R R 0 0 8 9 8 — 0 6 REPORT PERIOD May 1 1979 TO: April 30, 1980

SECTION A RESOURCE SUMMARY TABLE BIOTECHNOLOGY RESOURCES

RESOURCE COMPONENT	1 Number Subproj	2 Number Publica	3 Number Investigators	4 Usage Factor: Resource Technologies 1/	Hours Used 2/	Resource Staff Hrs	5 BRP Funds Allocated $	6 Resource Fees ($) Collected	7 Other Funds $
CORE RESEARCH & DEVELOPMENT				All: Computer Graphics System					
TOTAL:	6	2	1½	"	345	5425	277800	0	0
COLLABORATIVE RESEARCH & SERVICE									
TOTAL:	14	6	27**	"	1108	4337	64788	0	0
TRAINING									
TOTAL:	0	0	0	X	0	0	0	0	0
ADMIN/MISC									
TOTAL:			½	"	43	1420	14104		
DOWN TIME									
TOTAL:				"	(288*)	X	X		
GRAND TOTALS:			29	"	1496	11182	356692	0	0

* 12 24-hour days, not included in grand total, which is hours operated.

** 1 from GRIP team. The clients represented 14 principal investigators.

1/ Identify Resource Technology Used
2/ Give Hours Resource Technology Used
See Instructions, Page 9.

RT III, PROGRAM SPECIFIC DATA — BIOTECHNOLOGY RESOURCES PROGRAM

GRANT NUMBER P41RR00898-06

SECTION B RESOURCE PERSONNEL

NAME	POSITION	% of TIME or EFFORT			
		CURRENT BUDGET PERIOD		NEXT BUDGET PERIOD	
		Percent	Weeks	Percent	Weeks
Brooks, Jr., F.P.	Principal Investigator	25	52	33	52
Fuchs, H.	Senior Investigator	40	9	22	52
Leonarz, J.E.	Acting Resource Director	52	9	0	0
Brown, Jr., F.L.	Research Assistant	100	13	0	0
Cohen, J.S.	" "	100	7	0	0
Lipscomb, J.S.	" "	63	49	63	52
Pique, M.E.	" "	63	49	100	52
Voss, D.	" "	100	13	0	0
Wakabayashi, A.	" "	100	10	0	0
Williams, T.V.	" "	73	49	63	52
Hoffman, D.M.	" "	50	36	63	52 ?
Holmes, D.H.	" "	45	36	63	52 ?
Lumsden, M.W.	" "	13	6	0	0
Seaver, T.	" "	50	36	63	52 ?
Smotherman, M.K.	" "	13	36	0	0
Cronin, M.T.	" "	50	18	0	0
Middleton, D.J.	" "	50	18	0	0 ?
Stancil, P.	Electronics Engineer	100	11	100	52
Cuthrell, D.	Secretary (part-time)	50	17	0	0
Sams, J.	Secretary	100	20	100	52
Prevatte, L. } Ingram, T.	Student Assistant	10	34	0	0

SECTION C RESOURCE EXPENDITURES

TOTAL COSTS

BRP ALLOCATIONS			TOTAL RESOURCE EXPENDITURES		
BUDGET PERIOD			BUDGET PERIOD		
ACTUAL PREVIOUS	CURRENT	ESTIMATED NEXT	ACTUAL PREVIOUS	CURRENT	ESTIMATED NEXT
-05	-06	-07	-05	-06	-07
$ 127,582	$ 358,493	$ 241,226	$ 127,582	$ 356,692	$ 241,226

See Instructions, Page 9.