NCRR BIOMEDICAL COLLABORATORIES WORKSHOP REPORT

Pittsburgh Supercomputing Center
October 27-29, 2000

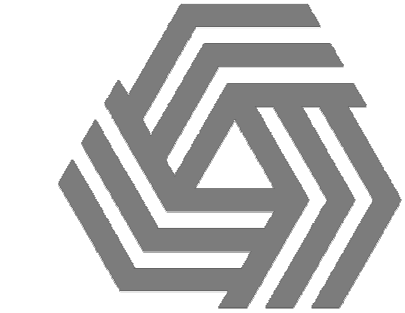

TABLE OF CONTENTS

Introduction

National Center for Research Resources (NCRR) awarded supplemental funding to seven current NCRR-supported Biomedical Technology resource centers to establish, demonstrate, and evaluate collaboratory (laboratory without walls) testbeds. These resource centers have a primary responsibility to collaborate with the research community at a regional and national level. The goal of these collaboratory testbeds was to determine whether this approach significantly enhances the efficiency and effectiveness of research activities and provides measurable improvements in the ability of these resource centers to serve the biomedical research community. In the second year of the program, the NCRR asked the Pittsburgh Supercomputing Center to organize a workshop in which researchers representing the seven biomedical collaboratory testbeds could explore together what works, what problems exist, and how we could help each other to analyze the impact collaboratory technologies may have on the efficacy of research resources. The seven participating biomedical collaboratories were:

- BioCoRE: A Collaboratory for Structural Biology, University of Illinois, Urbana-Champaign
- Collaborative nanoManipulator, University of North Carolina at Chapel Hill
- Collaboratories for Biomedical Research Software Development, Pittsburgh Supercomputing Center
- Microstructure Image-based Collaboratory, San Diego Supercomputing Center
- 3-D Image Visualization & Manipulation Collaboratory, University of California, San Francisco
- Collaboratory Testbed for Macromolecular Crystallography, Stanford Synchrotron Radiation Laboratory, Stanford University
- High Resolution Biological NMR Spectroscopy, University of Wisconsin

On October 27-29, 2000, 34 representatives of these biomedical collaboratories, several invited experts in collaboratory development, and two representatives from the NCRR met at the Mellon Institute facilities of the Pittsburgh Supercomputing Center for presentations and discussions spanning three days. The list of attendees with collaboratory affiliations and E-mail addresses is found in Appendix A. Two representatives from each collaboratory testbed site were compensated for travel expenses; however, additional representatives were welcome to participate in the workshop.

The workshop began on Friday afternoon with overview presentations from each site of their primary scientific problem and what their collaboratories are designed to do. These presentations provided the common framework for subsequent discussions. Saturday morning and afternoon were devoted to panel discussions from the perspectives of evaluators and users of collaborative tools, respectively. A panel discussion from the perspective of tools developers and implementers was held on Sunday morning. It was followed by a wrap-up session addressing key issues including lessons learned, common challenges and promising approaches, as well as shareable tools/resources and other opportunities for continued interaction among the biomedical collaboratories. The workshop agenda is found in Appendix B.

This workshop report is intended to provide the reader with an overview of the objectives and activities of the seven NCRR biomedical collaboratory initiatives. The perspectives of the scientific community to be supported, the tools developers and implementers, and the evaluators contribute to a concise description of each collaboratory. The concluding sections address the common theme of the workshop – the sharing of experiences about the challenges and successes met so far in this two-year-old initiative and the identification of opportunities to share promising approaches, tools, and resources among the collaboratory testbeds, with the goal of greater efficacy of research effort. We conclude by discussing the evaluation challenges present in determining whether collaboratories enhance the efficiency and effectiveness of research activities and provide measurable improvements in the ability of these resource centers to serve the biomedical research community.

BioCoRE: A Collaboratory for Structural Biology, University of Illinois, Urbana-Champaign

Principal Investigator: Klaus Schulten (kschulte@ks.uiuc.edu)
Collaboratory Web site: http://www.ks.uiuc.edu/Research/biocore

BioCoRE (Biological Collaborative Research Environment) is a Web-based collaborative environment that uses platform-independent technology and a secure infrastructure to ensure confidential scientific interactions between members of research project teams in structural biology, cellular biology, structural genomics, and pharmacology. These scientific communities' needs include access to analysis tools, remote simulation control, shared visualization sessions for 3-D cell structure, and data sharing and storage. Their needs also include joint document preparation, distant mentoring and training, and multi-channel communication (conferences, chat rooms, white boards, audio/video). A built-in evaluation component yields continuous data on user expectations and current needs, as identified by interviews, registration and feedback forms, users' comments, and bug reports.

The development of BioCoRE began in February 1999. BioCoRE was initially released for use in March 2000 and has been updated weekly since then. As of October 2000, there were 171 registered users in 13 projects, 46% of which are NIH funded. BioCoRE has played a role in the Human Frontier Science Program on Retinal Patients, with collaborators from the USA, Japan, Italy, Israel, and Germany.

BioCoRE is an environment consisting of four toolboxes: Workbench, Notebook, Conference, and Documents, within a Web-based collaborative framework that is platform independent and provides a secure infrastructure for private and confidential interactions. Functionality, simplicity, privacy, and flexibility are the primary specifications for these tools. The Notebook toolbox serves as a lab book, notice board, archive of project activity, and an automatic archive of chat sessions. The Conference toolbox provides real-time communication by way of a text-based chat tool with automatic archiving. The Workbench toolbox provides a common interface to visualization and simulation tools, as well as job submission and monitoring functions to gauge the health of ongoing simulations. The Documents toolbox will provide researchers with an easy way of producing multi-authored publications.

The evaluation component of the BioCoRE project is highly integrated into the BioCoRE environment, utilizing built-in evaluation mechanisms, such as unobtrusive data collection and a playback option, registration and feedback forms, users' comments, and bug reports. All the evaluation instruments are designed to obtain systematic data on how well the BioCoRE environment is meeting users' needs and expectations. Periodic surveys and interviews, and the permanent availability of a feedback form, assist in the acquisition of this information. The evaluation portion of the BioCoRE project account for both qualitative and quantitative data, and distinguishes between process and outcome data, treating each as important measure of BioCoRE success. Measures of outcome data include user satisfaction, attrition, resulting publications, citations of resulting work, participants' professional progress, and funding resources. Success is also gauged by the number of active users of the system, users' satisfaction and by the diversity of research activities supported.

In the first seven months since the initial release of BioCoRE, 171 users registered for BioCoRE accounts. BioCoRE has made contributions to the Human Frontier Science Program on Retinal Patients by bringing together collaborators worldwide in a shared virtual environment. BioCoRE has enabled training and mentoring opportunities in molecular modeling. Participants in a class at the European Molecular Biology Laboratory in Heidelberg were able to run molecular dynamics simulations at the University of Illinois using the workbench feature of the BioCoRE environment.

Current distribution policy requires that users register and use BioCoRE via the Resource's servers. It is anticipated that the BioCoRE server software will soon be made available for download and installation. This will give researchers the improved response time and better control that can only be achieved through the operation of a local BioCoRE server.

The Collaborative nanoManipulator, University of North Carolina at Chapel Hill

Project Lead Investigators: Diane H. Sonnenwald (dhs@sils.unc.edu) and Mary C. Whitton (whitton@cs.unc.edu)
Principal Investigator, nanoManipulator Project: Russell M. Taylor II (taylorr@cs.unc.edu)
Collaboratory Web site: http://www.cs.unc.edu/Research/nano/index.html

The Collaborative nanoManipulator is a multidisciplinary project, drawing expertise from Information Science, Computer Science, Physics, Chemistry, and Gene Therapy to design, deploy, and evaluate a version of the nanoManipulator (a virtual reality interface to an atomic force microscope) that supports distributed collaborations. The primary goal of the project is to see if and how the availability of the distributed version affects the process and outcomes of scientific collaboration. Initially, the system supports collaborations between two locations. The evaluation component of the collaborative nanoManipulator project is composed of: (1) an ethnographic study of current collaboration practices to provide data to guide system design and provide baseline data regarding scientific collaboration; (2) a controlled evaluation of the collaborative tool in a repeated measures study, and (3) a longitudinal ethnographic study of scientific collaboration as the system is deployed in scientists' offices and labs.

Ethnographic Study. An ethnographic study was performed to determine scientists' expectations, use, and perceptions of scientific collaboration in general and of the proposed collaborative nanoManipulator system. The study consisted of 28 interviews, 30 observation sessions, and five participant design meetings to determine system requirements. From the ethnographic study, the range of tasks and tools, the dynamics of shared and individual workflow, and issues relating to the role of situational awareness were discovered and used to guide system design.

The System. The system component most important for the success of shared scientific work in our context is the collaboration-enabled version of the nanoManipulator, running on a PC. Consequently, most project resources were applied to its development. During collaborative sessions, scientists sometimes work together and sometimes separately. The collaboration-enabled nanoManipulator supports this use model with shared and private work modes. When in private mode, the system works just as it does in single-user mode. When in shared mode, each user sees the same data visualization and both can, dynamically without explicit turn taking, control over 80 visualization parameters. The remote collaborator's pointer, tagged with mode of operation, is visible locally to provide awareness of the remote user's focus of attention.

A second PC is used for off-the-shelf video-conferencing and shared productivity applications. Users can select between two cameras: one is typically used to provide a view of the collaborating partner and the other, on a gooseneck, can be pointed at hands, notebook, physical models, or other materials used to aid communication between the collaborators. Video conferencing and shared applications are provided by Microsoft NetMeeting; audio is provided by standard telephony with wireless headsets. This PC also has a writing tablet so users may sketch out ideas and illustrate concepts for each other.

Controlled Experiment. This evaluation study was a repeated-measures, or within-subjects, controlled experiment with the order of conditions, working face-to-face and working distributively, counterbalanced. Twenty pairs of study participants conducted two scientific research activities using the system, one working face-to-face and one working distributively. The study participants, 19 males and 21 females, were junior and senior undergraduate science majors at research universities. The participants were randomly paired and were given up to 5 hours to complete the scientific research activities, including writing a scientific lab report. After each condition, every participant completed a survey instrument evaluating the system based on innovation diffusion theory and participated in an interview. Preliminary analysis of the survey data shows no significant difference in participants' scores that is attributable to condition (face-to-face or distributed). Analysis is ongoing, and results have been submitted for publication.

Longitudinal Ethnographic Study. The purpose of this study is to evaluate the system and any impact it may have on the scientific process and outcomes in the field. The system has been installed in labs or offices in four different locations. We are observing and interviewing scientists as they work on multi-disciplinary collaborative projects that utilize the nanoManipulator. This study is ongoing. In addition, this work has lead to the development of a new user interface, manuals, tutorials, including a teaching module and lab. Researchers are now using, and planning to use, the nanoManipulator system as an outreach tool in K-12 grades and university levels, including historically minority universities, to introduce students to collaborative scientific research. Plans for the future include the development of further synergy across research disciplines and outreach. In particular, emphasis will be placed on building on center resources to enable new collaborations and instrument access.

Collaboratories for Biomedical Research Software Development, Pittsburgh Supercomputing Center

Principal Investigator: Ralph Roskies (roskies@psc.edu)
Collaboratory Web site: http://collaboratory.psc.edu

The central goal of this collaboratory is to enhance the productivity and effectiveness of biomedical research collaborations engaged in software development by introducing collaborative technology. This is accomplished by the selection of promising tools, followed by an evaluation of their usefulness and impact in computational research testbeds. These testbeds include structural biology projects of *AMBER* and *CHARMM* code development, a computational pathology project in prostate modeling, and the Visible Human Project. This collaboratory is composed of three parts, users, a tools group, and an evaluation group.

The goals for the Structural Biology project include several improvements in the areas of efficiency and quality of code design/implementation/validation, access/utilization of codes by the user community, and data capture and collection methods (to enable 3-D prostate reconstruction, tumor location by feature detection, and LCM sampling.) Other goals include cross-fertilization of ideas between the developers of *AMBER* and *CHARMM*; and the design, implementation and validation of software for presenting these data to various classes of distributed users, in a compact and intuitive form. The goals for the Visible Human branch of the collaboratory include enabling the collaborative design and development of infrastructure to use the visible human data in a distributed anatomy laboratory of up to 40 simultaneous but independently operated viewing stations.

The users in the Structural Biology *AMBER* and *CHARMM* development project includes researchers from The Scripps Research Institute, the University of California – San Francisco, the Pittsburgh Supercomputing Center, the National Institute of Environmental Health Sciences, and the *AMBER* and *CHARMM* Communities. The users in the Pathology and Anatomy Distributed 3-D Viewers Development project come from the Pittsburgh Supercomputing Center, the University of Pittsburgh and UPMC Health System, the National Cancer Institute, and the University of Michigan. Collaboration with the University of Michigan is also part of the NGI/NLM Visible Human Project.

The Tools Group for the collaboratory is responsible for tool selection, deployment, and maintenance. There is a central service for tools support, including networking, based at the Pittsburgh Supercomputing Center. There are also local "toolmeisters" at participating sites.

The modes of activity between users vary significantly between projects. While the means of communication between Structural Biology project team members has been largely electronic (through E-mail, E-mail list systems, and Internet conferencing tools), both the Computational Pathology and Visible Human projects rely primarily on conference calls, application-sharing, and the *majordomo* E-mail list system. These differences reflect the dynamics and history of each project, as the structural biology project is well established, with most participants having worked closely with one another for several years. Frequent, close communication between structural biology project team members is seen as unnecessary, given that much work takes place on an individual level, with periodic episodes of collaboration for the sake of merging developed code modules and debugging. Both the Pathology and Visible Human projects are in the early and formative stages. There has been an emphasis on project management and planning activities, with a particular interest in distributed scheduling, meeting, and document-sharing technologies. Users have also expressed an interest in data-conferencing tools to facilitate algorithmic and coding discussions and to demonstrate applications to remote collaborators. As projects evolve, there is increasing interest in finding tools to facilitate the testing and integration of code modules that have been developed at different sites. *CVS*, a distributed software code management system, has been introduced to the structural biology project to aid in the control of code modifications within *AMBER* and *CHARMM*. A PSC-developed document-sharing program has been made available to the members of each collaboratory project, as have *SGImeeting, Microsoft NetMeeting*, and the *majordomo* E-mail list system.

The Evaluation Group is responsible for analyzing tool usage, monitoring collaboratory activities, and measuring the impact of the tools implemented. The evaluators bring the analytic resources of the University of Pittsburgh Center for Biomedical Informatics (CBMI) to the collaboratory. The evaluation group identifies appropriate measures of success for the collaboration tools and assesses the social and technological issues that influence collaboratory success. Evaluation is performed via participant observation, qualitative analysis of E-mail, electronic notebooks, and document sharing programs. The evaluation group continuously offers suggestions for improving collaboration.

Microstructure Image-based Collaboratory, San Diego Supercomputing Center

Principal Investigator: Mark Ellisman (mark@ncmir.ucsd.edu)
Collaboratory Web site: http://ncmir.ucsd.edu/MIBC/

The purpose of the Microstructure Image-based Collaboratory (MIBC) is to provide the opportunity for new science in the broad area of biological image collection and resulting structural analysis from molecule to cell. The collaboratory provides remote access and large-scale image management within a collaborative visualization environment. To accomplish this goal, the collaboratory is designing and implementing software tools that promote collaboration among scientists, students, and research resources connected to the Internet. To ensure broad applicability, the collaboratory tools are designed to have a kernel of reusable components to which application-specific components can be added. The tools integrate collaborative image visualization, high-performance computing, large-scale data storage and analysis, and access to remote instrumentation. In this application, experts in computation and microscopy at the National Center for Microscopy and Imaging Research (NCMIR) and National Biomedical Computation Resource (NBCR) are extending the existing Collaboratory for Microscopic Digital Anatomy to other imaging instruments and further developing the image-based collaborative environment. The MIBC permits researchers at different sites to interact during data acquisition and jointly analyze image data by accessing 3-D data in large-scale databases, employing high-performance computers to perform all the processing and analysis stages required to derive 3-D structural information. This is particularly valuable to researchers as few high-powered electron microscopes are available for use by biologists.

The developers of the Microstructure Image-based Collaboratory, NCMIR, and NBCR are mature resources with a 10-year history of collaboration. The collaboratory has links to three other projects, two of which include NCMIR and NBCR. Additionally, collaboration occurs among scientists within the US and scientists in Sweden, Finland, Switzerland, Brazil, Argentina, Scotland, Germany, Italy, Spain, Israel, and Japan. Users are able to engage in a high number of remote research and collaborative sessions using the large-scale data-archiving and management systems that the collaboratory has developed. This has greatly increased the pace of research, as users are no longer required to travel between sites to perform research tasks. The collaboratory stimulates new research interactions and expands opportunities for education and use of the resource.

Central to the collaboratory's efforts is the adoption and expanded availability of parallel computing resources. The *GTOMO* parallel tomography application provides distributed processing across the network, using components of the *Globus* toolkit. Additionally, it uses an application-level scheduler (*AppLes*) to achieve performance by simultaneously scheduling tasks over workstations and supercomputing nodes as they become available. This enables a lot of data to be gathered and processed in a much shorter time. Few researchers in this field would normally have such computing power available to them.

The collaboratory has migrated from simple telemicroscopy, which allowed the control of the microscope and information processing to occur at the same time, to a Web-based model called *VidCon*, which uses telemicroscopy Web tools that are *Java* based. Key aspects of the collaboratory include telescience portals, Web-based access, and distributed high-performance computing with shared databases. An example of a project performed via the collaboratory is the use of electron microscopy to reconstruct the interior of an object from its projections.

Evaluations, performed by the University of Wisconsin LEAD Center and based on observations, surveys, and data gathered by the software, are used to iteratively refine the collaboratory design and objectively measure its benefits for researchers using National Resource Centers. A major indicator of the collaboratory's success is the increased willingness of users to share data and methods, as well as the development of new research initiatives as a result of these collaborations.

3-D Image Visualization & Manipulation Collaboratory, University of California, San Francisco

Principal Investigator: Tom Ferrin (tef@cgl.ucsf.edu)
Collaboratory Web site: http://www.cgl.ucsf.edu/Research/collaboratory

This project seeks to develop a collaboratory environment for 3-D molecular modeling studies. The environment will allow multiple users in multiple locations to interact and share complex 3-Dmodels, and to access object data rather than just the graphical representation of the object. The collaboratory molecular-visualization environment currently under development at UCSF is called *Chimera.*

The goal of this collaboratory is to solve genomic and molecular recognition problems. The central challenge is to predict function and structure from a genetic sequence and engineer proteins for specialized function in hopes of understanding evolutionary changes. This has significant impact on drug discovery, as it may enable the prediction of what response a drug would yield, thereby helping to avoid toxic effects that would otherwise have been experienced by many individuals who would used the drug. The motivation for this collaboratory is three-fold:

1) to provide the benefits of face-to-face scientific collaboration through a common, visually based work environment,
2) to share its findings by extending this environment to remote scientists, and
3) to use the remote collaborative environment in new ways, such as for training and feedback purposes.

The initial design and implementation has been completed, and the collaboratory environment was introduced to users in the winter of 2000. A phased implementation approach is being used. The initial implementation was a 1:1 (single user to single user); it will be followed by the addition of 1:N and N:N functionality.

The *Chimera* collaboratory environment will be used by several testbed projects. The projects include: *Molecular Mechanisms of Mutagenesis and DNA Repair, Recognition of Damaged DNA; Drug Specificity of Dihydrofolate Reductase; Structural Aspects of Type 1 Collagen in Osteogenesis Imperfecta*; and one that provides feedback to *Chimera* developers. Multiple scientists at remote locations interactively manipulate shared, complex three-dimensional molecular models. Each collaboratory participant has access to the object's data, rather than just a graphic of the object. Participants may bring to the interaction operations they have performed on their own for discussion within the group interaction, or they may perform such tasks within the group setting without the need for advanced cueing. The results of input commands on one workstation can be simultaneously viewed by other participants within the *Chimera* molecular-modeling system. *Chimera* provides interactive manipulation of multiple molecular structures in real time in different types of formats, and it is compatible with its predecessor, *MidasPlus*. The benefit of *Chimera* over *MidasPlus* is that it allows the addition of new functionality without having to directly manipulate the source code; thus, new functionality can be tested and improved upon much more quickly. *Chimera* was built using *Python* and uses standard API's to ensure portability to many platforms. *Chimera* involves low-latency networking in which an initial high bandwidth is required to begin the program, but then only requires moderate bandwidth during the rest of the session. Consequently, *Chimera* can be run over Internet 2, a campus LAN, a DSL, or cable modem. Network issues such as latency and the need for a low rate of packet loss have affected performance. Developers are attempting to find ways around these problems, as the problems limit the scope of activity that can take place within the collaboratory environment.

Limited evaluation was begun with the collaboratory environment's early implementation efforts. It is expected that the evaluation efforts will ramp up as more testbed sites begin to use the environment. The collaboratory team wishes to broaden the community of users, as well as increase the number of new collaborative projects occurring within the environment. It is also anticipated that more frequent and spontaneous interactive sessions will occur, as well as new uses for such sessions, including training of new users.

Collaboratory Testbed for Macromolecular Crystallography, Stanford Synchrotron Radiation Laboratory

Principal Investigator: Peter Kuhn (pkuhn@stanford.edu)
Collaboratory Web site: http://smb.slac.stanford.edu

The overall goal is to enhance productivity and enable previously impossible experiments in macromolecular crystallography at the Stanford Synchrotron Radiation Laboratory (SSRL). Part of this goal is ensuring that the integrated resource is available to the scientific community within a collaborative and intuitive environment. For this to occur, procedures must be highly streamlined and systems well integrated. The development of the collaboratory environment started with an assessment of the basic needs of the users. This was evaluated by an Advisory Panel to define the project's priorities and plan for its development. The approach has been to take the collaboratory model and apply it over the entire development of the macromolecular crystallography beamlines at SSRL -- "if it's moveable, it gets a motor; if it has a motor, it's under software control; if it's under software control, the user should have an interface to control it remotely." BLU-ICE was designed to serve as the unified control and data collection environment at the macromolecular crystallography beamlines of SSRL.

Users are primarily structural biologists studying macromolecular structures, who utilize the resources at SSRL to collect diffraction data on single crystals. Facilitated user interactions include multi-client synching, and multiple video streams for each line, so that multiple users can communicate simultaneously. Database developments are underway to manage complex projects over the long term to ensure that data are not compromised when new collaborators join the project or researchers transfer between institutions.

In 2000 the collaboratory began offering tools for collecting and analyzing data while also providing image-viewing functions via a single user account with fully integrated file access from Web-applications, Windows and UNIX environments (local and remote). By November of 2000, there was a full launch of the collaboratory environment on all crystallographic beam lines. The implementation of a single OS for all user-system interactions, which is unified in a single user interface, has very significantly reduced the level of complexity in operations. A full suite of managed crystallographic software is available to users (local and remote) through a Windows Terminal Server platform. Raw data captured in experiments are currently written locally to a multi-TB RAID system and processed with high-performance multi-processor servers. A large-scale data archive systems is being developed, that will write data to a 1,000-terabyte archive system at the San Diego Supercomputer Center. There is a static Web site available to the public that includes beam line descriptions, software tutorials, and administrative information. For registered users, however, the central tool is a prototype Web application of the collaboratory environment, which can only be entered by logging on via an authorized UNIX account. The environment enables the user to browse the live data directory and view and manipulate images from that directory via the WebViewer.

Before the collaboratory developments, almost none of the equipment was motorized, and instrumentation and samples had to be manually aligned, necessitating extensive work by on-site scientific staff and visiting research groups. Furthermore, there were many different programs with crude user interfaces at each beam line to execute individual tasks such as moving motors, executing fluorescence scans, executing data collection, analyzing and managing data. All hardware has been motorized and is controllable locally or remotely, and all beam lines have identical, synchronized GUIs for local and remote users. This has set a standard for other synchrotron facilities, who are beginning to adopt the collaboratory's software.

Continued collaboratory development provides numerous challenges and opportunities. The exponential growth in structural biology poses challenges in user interaction, project management, and data handling, which all require careful assessment and addressing within the framework of the collaboratory. Only a truly integrated system will provide the tools required to perform next generation structural biology experiments that will focus on large macromolecular machines, dynamic detail of protein mechanisms at true atomic detail, and structural genomics. Rapid data growth will require using the base developments of the archive system to generate a database environment for all system parameters utilizing imgCIF. Work has now begun to integrate the overall system into a synchrotron structural biology pipeline that provides access to the users via a single BeamlinePortal to all administrative information, including proposals, addresses, time allocation, historic tracking information, experimental instrumentation (such as beamline and sample mounting robots), and data analysis systems for solving structures. This next-generation Collaboratory environment is building entirely on the existing infrastructure and will again significantly enhance the scientific effectiveness and efficiency of this research resource.

High Resolution Biological NMR Spectroscopy, University of Wisconsin

Principal Investigator: John L. Markley (markley@nmrfam.wisc.edu)
Collaboratory Web site: http://kamba.nmrfam.wisc.edu/Sesame/

NMR spectroscopy is uniquely capable of determining information about multiple areas of a molecule's structure. Approximately 50-60 publications result per year from the work done at NMRFAM, but there is much more demand for the NMR devices than can currently be met. This collaboratory is a means of streamlining the use of the NMR facility in order to meet as much of the need as possible. The goal of the collaboratory is to promote the development of biological NMR spectroscopy through core research projects that explore new technologies. This will be accomplished by providing state-of-the-art instrumentation and software to users, and by training in all aspects of biological NMR. This will aid in the goal to disseminate technology developed at NMRFAM and elsewhere to the larger scientific community.

Users originate from a variety of Biomolecular NMR projects. From November 1999 to September 2000, users could be separated into the following categories: 66 spectrometer users, 44 principal investigators (24 from UW-Madison campus and 20 from other institutions). Some of these institutions included: University of Rochester, University of Maryland, Institute for Human Virology, Purdue University, Agricultural University (As, Norway), Northwestern University, University of Lisbon, and the Mayo Research Institute. Training of users is a significant activity within the collaboratory. Experts train novice users on an individual basis, and training is tailored to the needs of the individual. Forty-two formal requests for training were given by unique users last year out of a total of 66 requests submitted. Advanced training at NMRFAM is typically for the analysis of macromolecules in a service or collaborative setting. Training covers several topics within the research process: experiment design and sample preparation, advanced operation of NMR spectrometers, processing of 1-D to 4-D NMR data, spectral assignment, structure determination and molecular modeling and visualization.

Use of the NMR resource can be broken down into categories as follows: Core, 15%; Collaborative, 41%; Service, 34%, and Maintenance, 10%. Data are recorded in electronic notebooks. Software that processes data then harvests information relevant to a structure-function investigation. All data are stored for later use and interpretation by other software. *LinuxNMR* has been introduced with the goal of demonstrating the viability of using a low cost UNIX platform and software tools available to academic users at little or no cost for the determination of biomolecular structures from NMR data. Other software introduced included: *Linux, bruk2pipe, nmrPipe, SPSCAN, XEASY, Sparky, NMRview, Garant, DYANA, MolMol,* and *Modelfree*.

The central tool for the collaboratory, however, is the *Sesame* data harvesting and experiment management system. *Sesame* is composed of several modules dedicated to specific functions: *Ouroborus* for expression plasmid management, *Lamp* for protein expression and purification, *Jar* for preparation of NMR sample, *Sand* for time requests and scheduling of data collection, and *Camel* provides the data collection protocol.

The evaluation objectives of the NMRFAM collaboratory are heavily based upon the goals of the collaboratory itself. The technology to be developed must meet three demands. First, it must capture and organize protocols involving the acquisition, processing, and analysis of data; second, the technology must provide methods for reviewing and evaluating intermediate and final results from structural NMR investigations; and third, it must enable the visualization of data and the development of a dictionary of standard visual icons in biomolecular NMR. Evaluators document ways in which use of Collaboratory tools change the way staff and clients conduct research and interact with each other. This is accomplished through a combination of formative and summative evaluation, including both quantitative and qualitative methods. Evaluators have found that clients are drawn to NMRFAM because of its high-field spectrometers, national focus, and knowledgeable staff. Good support is seen as essential, especially because of the interdisciplinary focus of many clients and the nature of NMR experimentation. For tools to be used consistently and repeatedly, collaboratory tools must yield an improvement in time or money expenditure, and the tools must complement staff, not replace them.

Collaboratory Needs Assessment – Issues and Methods

One of the pervasive themes of the workshop was the sharing of experiences about the challenges and successes met so far in this initiative to support collaborative science. Table 1 uses the types of functionality that were common to many of the participating collaboratory initiatives to organize the shared experiences to date. This section concludes with a discussion of the needs and solution implementations/plans of specific collaboratories.

Table 1 Collaboratory Needs – Functionality Requirements and Solutions

Issue	Solutions Attempted	Did it meet the need?	Capabilities and Drawbacks
Audio communication	• NetMeeting	• No	• Poor audio transmission quality • Extended latency makes synchronous communication impossible
	• Conference phone	• Partially	• No training required • Easily incorporated into existing patterns of interaction • Expensive if used frequently or on an international scale
	• Dedicated audio line	• Yes	• Improved audio transmission quality • Enables synchronous communication • Expensive • Not available to everyone due to resource constraints
Video communication	• NetMeeting	• Partially	• Significant latency in video transmission, which is compounded during application sharing • Small video window; low resolution
	• Polycom	• Yes	• Integrated hardware and software solution for use over the Internet
	• Access Grid	• Unknown	• Emerging group-to-group (room-to-room) capability
Data archiving and management	• Electronic notebooks	• Partially	• Easy to use • Freeware • Users determine what will be logged • No support for synchronous updating
	• GridManager	• Yes	• Archives images from collaboratory sessions for later use
	• Sesame Toolbox: Ouroborus, Lamp, and Jar	• Yes	• Each module houses a separate type of data • Modules store experiment information, but also act as a reference library for NMR researchers
	• CVS	• Yes	• Versioning control tool • Streamlines the code reconciliation process • Reduces the potential for harmful impact to overall code brought on by the introduction to new code sections
Shared models and applications	• Edgewarp	• Yes, mostly	• Shared 3-D model navigation • Gets bogged down with very large data sets
	• Chimera	• Yes	• Interactive manipulation of modeled molecular structures
	• CORES Image Processing software	• Yes	• Provides center and boundary tracing functions for the creation of models from images
	• Diffraction Image Viewer	• Partially	• Implementation ongoing – the next generation of BeamlinePortal will meet the needs fully

Table 1 Collaboratory Needs – Functionality Requirements and Solutions (continued)

Issue	Solutions Attempted	Did it meet the need?	Capabilities and Drawbacks
Shared models and applications (continued)	• BLU-ICE/DCS	• Yes, mostly	• Shared access to instrumentation while adhering to strict access control lists for safety
	• NetMeeting	• Partially	• Requires network fine-tuning to bring latency into acceptable range • Explicit turn-taking hinders work process
	• nanoManipulator	• Yes	• Opportunistic floor control allows scientists to perform interactive manipulation and use tools such as haptic feedback to synchronously analyze and compare experiment data
Platform compatibility	• Web-based	• Yes	• Universal accessibility via browser
	• Linux-based	• Yes	• Interface is Web-based, though built from Linux • Linux emphasizes the low-cost availability of NMR tools
	• Windows Terminal Server	• Yes	• Allows for server side management and simple client application installation • Full access to legacy applications through familiar environments • Session shadowing is not as powerful as would be required for full collaboration
	• Direct connection applications (NetMeeting)	• Partially	• In collaboratories where multiple platforms must be used, some conflicts have arisen • SGI Meeting and NetMeeting are incompatible at some version levels; must revert to earlier version to retain functionality
Scheduling	• Corporate-Time	• Unknown	• Not yet implemented • Web-based coordination of users' existing calendar programs • Reviews schedules to find mutually available times for meetings • Commercial-product; licensing issues for associated users not at main site
	• AppLes	• Yes	• Schedules data flow for optimal processor use • Makes improvements in task scheduling plan as new resources (supercomputing nodes and workstations) become available
	• Sand	• Yes	• Allows users to schedule Resource use, specifically, NMR time, to perform experiments

Four of the seven collaboratories utilized shared models (e.g., data, image renderings, experimental tasks). An additional two were still in the planning stages of incorporating shared models into their projects. The collaboratories with modeling systems already in place used the following programs to meet their modeling needs. UCSF used the *Chimera* modeling system; Urbana-Champaign used functions found in its workbench module; UNC used locally developed *CORES* image-processing software, and PSC's Structural Biology Collaboratory promoted the use of *CHARMM* and *AMBER* for such modeling. Both the Visible Human and Pathology collaboratories at PSC used *Edgewarp* for model manipulation.

Six of the seven collaboratories provided access to both object data and graphics, usually through their modeling software, though Stanford is using the *Diffraction Image Viewer*, and Urbana-Champaign used the *Notebook* module of their collaboratory environment for this. San Diego was still in the planning stages of providing such functionality.

Several projects tried to use real-time video interaction between participants but found their efforts largely unsuccessful, because bandwidth and lag issues within *NetMeeting* were insurmountable. UNC uses *NetMeeting* for video and

provides two video cameras per workstation to capture both the communicant's body language and any paper-based drawing or explanations given during the conversation. Video is transmitted over the local Internet2 network to help decrease transmission lag. In practice, UNC finds that while audio is used heavily, video is used less frequently. Although scientists tend to keep their visual focus on the display of their scientific data, video is used and can be an important tool for resolving differences of opinion. Both San Diego and the University of Michigan reported having used *Polycom* successfully over the Internet.

Solving the "audio problem" continues to be an elusive goal for collaboratories. Conference phones as the primary auditory media are an interim solution, but all sites articulated the need for a more integrative approach. For those that have experimented with Internet solutions there was consensus that multipoint communication is more challenging than point-to-point. The value of having at least two modes of communication between collaborators (e.g., shared application, *Polycom* over IP, telephone) was emphasized.

The majority of the collaboratories have avoided platform compatibility issues by making their central user interface entirely Web-based and accessible via a browser. Developers in the PSC collaboratory have faced many platform compatibility issues because the different communities are used to different platforms, including SGI, Windows, and Macintosh. Although *NetMeeting* is available in SGI and Windows versions, attempts to run cross-platform sessions with this tool have been largely unsuccessful.

Most of the collaboratories suffer from high bandwidth demands, noting that information transfer is too slow over the network. UCSF's *Chimera* program requires high bandwidth initially, but the need moderates after the beginning phase of use. Stanford is unusual in that it claims virtually no bandwidth problems, and that bandwidth is used very efficiently. High-bandwidth applications at Stanford include the *Large Scale Archival* system, which will be operated in the background; hence, there is a clear separation of high-efficiency and real-time network use vs. high-bandwidth and long-term network use. Urbana-Champaign believes that it will soon overcome bandwidth issues that have occurred from the number of users exceeding available resources. Users will soon be able to host BioCoRE on their own servers, thereby reducing the traffic burden on the BioCoRE servers.

None of the collaboratories reported that user interactions using collaboratory tools were spontaneous or frequent. Most required a level of advanced planning to avoid schedule and other conflicts. The ability to have successful spontaneous collaboratory sessions, and the desire of users to have these sessions (rather than planned meetings or individual directed E-mail or telephone calls), is the goal of any collaboratory system. It is a marker of seamlessly integrating collaboratory tools into the research process.

Three of the collaboratories have implemented, or are in the process of implementing, a scheduling program into the set of collaboratory tools. San Diego uses *AppLes* for this purpose. *AppLes* schedules the movement of large data chunks between processors in order to streamline the data-processing flow and reduce the amount of dead time between processing tasks. Wisconsin's *Sand* module of its *Sesame Toolbox* allows users to schedule NMR time. UNC also has a Web-based scheduling program. Since scheduling collaboratory sessions currently consumes many communication cycles between users, PSC is searching for a scheduling program that will easily integrate with users' existing calendar programs.

A highly organized database is an asset several of the collaboratories have worked to achieve. San Diego's *GridManager* archives images that are shared during collaboratory sessions. These images are later accessible to password holders who wish to review the images outside of the session. Project team members consider this database to be the "resource of resources" because in addition to storing data, it also acts as a portal to microscopy resources worldwide. PSC, Urbana-Champaign, and Wisconsin all use electronic notebooks with archival systems to store data. PSC's Structural Biology projects also use a versioning control software program called *CVS* as a means of archiving changes users make within the *CHARMM* and *AMBER* codes. Wisconsin's modules, including *Ouroborus* (dedicated to plasmid management information), *Lamp* (protein expression) and *Jar* (for NMR sample preparation information), use a common database for archiving and retrieving information. Stanford's databases ensure that data are not lost or disrupted when researcher/users transfer between institutions, as raw data are copied to a 1,000-terabyte tape-storage system at San Diego Supercomputing Center.

Areas of Ongoing Concern for Collaboratory Development and Evaluation

The workshop was an opportunity for collaboratory developers and evaluators to identify the issues that continue to challenge their efforts. Table 2 organizes these areas of concern into communication, tools, and evaluation issues, further delineating each along technical and social/organizational lines.

Table 2 Ongoing Collaboratory Questions and Concerns

Areas of Concern	Shared Questions and Concerns	Underlying issues

Communication issues (technical)	• Synchronous communication
	  • How do we overcome the problems associated with Internet audio and video functions?
	  • Can communication be effective even in situations of high latency?
	  • What elements contribute to the differences seen between face-to-face and distributed (online) communication?
		Face-to-face communication is frequently considered to be the "gold standard" for effective synchronous communication; therefore, a great deal of effort has been devoted to achieving the benefits of face-to-face communication without the associated drawbacks of travel, time, and money. Successful collaborative tool development for synchronous communication involves discovering how to optimally balance the features that will yield such benefits with the resources available.
		Internet-mediated interaction is arguably superior, in some ways, to face-to-face for asynchronous communication.

	• For which tasks in scientific collaborations is asynchronous communication as effective as, or preferred to, synchronous communication?	
	• How necessary are back-up methods of communication?	
Communication issues (social/organizational)	• Collaboration may represent a major paradigm shift for scientists.	Participants must not only be technologically ready to collaborate, but also socially and organizationally ready to collaborate. These new models of collaboration may be initially threatening or devalued by scientists whose careers have been primarily spent in independent research. Tools for maintaining presence awareness and resource scheduling (including people) are not yet facile. For shared-resource collaboratories, communication methods that are successful among the developers may not translate well to customer/user support.
	• How do we overcome the ownership and control issues that arise during application sharing and other collaborative tool use?	
	• How do we facilitate opportunities for ad hoc and scheduled collaborative sessions that integrate seamlessly into existing work routines?	

Table 2 Ongoing Collaboratory Questions and Concerns (continued)

Areas of Concern	Shared Questions and Concerns	Underlying issues
Tool issues (technical)	• How often do the tools fail?	Tools that are not reliable, or that present challenges to usual work routines, are not used. Obstacles cause tool use to regress to the lowest common denominators: telephone and E-mail. Without an adequate means of logging tool-use problems as they occur, it becomes difficult to pinpoint the source of difficulty. Ad hoc use of tools (e.g., shared applications and video) presents novel user-support challenges.
	• How do we incorporate monitoring and logging functions into the tools introduced?	
	• How do we address the need for presence awareness mechanisms during ad hoc tool use?	
	• How do we overcome latency and bandwidth issues in collaborative tools?	
Tool issues (social/organizational)	• How do we encourage the adoption and use of newly introduced tools?	What is the "Tipping Point" for tool use? What is the key ingredient that controls whether a tool will be embraced? Complacency and the reluctance to adopt and regularly use new tools, may be central to a collaboratory's efficiency and its efficacy.
	• Do the tools enable new functions or do the users just wind up doing the same things they did before tool implementation?	
	• If tools aren't vitally necessary, will collaborators use them?	
	• How do we overcome frustration association with the use of imperfect tools?	
Evaluation issues (technical)	• What information should be captured in evaluation?	It is difficult to use traditional scientific methods to evaluate the progress of a collaboratory; neither control groups nor "dummy" tools can be implemented as an adequate means of comparison. However, a broad spectrum of quantitative and qualitative methods of evaluation is available and can be applied to improve the validity and objectivity of the evaluation process. Low-intensity evaluation efforts yield low response rates. However appropriate investment in evaluation can produce high response rates and quality results.
	• How do we define success if we cannot determine what the outcome would have been without the intervention of tools?	
	• Should evaluation and tool changes occur simultaneously or separately?	
	• How does the use of collaboratory tools affect the amount of time spent on various phases of research if we do not know what time would be expended without collaboratory tools?	
	• How can we increase the response rates for evaluation surveys?	

Table 2 Ongoing Collaboratory Questions and Concerns (continued)

Areas of Concern	Shared Questions and Concerns	Underlying issues
Evaluation (social/organizational)	• How do you disentangle the health of the collaboratory from the health of the resource?	Evaluation helps convince "non-believers" of the value of collaboration. Collaboratories that are closely integrated with their NCRR resource may be difficult to evaluate separately from the resource itself because of considerable overlap in function, personnel, and scope. Evaluators may encounter considerable difficulty in trying to find comparable collaboratory environments for comparison because of the strong impact that interpersonal factors have on collaboration.
	• What focus should be given to the evaluation of user needs and requirements vs. evaluation of the success of the collaboratory, which represent two distinct sets of evaluation issues?	
	• What are the roles of scheduled and unscheduled collaboration in the research process, and how do we best assess the impact of collaboratory tools on each type?	
	• How do we develop comparable environments to facilitate comparisons between collaboratory environments?	

Evaluation of Biomedical Collaboratories

Tom Finholt and Stephanie Teasley led a discussion of the challenges associated with evaluating collaboratories at the conclusion of the Evaluators' Perspective Panel session. They used the two-by-two diagram shown in Figure 1 to illustrate some diverse ways in which collaborative use is made of biomedical research resources. That evaluation benefits a collaboratory's effectiveness is not arguable. However, different levels and types of evaluation approaches may be appropriate to each quadrant. Therefore developers and evaluators must be sensitive to these differences in designing evaluation studies and gauge expectations accordingly.

Figure 1 A Typology of Collaboratories (T. Finholt, S. Teasley)

		Types of biomedical research resources that are the focus of collaboration	
		Independent/single	***Dependent/multiple***
How the resource is used	***Community-wide use***	Protein Data Bank, GenBank (databases to be universally shared)	Linux development
	PI-generated use	Teleoperation of electron microscope, synchotron, visualization and modeling software tools	Collaboratories as commonly defined in the literature

Which evaluation measures to use in assessing collaboratory success continues to be the subject of much discussion. Basic measures of collaboratory tools use include numbers of users, number of collaborative sessions, and hours of use, among others. However, the relationships between usage statistics and measures of benefits to users depends on many contextual factors, including alternative access to collaborative resources. Other evaluation measures, such as usability and user satisfaction, are relevant to all collaboratories. Still other measures, those that focus on the benefits of collaboratories, are more dependent on the specific characteristics and objectives of each collaboratory. Process effects, such as how control is shared during application sharing or changes in how scientists spends their time, and cultural changes, such as more open sharing of data and results, can be observed and measured. However, the evaluation has to be methodologically diverse and open to both anticipated and unanticipated effects, as reflected by the range of evaluation approaches in the collaboratories represented at this workshop.

Evaluation continues to be seen as an important motivator of future funding of collaborative efforts and there is always pressure for "harder" results (e.g., use of controls or "gold standards"). Again, the collaboratory type, as well as its lifecycle phase of development, influences the questions that are appropriate to ask and the methods that are appropriate to use to answer them. Regardless of particular methodology utilized, quality evaluation requires a great deal of effort. Low-intensity evaluation efforts yield sub-optimal results, such as low response rates to user surveys. With the appropriate investment (e.g., adequate staff to conduct call-backs of survey non-respondents), the resulting evaluation data can be of very high quality.

Participants in this discussion expressed their thoughts regarding several hard methodological realities of evaluating collaboratories and raised some difficult philosophical questions.

- How do you disentangle the collaboratory from the research resource for the purpose of evaluating its contributions, problems, etc.? (i.e., what is the value-added by the collaboratory?)
- What is the value of custom-developed collaborative tools over the more generally available alternative?
- To what are you comparing collaboratory experiences? (e.g., remote access using traditional methods, on-site use of the resource)
    - Can comparable collaborative environments be developed to facilitate comparisons between them?
    - What are appropriate measures of success if we don't know what the outcome would have been without the intervention of the tools?
    - Is it easier to evaluate a collaboratory when the research task cannot be accomplished without collaboration? Or, is it harder because the baseline and desired end-state are so different?
- Does collaboration improve science, and do collaboratories improve collaboration?
- Is "better science through better tools" the answer?
- Can collaboratories change the process of science?
- What is the impact of a collaboratory on the time that scientists devote to various research processes (e.g., problem formulation, data collection)?

Acknowledgements

The Pittsburgh Supercomputing Center (PSC) would like to thank NCRR for supporting this workshop and for the opportunity to assist the scientific community through the introduction of collaborative technologies. PSC would also like to thank the collaboratories and their representatives who attended the workshop and shared their insights and experiences. Workshop report preparation, led by Cynthia Gadd with much assistance from Shelly Ozark, has greatly benefited from the many helpful comments provided by workshop participants on earlier drafts of this document. This shared knowledge will yield greater efficacy for the Research Resources and contribute to the progress of the scientific projects they support.

References

Information of General Interest to Collaboratory Developers

CSCW2000 Workshop on Lifecycle Support for Collaborative Science. This workshop explored how CSCW tools can be used to support and integrate work performed throughout the scientific lifecycle – from proposal generation through experiment design, experimentation, data collection, analysis, and publication. The workshop Web site (http://wind.arc.nasa.gov/cscw2000/) includes presentations.

A workshop series being organized at University of Michigan under the auspices of its ITR award will focus on a broad array of collaboratory issues (technology, adoption, domain community use, evaluation) and will include participation from the NCRR awardees. The ITR Web site (http://intel.si.umich.edu/crew/Research/resrch_ITR.htm) will soon have a link to information on the workshop series.

BioCoRE: A Collaboratory for Structural Biology, University of Illinois, Urbana-Champaign

Milind Bhandarkar, Gila Budescu, William F. Humphrey, Jesus A. Izaguirre, Sergei Izrailev, Laxmikant V. Kalé, Dorina Kosztin, Ferenc Molnar, James C. Phillips, and Klaus Schulten. "BioCoRE: A collaboratory for structural biology." In Agostino G. Bruzzone, Adelinde Uchrmacher, and Ernest H. Page, editors, Proceedings of the SCS International Conference on Web-Based Modeling and Simulation, pages 242-251, San Francisco, California, 1999.

Additional information can be found at http://www.ks.uiuc.edu/Research/biocore

Collaborative nanoManipulator, University of North Carolina at Chapel Hill

Sonnenwald, D.H., Bergquist, R., Maglaughlin, K.A., Kupstas-Soo, E., & Whitton, M. (2001). Designing to support collaborative scientific research across distances: The nanoManipulator example. In E. Churchill, D. Snowdon, A. Munro (Eds.), *Collaborative Virtual Environments* (pp. 202-224). London: Springer Verlag.

Sonnenwald, D.H., Maglaughlin, K.L., Whitton, M. C. (June, 2001). Using innovation diffusion theory to guide collaboration technology evaluation: Work in progress. IEEE 10th International Workshops on Enabling Technologies for Collaborative Enterprises (WET ICE). NY: IEEE Press. 7 manuscript pages.

Hudson, T., Sonnenwald, D.H., Maglauhlin, K., Whitton, M.C., Bergquist, R. (2000). Enabling distributed collaborative science. ACM 2000 Conference on Computer Supported Cooperative Work: Video Program.

Additional information can be found at http://www.cs.unc.edu/Research/nano/index.html

Collaboratories for Biomedical Research Software Development, Pittsburgh Supercomputing Center

Additional information can be found at http://collaboratory.psc.edu

Microstructure Image-based Collaboratory, San Diego Supercomputing Center

Additional information can be found at http://ncmir.ucsd.edu/MIBC/

3-D Image Visualization & Manipulation Collaboratory, University of California, San Francisco

Additional information can be found at http://www.cgl.ucsf.edu/Research/collaboratory

Collaboratory Testbed for Macromolecular Crystallography, Stanford Synchrotron Radiation Laboratory

Additional information can be found at http://smb.slac.stanford.edu

High Resolution Biological NMR Spectroscopy, University of Wisconsin

Zs. Zolnai, P.T. Lee, W. M. Westler, B. F. Volkman, M. Livny and J. L. Markley, "SESAME - an experiment management system for NMR spectrometers," Frontiers of NMR in Molecular Biology, Breckenridge, Colorado, January 9-15, 1999.

P.T. Lee, W. M. Westler, M. R. Chapman, J. L. Markley and Zs. Zolnai "SESAME - an experiment management system for NMR spectrometers," 40th Experimental NMR Conference, Orlando, Florida, February 28 - March 5, 1999.

P.T. Lee, J. Li, M. R. Chapman, B. F. Volkman, Y. K. Chae, J. L. Markley and Zs. Zolnai "SESAME - an experiment management system for Biomolecular NMR," 41th Experimental NMR Conference, Asilomar, California, April 9 - 14, 2000.

Additional information can be found at http://kamba.nmrfam.wisc.edu/Sesame/

Appendices

Appendix A – Workshop Attendees

Attendees at the NCRR Biomedical Collaboratories Workshop – October 27-29, 2000

Name	Project	E-mail
Bair, Raymond	PNL/DOE	raybair@pnl.gov
Blankenstein, Nancy	Pittsburgh	blankens@psc.edu
Bourne, Phillip	San Diego	bourne@sdsc.edu
Brandon, David	Illinois	brandon@ks.uiuc.edu
Brunner, Robert	Illinois	rbrunner@uiuc.edu
Budescu, Gila	Illinois	gila@ks.uiuc.edu
Clifton, William	San Diego	wclifton@facstaff.wisc.edu
Crowley, Mike	Scripps/Pittsburgh	crowley@scripps.edu
Daffinrud, Susan	Wisconsin	smdaffin@facstaff.wisc.edu
Deerfield, David	Pittsburgh	deerfield@psc.edu
Ellisman, Mark H.	San Diego	mark@ncmir.ucsd.edu
Farber, Greg	NCRR	farberg@ncrr.nih.gov
Ferrin, Thomas	San Francisco	tef@cgl.ucsf.edu
Finholt, Thomas	Michigan/NSF	finholt@umich.edu
Friedman, Charles	Pittsburgh	cpf@cbmi.upmc.edu
Gadd, Cindy	Pittsburgh	csg@cbmi.upmc.edu
Hacker, Tom	Michigan/Pittsburgh	hacker@umich.edu
Huang, Conrad	San Francisco	conrad@cgl.ucsf.edu
Jarzynka, Lucille	PSC	jarzynka@psc.edu
Konerding, David	San Francisco	dek@cgl.ucsf.edu
Kuhn, Peter	Stanford	pkuhn@stanford.edu
Levine, Michael J.	PSC	levine@psc.edu
Madrid, Marcela	Pittsburgh	mmadrid@psc.edu
Marron, Michael	NCRR	marron@nih.gov
McGinnis, Laura	Pittsburgh	lfm@psc.edu
Ozark, Shelly	Pittsburgh	sdo@cbmi.upmc.edu
Prologo, Elvira	PSC	prologo@psc.edu
Roskies, Ralph	Pittsburgh	roskies@psc.edu
Sanielevici, Sergiu	Pittsburgh	sergiu@psc.edu
Schulten, Klaus	Illinois	kschulte@ks.uiuc.edu
Sonnenwald, Diane H.	North Carolina	dhs@ils.unc.edu
Stock, Robert	PSC	stock@psc.edu
Stone, Nathan	Pittsburgh	nstone@psc.edu
Teasley, Stephanie D.	Great Lakes AIDS Study	steasley@umich.edu
Terzian, Alex	Michigan/Pittsburgh	terzian@umich.edu
Ulrich, Eldon	Wisconsin	elu@bmrb.wisc.edu
Vandivort, Kirby	Illinois	kvandivo@ks.uiuc.edu
Volkman, Brian F.	Wisconsin	bvolkman@mcw.edu
Wetzel, Art	Pittsburgh	awetzel@psc.edu
Weymouth, Terry	Michigan/Pittsburgh	weymouth@umich.edu
Whitton, Mary	North Carolina	whitton@cs.unc.edu
Wilkens, Steven J.	Wisconsin	wilks@nmrfam.wisc.edu
Zolnai, Zsolt	Wisconsin	zsolt@nmrfam.wisc.edu

Appendix B – Workshop Agenda

Agenda for the NCRR Biomedical Collaboratories Workshop – October 27-29, 2000

FRIDAY, OCTOBER 27 (Half Day)

1:15 PM	Welcome: Michael Marron (NCRR) and Ralph Roskies (PSC)
	Presentations from each site of their scientific problem and what their collaboratories are designed to accomplish. Chair: Ralph Roskies (Pittsburgh)
1:30 PM	Illinois Project Overview: Klaus Schulten
2:00 PM	North Carolina Project Overview: Diane Sonnenwald
2:30 PM	Pittsburgh Project Overview: Sergiu Sanielevici
3:00 PM	Break – Informal Discussion
3:15 PM	San Diego Project Overview: Mark Ellisman
3:45 PM	San Francisco Project Overview: Thomas Ferrin
4:15 PM	Stanford Project Overview: Peter Kuhn
4:45 PM	Wisconsin Project Overview: Eldon Ulrich

SATURDAY, OCTOBER 28

	Panel discussion from the evaluators' perspective. Chair: Ray Bair (PNNL/DOE)
9:00 AM	Panel discussion from the evaluators' perspective:
	Statements by Panelists (one evaluator from each of the seven Collaboratories)
10:15 AM	Break – Informal Discussions
10:45 AM	Panel discussion continues: Statements from the floor; Q &A; Discussion
Noon	Lunch
	Panel discussion from the biomedical researchers' (tool users') perspective. Chair: Gregory Farber (NCRR)
1:30 PM	Panel discussion from the tool users' perspective:
	Statements by Panelists (one Researcher/User from each of the seven Collaboratories)
2:45 PM	Break – Informal Discussions
3:15 PM	Panel discussion continues: Statements from the floor; Q&A; Discussion
4:30 PM	Discussion: How to report on this workshop? Leader: Cindy Gadd (Pittsburgh)
5:00 PM	Session Wrap-up and Concluding Remarks: Michael Marron (NCRR)

SUNDAY, OCTOBER 29 (Half Day)

	Panel discussion from the tools development and support perspective. Chair: Tom Finholt (U. Michigan)
9:00 AM	Panel discussion from the tools development and support perspective:
	Statements by Panelists (one tools person from each of the seven Collaboratories); Statements from the floor; Q&A; Discussion
11:30 AM	Workshop Wrap-up and Concluding Remarks: Greg Farber (NCRR)
Noon	Lunch
1:30 PM	End of Workshop