DEPARTMENT OF HEALTH AND HUMAN SERVICES
PUBLIC HEALTH SERVICE
NATIONAL INSTITUTES OF HEALTH

NATIONAL CENTER FOR RESEARCH RESOURCES
BIOMEDICAL RESEARCH TECHNOLOGY PROGRAM

ANNUAL PROGRESS REPORT

1. PHS GRANT NUIMBER: P41 RR02170-16

2. NAME OF RECIPIENT INSTITUTION:
   UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL

3. HEALTH PROFESSIONAL SCHOOL: DEPARTMENT OF COMPUTER SCIENCE

4. REPORTING PERIOD:
   A. FROM MAY 15, 1999
   B. TO MAY 14, 2000

5. PRINCIPAL INVESTIGATOR:

   A. RUSSELL M. TAYLOR II

   B. TITLE: RESEARCH ASSISTANT PROFESSOR

   C. SIGNATURE:

6. DATE SIGNED: March 30, 2000

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10. WAS PATENT OR COPYRIGHT AWARDED THIS GRANT YEAR? NO.

11. TOTAL % EFFORT RELATED TO AIDS RESEARCH: 0%

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IIA. SUMMARY OF RESEARCH PROGRESS

Our Resource continues to provide tools that are as powerful and as versatile as contemporary computing technology can make them – tools that enable direct viewing of and interaction with real and simulated macromolecules, viruses, and cells. Virtual filters enable superposition and transformation of images in order to map them from the raw instrument data formats onto more natural and useful views. Computer graphics enables *direct visual comparisons* between a scientist's conception of an object (as seen in the mind's eye) and the object of study – either a model stored within a computer or a real, physical molecule scanned by a microscope. Haptic (force-feedback) display coupled to the microscope's tip enables *real-time exploration* of the properties of real and simulated objects, touching and moving them to feel how they respond. We continue our work to allow the scientist to pay great attention to the experiment and little to the tools, rapidly and easily chasing down "what if" scenarios as they present themselves.

In response to emerging opportunities and strong encouragement from our advisory board, we have shifted our focus over the current grant period from probing simulated molecules to probing real biomolecules and structures – enabling our collaborators to directly interact with and manipulate them and measure their properties. Our long experience with the simulation and visualization of macromolecules positions us well to merge this capability with our new direct manipulation capabilities to enable direct comparisons between theory and experiment.

We continue in our *trailblazer* role to investigate the usefulness of new instrumentation and techniques to biological scientists, inviting them to use our leading-edge facilities (both providing new capabilities for the scientists and honing the usefulness of our tools on actual problems). The winning ideas are then developed more fully, either spun off to obtain their own funding or made available commercially.

As always, we continue to explore advanced technology research and development in computer graphics--the close coupling of computers and their users.

The Resource has the following specific aims for the next year:

- Continue to bring cutting-edge devices, techniques, and research in computer science to bear on biomedical research;
  - Design and implement techniques which display models aligned in space with experimental results;
  - Continue to develop visualization and manipulation interfaces for a new probe microscope system that is capable of operating inside a living cell;
  - Develop techniques and algorithms required for a combined SEM/AFM optimized for the viewing and manipulation of biomolecules;
- Continue to advance the art of controlled SPM manipulation of biomolecules;
  - Work with our collaborators to develop techniques for AFM imaging in liquids;
  - Work with our collaborators to develop AFM tips optimized for the lifting and placement of biomolecules;
- Support our collaborators work to advance knowledge in:
  - base excision repair
  - mucociliary clearance for cystic fibrosis
  - microtubule mechanics within live cells

- – the infectivity pathway for adenovirus
- – mechanical and electrical properties of DNA
- – mechanical properties of fibrin
- – applying DNA to self-assembled circuitry;

- Continue our service to the national community through publication, the release of software, and hosting visiting scientists;
  - – Cooperate with the commercialization of the nanoManipulator system in order to provide a robust, supported system for use by biomedical researchers in their own laboratories;
  - – Continue training graduate and undergraduate students to work in multidisciplinary teams, exposing computer scientists to the wealth of biomedical applications;
  - – Continue outreach to K-12 students to increase their awareness of and excitement about cutting-edge biological science.
- Funded by the supplemental award, continue developing and evaluating telecollaboration technologies for distributed collaborative use of the nanoManipulator.

Summary of Progress on Controlled Manipulation with Scanning Probe Microscopes

- Instrumentation development
  - – Completed installation of an optical fluorescence microscope on our Explorer AFM.
  - – Constructed initial prototype for a new 3D force microscope
  - – Under separate funding, completed the installation of a combined SEM/AFM system.
- Multivariate visualization
  - – Conducted first-stage user studies on the two visual methods of data presentation and second-stage user studies on haptic presentation techniques.
  - – Completed the integration of the visual and haptic multivariate presentation methods into the nanoManipulator system.
- Developed new techniques as required supporting active areas of collaborators' research
  - – Implemented "force curve" measurements at specified locations or along lines on the surface.
  - – Implemented a prototype 3D tip control mode, with haptic feedback to the user.
- Other Progress
  - – Completed the previous year's goal of porting the nanoManipulator system to lower cost hardware. The system now runs well on a dual-processor PC with a $250 Nvidia GEForce graphics card, bringing it within a range that will allow it to be deployed as a visual-only system on a scientist's desk.

Next Year's Objectives for Controlled Manipulation with Scanning Probe Microscopes

- Instrumentation Development
- Develop and build an "optical tweezers" 3D force microscope that is capable of positioning and measuring a submicron bead within liquids. Provide haptic display of the data and control over the bead's position. Develop sparse volume-rendering techniques and scan algorithms to provide visualization.
- Develop automatic registration algorithms for data from the combined SEM/AFM. Develop real-time visualization (with SEM) of manipulation with an AFM tip. Implement direct 3D force mode within the combined instrument.
- Continue to develop new measurement and manipulation techniques as required by our collaborators' experiments.
- Overlay of model and experiment data
  - Develop and apply inverse Solvent-Accessible Surface algorithms to determine which parts of an AFM image are reliable and which are likely to be artifact. Trim away the parts of the surface that are likely to be artifact.
  - Develop methods to simultaneously display AFM scans and models of macromolecules (such as adenovirus particles, proteins, DNA and carbon nanotubes).
- Multivariate Visualization
  - Complete and report on user studies on the two visual methods of data presentation and second-stage user studies on haptic presentation techniques.

Summary of Progress on Evaluating Telecollaboration for Science

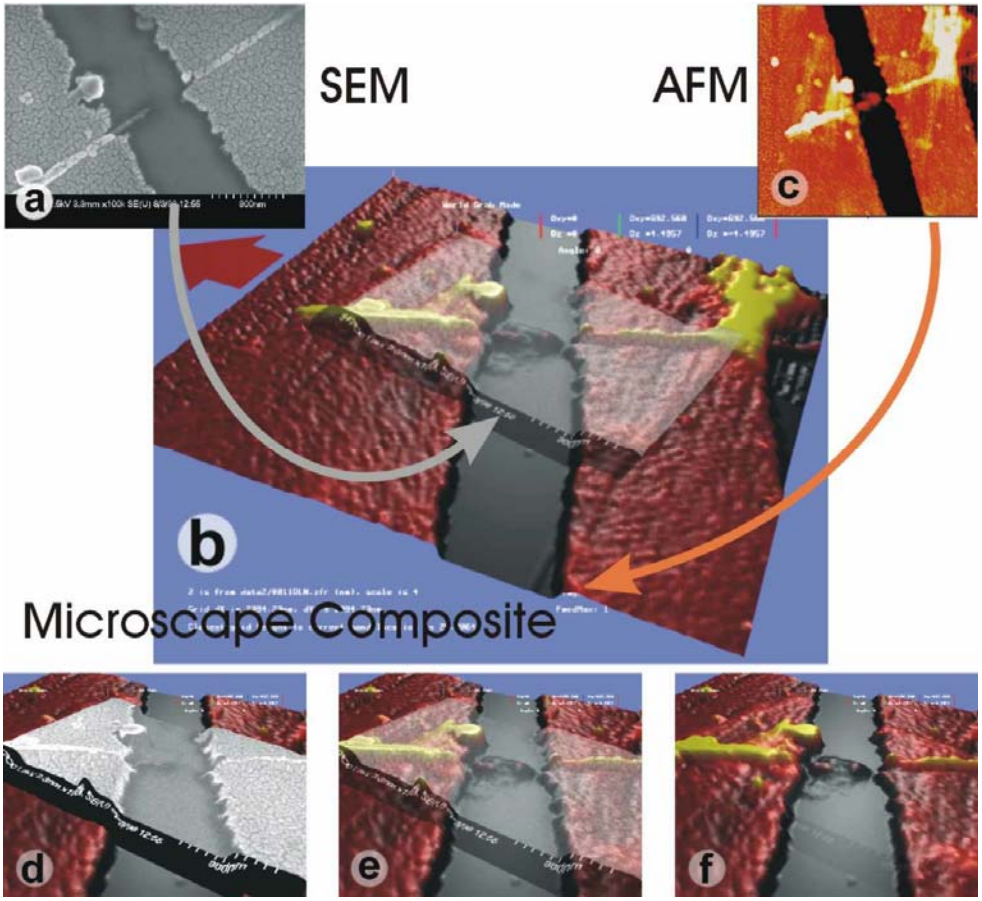
- System Components
  - Developed networking, microscope, and collaboration techniques and protocols that enable distributed control of the nM interface by two distributed users. We expect to enable 3 users and to control the live microscope by the end of Spring semester 2000.
  - We have completed installation of systems in Physics and Chemistry; hardware has been configured for Gene Therapy and bought (independently of the grant) at NIEHS. The latter two installations will be completed in April 2000.
- Prototype Demonstration
  - We performed a demonstration between UNC-CH and Washington, DC as part of the Internet 2 demos in April 1999.
- Networking
  - Devised and instrumented experiments on dedicated-service network to characterize network traffic and performance during live use of the system for collaboration. Measurements are being made concurrently with the telecollaboration evaluation study.
  - Began investigations of various network quality-of-service (QoS) improvement mechanisms.
- Evaluation of Telecollaboration
  - We have begun our study comparing results of face-to-face and distributed collaborations between undergraduate lab partners. This study is expanded in scope from the original proposal.
  - We continue gathering data by observation, questionnaire, and interviews with working, collaborating scientists.
- Other progress.
  - Formulated a theory of the design of distributed collaborative systems and reported it in a book chapter.
  - Completed a menu-based GUI for the reduced functionality nanoManipulator used for collaboration study.
  - Produced a user's manual for the reduced functionality nM and distributed collaboration tools for study.
  - Designed two laboratory experiments using the nM. These can be used as tutorials for new users.

Next year's plans for Evaluating Telecollaboration for Science

- System Components
  - Installations in Gene Therapy and at NIEHS
  - Complete user interface redesign of all 101-functions and user manual for all nanoManipulator functionality
  - Complete a user manual for the full set of nM functionality.
  - Refine system based on user feedback.

- Networking
  - Conduct experiments using the dedicated network to investigate tradeoffs among several alternatives for providing differing levels of quality of service (Q0S) to the data flows in the nanoManipulator system.
  - Provide network-related support for outreach projects with off-campus users of the nanoManipulator
- Evaluation of Distributed Collaboration for Science
  - Complete the formal study: run subjects, analyze data, and write up.
  - Continue collecting ethnographic data on distributed and local scientific collaborations.
  - Begin analysis of data collected via observations, interviews, and questionnaires.

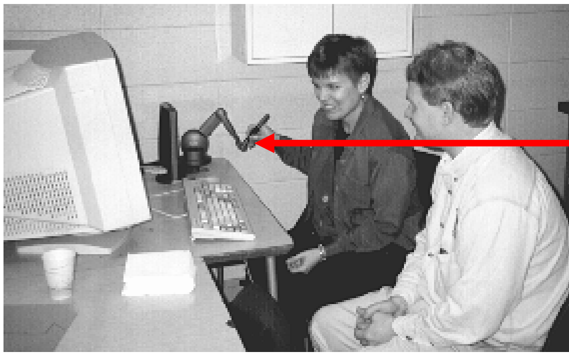
Highlight 1. New Microscopy Techniques

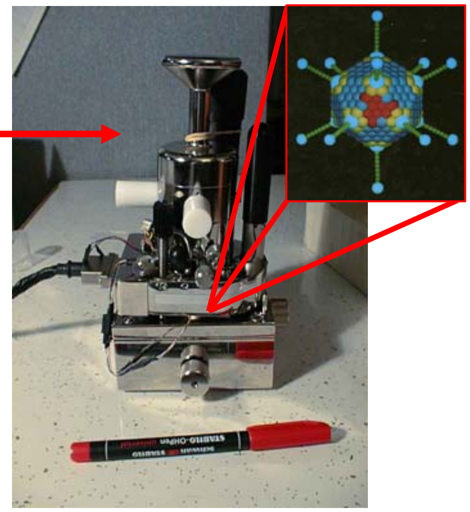


SEM/AFM. Our Resource has designed and built a prototype instance of a new form of microscope that combines a Scanning Electron Microscope (SEM) with an Atomic Force Microscope (AFM). This system, shown in the image to the left, allows the user to manually align and then overlay the data coming from the AFM (c) which gives direct but distorted measurements of topography with data from the SEM (a) which is capable of measuring material boundaries and tell which elements are present across the surface. The relative mixture of each displayed surface can be adjusted, as shown in (d)-(f), allowing the user to weight the visualization towards the technique of interest for a particular problem. The SEM and AFM are co-located and have been combined into a single virtual instrument; this allows viewing with SEM while manipulating the surface with AFM. This is particularly relevant when doing true 3D manipulations with *3D touch mode* (described next).

3D Touch Mode. The Resource has developed a technique that allows direct control of the tip of an AFM in all three motion directions (X, Y parallel to the surface and Z perpendicular to it), while still preventing damage to the tip or sample due to uncontrolled forces. This extends our earlier 2D+force control mode and allows both experimentation on more delicate samples and manipulation of objects in three dimensions (lifting them off the surface).

Highlight 2. Science Outreach at Orange High School Gives Proof-of-Concept for Teleoperation of the nanoManipulator





A nanoManipulator control and display system (graphics plus haptics) was taken to Orange High School for a second time in order to allow freshman and sophomore Biology classes to experience cutting-edge science. The students used the system across the Internet to touch and manipulate adeno virus particles located in an atomic force microscope 20+ miles away in the UNC-CH department of Physics and Astronomy.

This outreach project was the result of collaboration between Orange High School, the UNC School of Education, the Department of Computer Science (including the Research Resource), and the Department of Physics and Astronomy. The students were taken through a program of lectures, model building and hands-on operation of the AFM through the nanoManipulator interface. The students experienced first-hand the interdisciplinary nature of modern science and saw themselves as doing experiments that no one had ever done before. It included a study of the effectiveness of haptic feedback compared to visual-only feedback in teaching about virus morphology. It also supported the pre- and post- testing required to determine the effectiveness of the project in teaching students and in increasing their interest in science.

After this visit, the students wrote articles describing what they experienced. Here are some quotes from these articles: “When other people get to work with the nanomanipulator like we did, they will think about viruses and biology in a whole different way.” “When I pushed it into the virus it stopped, and I could actually feel the force like I was really touching it. That was awesome. I have never done anything like that before.” “When I compare it to labs and other working assignments, it was the best thing we have done here in our class ever.” “To put it in plain words, it was the trippiest experience I have ever had ... The fact that we knew that we were actually touching a live virus that was somewhere else was half the trip.” “I realized that I had really been fooled by a false stereotype of what a scientist had to look like. There were all different kinds of people here, of different ages as well as of different races.” “I thought when you went to do an experiment, you would just take your tools and do what ever it was you set out to do. Boy, was I wrong!” “In the course of a week, I have learned so much. Coming into this experiment we knew so little about viruses, and now we can describe their size, some of their characteristics, and how viruses infect you and make you sick. The visiting scientists have inspired me and so many others to join a field in science. They have lit a flame that cannot be put out. There are so many unanswered questions out there just looking for a solution. This experiment is just the beginning of a long line of discoveries.”

Highlight 3. Tools at Work: Science enabled by the nanoManipulator
Material properties of fibrin fibers, principal building blocks of blood clots

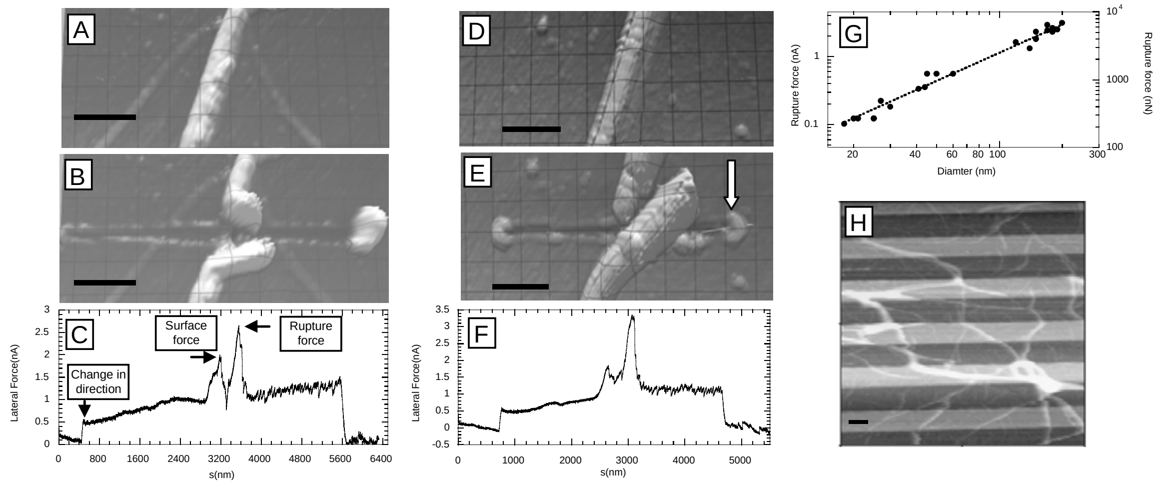


Fig. 1 Manipulation of fibrin. (A-C) Manipulation of fibrin fiber 1, (diameter: 150 nm) in ambient condition (C) Lateral force trace for manipulation of fiber 1. (D-F) Manipulation of fibrin fiber 2(diameter: 180 nm) in ambient conditions. (F) Lateral force trace for manipulation of fiber 2. (G) Rupture force vs. diameter of fiber (logarithmic scale). The deduced exponent is about 1.4. (H) Fibrin fibers on grid surface imaged in buffer. Scale bar in all images is 1 μm.

Fibrin fibers are the major structural component of blood clots. Thus, determining the strength and mechanical properties of blood clots may provide new insights into the wound healing process and will advance our understanding of heart attacks and strokes. In the study described here, the rupture force and mechanical properties of individual fibrin fibers are being measured (Fig. 1). Images of two typical manipulations of these fibers are shown in Fig 1 (A) & (B) and (D) & (E). (A) and (D) show the fibers before the manipulation during which a lateral force was applied to the fiber until it ruptured. Images (B) and (E) depict the fiber after the manipulation and (C) and (F) show the respective lateral force traces that were recorded during the manipulations. From such curves the rupture force and other mechanical properties of human fibrin were determined. In Fig. (G) it can be seen that the rupture force increases proportional to $R^{1.4}$, which might indicate that the inside of the fiber is inhomogeneous. Furthermore, the manipulation depicted in (D) and (E) suggests that the deformation in the fibrin fiber is - at least partially - elastic since the fiber moved back towards its straight configuration due to a restoring force. From several force curves a Young's modulus of about 0.4 GPa was estimated. The image in (H) shows fibrin fibers that were deposited onto a silicon grid (1 μm troughs and 2 μm wide and 100 nm tall ridges) and imaged in buffer (10 mM $CaCl_2$, 130mM NaCl, 20 mM Hepes, pH 7.4). The goal is to have fibers spanned over the troughs, so that the surface does not interfere with measurements on the fibers.

Future plans

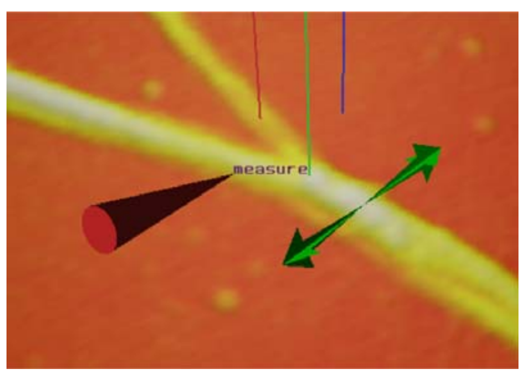
The goal of future studies over the next couple of years is to investigate the mechanical properties of wild-type and mutant fibrin fibers (e. g. from thrombic patients) and to test the effect of drugs and other factors on the properties of these fibers.

Highlight 4. Evaluating Telecollaboration for Science (Funded by Supplement)

We began our research by conducting an ethnographic study to develop an understanding of the scientific research process, current collaborative work practices, the role of a nM as a scientific instrument, scientists' motivation for multi-disciplinary collaboration across distances, and scientists' expectations regarding technology to support scientific collaborations across distances. This understanding suggests that collaborative scientific research in the nM context is cognitive work that is supported by social and physical activities, and our collaborative environment should support the cognitive work and its supporting, or enabling, social and physical activities. This is in comparison with other approaches that primarily support social interaction with the expectation that the social interaction will support cognitive work. The design was further guided by a synthesis of social awareness literature and our empirical data. This synthesis suggests that social awareness is comprised of contextual, situational and discrete levels of social awareness. Control, sensory and distraction factors appear to contribute to enhancing these levels of social awareness in a collaborative environment.

In addition to the traditional nM features that provide a 3-D visualization of a sample magnified by a factor of about a million to one and the ability to touch and modify a sample, the collaborative nM environment we designed includes: consistent shared and private work modes, or spaces; the ability to customise an individual view of a shared work space; the ability to switch between shared and private work modes; multiple cursors that show each collaborator's focus of attention and mode of operation simultaneously when in shared mode; audio communications; video conferencing that provides views of hand gestures and other physical objects scientists use during experiments in addition to facial views of collaborators; and shared access to data analysis tools and other applications that are used during the scientific process. The figure below shows that the remote collaborator (red cone) is in measure mode and the local collaborator (green arrows) is in zoom out mode as they examine a sample of fibrin fiber.

As part of our evaluation of telecollaboration we are performing a repeated measured factorial design experiment comparing scientific results generated in face-to-face settings and in telecollaborative settings. The pairs of participants work as lab partners and do one lab side-by-side and the other in separate rooms, using the collaborative tools. We will use the quality of their lab reports, as well as surveys, observations, and interview data to evaluate the effectiveness of our telecollaboration environment for science.



SUBPROJECT SUMMARY: PRIMARY AWARD

	Tech Research and Development(T)	Collab Research and Service (C)	Dissemination and Training (D)	Totals
Number of Publications	16	13	0	29
Number of Subprojects	10	6	5	21
Number of Investigators	17	11	14	42*
Percent of BRTP Funds Allocated	58%	23%	19%	100%
Percent of BRTP Funds Allocated for AIDS	0	0	0	0
Service Fees Collected	0	0	0	0
Other Funds ($)	0	0	0	0

*** A total of 27 investigators worked on the 21 primary subprojects. Several investigators worked on multiple projects within one (or more) of the categories.**

SUBPROJECT SUMMARY: SUPPLEMENTAL AWARD

	Tech Research and Development(T)	Collab Research and Service (C)	Dissemination and Training (D)	Totals
Number of Publications	6	0	0	6
Number of Subprojects	4	3	1	8
Number of Investigators	7	6	4	17*
Percent of BRTP Funds Allocated	74%	16%	10%	100%
Percent of BRTP Funds Allocated for AIDS	0	0	0	0
Service Fees Collected	0	0	0	0
Other Funds ($)	0	0	0	0

*** A total of 12 investigators worked on the 8 supplemental subprojects. Several investigators worked on multiple projects within one (or more) of the categories.**

GEOGRAPHICAL DATA: PRIMARY AWARD

State or Country	Number of Investigators
NC	21
CA	3
AZ	2
Belgium	1

GEOGRAPHICAL DATA: SUPPLEMENTAL AWARD

State or Country	Number of Investigators
NC*	12

* Includes two at NIEHS.

INVESTIGATOR SOURCES OF SUPPORT: PRIMARY AWARD

BRTP UNIT: T

Brooks, Frederick P., Jr.	Ph.D.	CS	UNC	FED	NIH, NSF, LLL
				SCCF	UNC-CH
Falvo, Mike	Ph.D.	Phy&Astron	UNC	FED	NSF
Guthold, Martin	Ph.D.	CS	UNC	FED	NIH
Healey, Chris	Ph.D.	CS	NCSU	OTH	Angelsstreet.com, Inc.
				SCCF	NCSU
Helser, Aron	MS	CS	UNC	FED	NIH, NSF
Hollins, Mark	PhD	Psych	UNC	FED	NSF, NIDR
				SCCF	UNC-CH
Jeffay, Kevin	Ph.D.	CS	UNC	IND	Cabletron
				SCCF	UNC-CH
				FED	NIH,NSF
Lin, Ming	PhD	CS	UNC	FED	NSR, USARO
				SCCF	UNC-CH
Manocha, Dinesh	PhD	CS	UNC	FED	NSF, USARO, DOE, ONR
				SCCF	UNC-CH
Pizer, Stephen	PhD	CS	UNC	FED	NSR, USARO
				SCCF	UNC-CH
Robinett, Warren	M.S.	CS	UNC	FED	NIH,NSF
Smith, F.D.	Ph.D.	CS	UNC	FDN	MCNC
				FED	NIH,NSF
Superfine, Richard	Ph.D.	Phy&Astron	UNC	FED	NIH,NSF,ONR,ARO
				SCCF	UNC-CH
Taylor, Russell M.	Ph.D.	CS	UNC	FED	NIH, NSF, ONR, ARO
Vicci, Leandra	BS	CS	UNC	SCCF	UNC-CH
Washburn, Sean	Ph.D.	Phy&Astron	UNC	FED	NSF,ONR, ARO,
Whitton, Mary C.	M.S.	CS	UNC	FED	NIH, LLL

INVESTIGATOR SOURCES OF SUPPORT: SUPPLEMENTAL AWARD

BRTP UNIT: T

Helser, Aron	MS	CS	UNC	FED	NIH, NSF
Jeffay, Kevin	Ph.D.	CS	UNC	IND	Cabletron
				SCCF	UNC-CH
				FED	NIH,NSF
Smith, F.D.	Ph.D.	CS	UNC	FDN	MCNC
				FED	NIH,NSF
Sonnenwald, D.H.	Ph.D.	ILS	UNC	FED	NIH,NSF
				SCCF	UNC-CH
				FDN	Howard Hughes Medical Ins
Superfine, Richard	Ph.D.	Phy&Astron	UNC	FED	NIH,NSF,ONR,ARO
				SCCF	UNC-CH
Taylor, Russell M.	Ph.D.	CS	UNC	FED	NIH, NSF, ONR, ARO
Whitton, Mary C.	M.S.	CS	UNC	FED	NIH, LLL

INVESTIGATOR SOURCES OF SUPPORT: PRIMARY AWARD

BRTP UNIT: C

Craig, Lisa	PhD		CALF	FND	Scripps
Erie, Dorothy	Ph.D.	Chemistry	UNC	FED	NIH,
				SCCF	UNC-CH
Falvo, Mike	Ph.D.	Phy&Astron	UNC	FED	NSF
Friedlander, Sheldon	PhD	ChemE	CALF	SCCF	UCLA
Guthold, Martin	Ph.D.	CS	UNC	FED	NIH
Lord, Susan	PhD	Pathology	UNC	FED	NIH
Superfine, Richard	Ph.D.	Phy&Astron	UNC	FED	NIH,NSF,ONR,ARO
				SCCF	UNC-CH
Tainer, John	PhD		CALF	FND	Scripps
Taylor, Russell M.	Ph.D.	CS	UNC	FED	NIH, NSF, ONR, ARO
Vicci, Leandra	BS	CS	UNC	SCCF	UNC-CH
Washburn, Sean	Ph.D.	Phy&Astron	UNC	FED	NSF,ONR, ARO,
				SCCF	UNC-CH

INVESTIGATORS SOURCES OF SUPPORT: SUPPLEMENTAL AWARD

BRPT UNIT: C

Erie, Dorothy	Ph.D.	Chemistry	UNC	FED	NIH,
				SCCF	UNC-CH
Guthold, Martin	Ph.D.	CS	UNC	FED	NIH
Kunkel, Thomas	PhD		NC	FED	NIEHS
Samulski, Jude	PhD	Gene Therapy	UNC	FED	NIH, LLL
				OTH	YALE
Superfine, Richard	Ph.D.	Phy&Astron	UNC	FED	NIH,NSF,ONR,ARO
				SCCF	UNC-CH
Wilson, Samuel	PhD		NC	FED	NIEHS

INVESTIGATOR SOURCES OF SUPPORT: PRIMARY AWARD

BRTP UNIT: D

Brooks, Frederick P., Jr.	Ph.D.	CS	UNC	FED	NIH, NSF, LLL
				SCCF	UNC-CH
de Shryver, Frans	Ph.D.		KU Leuven	OTH	Flemish Government
England, Nick	EE	CS	UNC	FED	NSF
Falvo, Mike	Ph.D.	Phy&Astron	UNC	FED	NSF
Helser, Aron	MS	CS	UNC	FED	NIH, NSF
Jeffay, Kevin	Ph.D.	CS	UNC	IND	Cabletron
				SCCF	UNC-CH
				FED	NIH,NSF
Jones, Gail	Ph.D.	Education	UNC	SCCF	UNC-CH
				OTH	Eisenhower Grant
Ramakrishna, B.L.	Ph.D.	Solid Science	ASU		
Razdan, Anshuman	Ph.D.	CS	ASU		
Smith, F.D.	Ph.D.	CS	UNC	FDN	MCNC
				FED	NIH,NSF
Superfine, Richard	Ph.D.	Phy&Astron	UNC	FED	NIH,NSF,ONR,ARO
				SCCF	UNC-CH
Taylor, Russell M.	Ph.D.	CS	UNC	FED	NIH, NSF, ONR, ARO
Washburn, Sean	Ph.D.	Phy&Astron	UNC	FED	NSF,ONR, ARO,
				SCCF	UNC-CH
Whitton, Mary C.	M.S.	CS	UNC	FED	NIH, LLL

INVESTIGATOR SOURCES OF SUPPORT: SUPPLEMENTAL AWARD

BRTP UNIT: D

Jeffay, Kevin	Ph.D.	CS	UNC	IND	Cabletron
				SCCF	UNC-CH
				FED	NIH,NSF
Smith, F.D.	Ph.D.	CS	UNC	FDN	MCNC
				FED	NIH,NSF
Taylor, Russell M.	Ph.D.	CS	UNC	FED	NIH, NSF, ONR, ARO
Whitton, Mary C.	M.S.	CS	UNC	FED	NIH, LLL

PUBLICATIONS: Primary Award

BRTP UNIT: T

NUMBER OF PUBLISHED -

BOOKS:	1 (chapter)	PAPERS:	12	ABSTRACTS:	0

NUMBER IN PRESS -

BOOKS:	0	PAPERS:	3	ABSTRACTS:	0

NUMBER IN REVIEW -

BOOKS:	0	PAPERS:	0	ABSTRACTS:	0

BOOK CHAPTERS PUBLISHED:

* R. M. Taylor II and R. Superfine. "Advanced Interfaces to Scanned-Probe Microscopes." Handbook of Nanostructured Materials and Nanotechnology, H. S. Nalwa, Ed. (Academic Press, San Diego). 2: 271-308 (1999).

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* D. Aliaga, J. Cohen, A. Wilson, E. Baker, H. Zhang, C. Erikson, K. Hoff, T. Hudson, W. Stuerzlinger, R. Bastos, M. Whitton, F. P. Brooks, Jr and D. Manocha. "MMR: An Interactive Massive Model Rendering System using Geometric and Image-Based Acceleration." Proceedings of ACM Symposium on Interactive 3D Graphics (Atlanta, GA, April 26-28, 1999), pp. 199-206, 237.

* R. Bastos, K. Hoff, W. Wynn and A. Lastra. "Increased Photorealism for Interactive Architectural Walkthroughs." Proceedings of ACM Symposium on Interactive 3D Graphics (Atlanta, GA, April 26-28, 1999), pp. 183-190, 235.

F. P. Brooks, Jr. "Fourteen Years of Interactive Walkthroughs." ACM SIGGRAPH 99 Course Notes, course #20. (Los Angeles, CA: ACM SIGGRAPH, 1999), pp. H1-H22.

F. P. Brooks, Jr. “What's Real About Virtual Reality?” IEEE Computer Graphics and Applications. 19(6) (Nov/Dec 1999): 16-27.

* C. Erikson and D. Manocha. "GAPS: General and Automatic Polygon Simplification." Proceedings of ACM Symposium on Interactive 3D Graphics (Atlanta, GA, 1999): 79-225.

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BRTP UNIT: C

NUMBER OF PUBLISHED -

BOOKS:	0	PAPERS:	4	ABSTRACTS:	4

NUMBER IN PRESS -

BOOKS:	0	PAPERS:	3	ABSTRACTS:	1

NUMBER IN REVIEW -

BOOKS:	0	PAPERS:	1	ABSTRACTS:	0

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PUBLICATIONS: Supplemental Award

BRTP UNIT: T

NUMBER OF PUBLISHED -

BOOKS:	0	PAPERS:	5	ABSTRACTS:	0

NUMBER IN PRESS -

BOOKS:	1 (chapter)	PAPERS:		ABSTRACTS:	0

NUMBER IN REVIEW -

BOOKS:	0	PAPERS:	0	ABSTRACTS:	0

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M. Clark and K. Jeffay. "Application-Level Measurements of Performance on the vBNS." Proceedings of IEEE International Conference on Multimedia Computing and Systems. Vol 2. (Florence, Italy, 1999): 362-366.

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* D. H. Sonnenwald, R. Bergquist, K. L. Maglaughlin, E. Kupstas Soo and M. C. Whitton. "Designing to Support Scientific Research Across Distances: The nanoManipulator Environment." To appear in Collaborative Virtual Environments. E. Churchill, D. Snowdon and A. Munro (Eds). (London: Springer Verlag, 2000).

III.F. Report of the Advisory Committee Meeting April 12, 1999

1.0 Nanomanipulator Advisory Board Report

April 12, 1999

The GRIP advisory committee is very impressed with the progress made in the last two years. The project leaders have assembled an excellent team of people who together posses the necessary combination of scientific background and technical expertise.

1.1 Specific Comments and Recommendations

1.2 Biology

To ensure the continued success of the nanomanipulator project, we find it absolutely necessary to continue pursuing high visibility biochemical/biological applications and attract more usage from biological scientists. The committee recommends that the team publicize the scientific advantages offered by the nanomanipulator in the domain of biological science. Toward this end we suggest:

1) Work towards the biological "killer app" of the nanomanipulator. The team should focus on understanding and controlling interactions between the tip and the sample so that biological molecules can be reliably picked up, moved, and put down in another location. This is a basic capability that will enable many experiments for which the nanomanipulator is uniquely suited. One carefully done experiment published in a leading journal will demonstrate the utility of the nanomanipulator for biology, biochemistry, and biophysics. Collaborations with biological AFM groups will be helpful for this purpose.
2) Aim to write at least two high profile journal publications in biology per year. We hope this goal will demonstrate the power and potential of the nanomanipulator in biology.
3) Bring in more external collaborators by using one or more of the following venues:
   - Organize a 1-2 day workshop. Invite current leaders in imaging technologies, such as David Agaard at UCSF, Mark Ellisman at UCSD, Steve Smith at Stanford, Scott Frasier at Caltech and demonstrate the powers of the nanomanipulator.
   - Make contact with people doing "single-molecule manipulation" experiments (Steve Block, Jeff Gelles, Jim Spudich, Carlos Bustamante, Herman Gaub, Paul Hansma, Ron Vale, David Bensimon, etc) and attend meetings where laser tweezers, AFM, single molecule fluorescence and other such methods are being presented. This community is likely to suggest the best applications, provide the best collaborations, and be most interested,.
   - Offer a course at Woods Hole or a Gordon Conference. These venues are commonly attended by biologists just for learning new techniques.

- Publish or demonstrate at one of the major biological meetings: Microscopy Society of America, Cell Biology Meetings, Society for Neuroscience

4) Add a section to the nanomanipulator web site that invites biologists to use the system. We suggest that you require a one-page proposal describing the science that will be done, and request a final report detailing the experience and the progress made. Make explicit that a biochemist postdoc is available for making the system work.

1.3 Material Science

The committee is very pleased with the progress in physics and material science applications. The two Nature publications on the bucky tube are a concrete metric of the success in this area. We look to these applications to deepen the understanding of tip-sample interactions and the measurement of forces involved. We encourage the development of surface technologies to allow the manipulation of biological samples, e.g. silicon-HMDS-silicon patterning.

1.4 Technology

We particularly like the level of integration between the AFM and the nanomanipulator interface. The committee is impressed that the software team does not try to reinvent every analysis package and integrate it into their system. We were especially pleased to see the improvements in the field of data visualization as recommended by the 1997 committee. The multiple data set visualization of bumps and dots is very effective and certainly not an expected result. We encourage the plan to combine the SEM and the AFM to allow manipulation with simultaneous imaging. The committee thought this was a particularly good idea.

There is a need to characterize the limitations of the instrument in the user interface. We feel it is crucial to understand how much of the image the user sees is due to instrument artifacts, visualization artifacts or molecular properties. Try to list the limits of the instrument (e.g. lowest measurable lateral force) and put them into relations that biologists understand, for example, normal force compared to binding strength of a hydrogen bond. Any information along these lines should be conveyed to the end user, preferably in the visual interface.

The 1997 advisory committee recommended adding another perception dimension to the topographical information (i.e. friction by audio). This item is reiterated here.

The nanomanipulator should provide more automatic manipulations. The team has a good start in that straight lines are now supported as recommended by the 1997 committee. We recommend that you continue investigating the use of macros to increase productivity. One application is Dorothy Erie's need to "herd" her DNA into close proximity to the proteins.

The committee is glad to see that investigating true XYZ control is listed in the future plans. This was a recommendation of the 1997 committee and is reiterated here.

Take advantage of newer developments/tricks in AFM technology, such as modified tips, electrical potentials between sample and tip, lateral modulation to vary friction in a controlled fashion.

1.5 Remote Control and Collaboration

Adding remote control capabilities to the nanomanipulator is a good plan for servicing the national community. We understand that this is a new endeavor and that you have funding to specifically accomplish this task. With that in mind, we list here some comments in the hope they will help jump-start your efforts.

We recommend continuing evaluation of remote application use, both for individual users and for multi-user, distributed, collaborative interactions. The committee feels that this evaluation should use multiple empirical and analytic methods with continuing consideration given to domain (i.e. biology), technology and user issues. Currently we are concerned that technological solutions are being considered and recommended without a justification of need or efficacy for the problems at hand i.e. because they can be done rather than that they should be done. To this end we recommend increasing the user centered design methods which the team have already begun to develop. In particular we recommend a better understanding of the work practices of domain experts, i.e. biological scientists. We see a need for a deeper understanding of (1) the nature of collaborations for the current research domains, and (2) the role of graphical and textual representations in individual and collaborative problem solving in these areas. With regard to (1), we feel it is necessary to know more than "who talks to who" - but also the nature and content of such interactions – to know how they talk to each other, what kinds of information are shared, how that information is shared, and the role of shared visualizations in the co-construction of results and understandings in this domain.

We advocate that the team supplements observational studies by focusing the planned experimental studies on developing an understanding of the effects of computer mediation on individual and collaborative activities in biology and scientific discourse. In particular, the evaluation team needs to do a thorough literature search on collaborative methods, technologies, and remote collaboration. We also recommend discussions with existing groups that have expertise in remote instrument control and collaboration. Examples are the DOE2000, Beckman Institute at UIUC, Scripps Institutes, Pacific Northwest Lab.

It is encouraging to see that the nanomanipulator has matured to the point of defining stable interface specifications between the major components. These interfaces need to be published and discussed among other groups active in remote instrument control, such as DOE200, Beckman Institute at UIUC, Scripps Institutes, and PNL. A set of existing interface specifications that have been proven by a large number of users is a key factor in getting manufacturers to begin offering these interfaces on their instruments.

The nanomanipulator project resources should be focused to allow the solidification of the system locally for the researchers at UNC and Triangle Park before moving to wide area networks. The interface specifications are an excellent first step in allowing large pieces of the nanomanipulator to be run in simulation instead of requiring the entire system be up and running to test any new software.

The use of networking simulation tools such as the *Network in a box* available from NIST will allow repeatable network experiments to be performed. This will facilitate the changes to the interfaces to be tested in isolation of any variability of the network.

1.6 Summary

The advisory committee is very impressed with the amount of progress that has been made in the last two years. The nanomanipulator team has taken a system that was barely working and made it usable, improved it, and gotten new scientists involved. We are particularly pleased that some biochemists are now actively pursuing research with the system, also we are impressed with the successfully funded spin-off projects such as Dorothy Erie's DNA repair.

The nanomanipulator team has done an excellent job of following the recommendations of the 1997 committee. Nearly all points have been investigated and/or implemented. We have reiterated the 1997 recommendations that we feel still need attention.

This report has listed many specific recommendations. This is due in part to the team's success in the last two years and it's growth along many different frontiers. But the committee would like to reemphasize the core recommendations:

1) Continue pursuing high visibility biological applications
2) Improve visibility of the resource, in particular as you move into your service phase
3) Communicate with other groups across the nation doing similar work.

Overall the nanomanipulator team has done an excellent job. Please continue the good work and keep focused on the mission of the research center.

IV. A. Allocation of Resources

Scientists engaged in work for which our systems are suitable and whose results will be made available to the scientific community and the general public are welcome to use the resources supported by this grant. Should the demand for our services exceed our capacity to work with the applicants, we will select those clients whose needs our systems will best serve. Our Advisory Committee helped us set this policy for resource allocation. We have been able to accommodate all requests during this reporting period.

We have been promoting the availability of the Resource through personal contact and announcement at various appropriate conferences. We have found that this is the most effective method of recruiting users. Our one-time placement of an advertisement resulted in no new users, so we are, in the budget for the coming year, requesting additional travel funds to allow attendance (and where possible demonstrations) at appropriate conferences and workshops.

Our **Research Resource Advisory Board,** as of last year representing scanning probe microscopy and telecollaboration experts, met last year on April 12, 1999. Their report is included in this document. The Board will meet this year in early May. In addition to the annual Board meeting, we met or conversed informally with several of the committee members on occasion during the year to discuss how to direct our system development and competitive renewal proposal efforts.

The members of the Resource Advisory Board who will meet in May 2000 include:

Ms. Rachel Brady, Chair
Beckman Institute, NCSA
Urbana, IL
rbrady@ncsa.uiuc.edu

Dr. Elizabeth Churchill
FX Palo Alto Laboratory
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Dr. Elizabeth Getzoff
The Scripps Research Institute
La Holla, CA
edg@scripps.edu

Mr. Mike Pique
The Scripps Research Institute
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mp@scripps.edu

Dr. Paul West
ThermoMicroscopes
Sunnyvale, CA
paulw@thermomicro.com

Dr. Stanley Williams (tentative)
UCLA Dept. of Chemistry & Biochemistry
Los Angeles, CA
williams@chem.ucla.edu

IV. B. Dissemination of Information

Our Resource disseminates our results and our systems through publication and presentations in journals and at conferences, through distribution of working software libraries and applications (some freely, others through technology transfer to commercial entities), through technology demonstrations at various technical and public venues, through our Web pages, through our organized local demonstrations to a wide range of visitors, and through the popular press.

Publications and Conferences. We are meeting the goals set by our advisory board of writing at least two journal publications in biology each year and of publishing at biological conferences. The rate of such publications is up sharply from previous years. We publish also in the computer science, physics, chemistry, materials science, and education literature. Details of the publications appear elsewhere in this report. In the past year we have been invited speakers at:

- AFM’99, Pontresina, September 1999
- Biophysical Society Meeting, New Orleans, February 2000
- Symposium on Interdisciplinary Nanoscience, Hamburg, January 2000

Software distribution

Free Software Library, VRPN. This library, for control of peripherals in virtual reality environments, has been placed into the public domain and is distributed on the web. We provide new releases as soon as new features are included in the Resource version of the code. We had 1279 visits to our main VRPN page and 145 visitor to our VRPN download page in the six months since July of 1999; 20 outside users have asked to be included on the mailing list (several of these groups have contributed updates to the library).

Free Applications. The nanoManipulator system has until recently been provided free (without a guarantee of support) to all takers. In the past year resource personnel visited and upgraded the systems at Catholic University of Leuven and Arizona State University, which is using the nM to develop web-browser-based remote access to SPMs.

Technology Transfer. We are in the process of licensing the nanoManipulator technology to a start-up company to sell as a product. We had discussed this possibility a few years ago, but all of the researchers were more interested in continuing the research. Aron Helser, a member of our technical staff, recently expressed interest in taking up this opportunity, and we are cheering him on. Licensing agreements are still being worked out, but the basic structure of the agreement will allow free Resource access to the improvements, documentation and maintenance of the system provided by the commercial entity. This is a real win-win-win situation for the Resource, the start-up, and scientists who will benefit from the ability to have a commercial-quality, supported nanoManipulator in their laboratories.

Public and Invited Demonstrations

Internet 2 Demonstration, April 1999, Washington, D.C. We presented the system running across the Internet2 at the Internet2 conference, courtesy of NCNI. This conference was held to demonstrate the variety of applications that will take advantage of the Internet2 and was widely attended by program managers and congressional staff members, as well as technical contacts from several universities.

Foresight Conference on Nanotechnology, October 1999, Santa Clara, CA. Graduate student Chris Dwyer was invited by the conference to show the nanoManipulator running in a demonstration session for three days during this conference, as well as presenting a lecture about the system.

Demonstration for Congressman Taylor, December 1999, Asheville, NC. The nanoManipulator was one of eight systems that were shown at this session. The session was a meeting of educators from K-12, community college and 4-year universities and was part of Congressman Taylor's technology for education initiative.

America's Millennial Celebration on the Mall, December 31, 1999, Washington, DC. We were part of a *Future Visions* session entitled "Glimpsing the Future: Technologies for the Millennium" on stage at the Hirshhorn Museum in the 12-1 hour. The show was broadcast on C-Span on January 1, 2000.

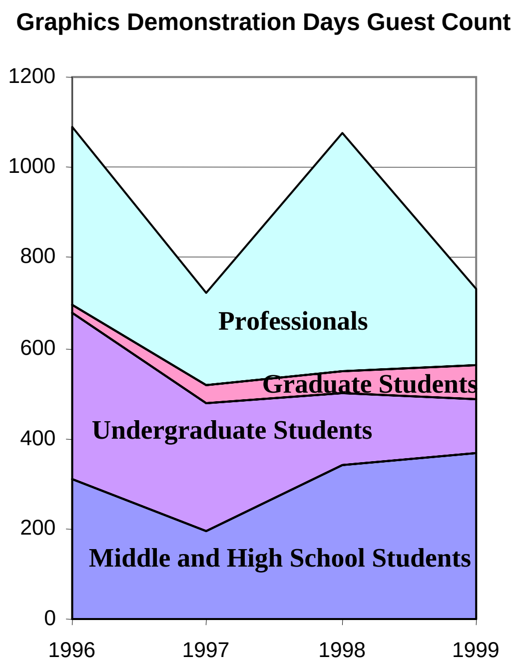
Dissemination of Information: Web Pages

We have a policy of attempting to answer all queries by posting the information on a web page, both for within-group questions and external questions. This provides a growing base of information available both to Resource collaborators and to the general public. To facilitate this, and to maintain the pages with up-to-date information, one of the research assistants spends ¼ time as the project Webspinner.

Our web pages have been well visited, with over 20,000 hits from users outside UNC on Resource starting pages in the period from July 1999 through January 2000. This represents over 100 visits per day to the Resource by outside researchers, and does not count hits by on-campus collaborators or by team members. (The average daily use was skewed by over 4000 hits in the week after we were listed on the popular web-based news site *Slashdot*, we run just under 100 hits per day when this is taken into account.) The visitors were from academic, industry and government sites from across the U.S. and abroad.

Outreach to Students and Professionals: Graphics and Image Demonstration Days

The Graphics and Image Cluster has regularly scheduled demonstration days in our laboratories. The nanoManipulator demo is one of the highlights of the visits. Over 300 undergraduate and graduate students and professionals were exposed to this exciting technology and science through these demonstrations.



IV. C. Training

The Research Resource carried out its education and training role in several ways during the 1999-2000 project year: we trained computer scientists in scanning probe microscopy techniques and we helped train physics and chemistry graduate students in computer techniques in aid of their disciplines. Dr. Taylor gave lectures on haptic display, virtual-environment libraries and the nanoManipulator as a scientific visualization tool in several computer science courses throughout this period (including a seminar tele-class that is broadcast to Utah, Brown, Caltech and Cornell).

Dr. Taylor was one of the speakers in a course on Haptic Interfaces at SIGGRAPH 99.

At UNC, we believe that graduate students best learn to do research through their apprenticeships working on projects such as those of the resource. This year the resource provided 22 graduate student research assistants the opportunity to "learn by doing" research.