BioCoRE:
A Collaboratory for Structural Biology

Final Report

National Institutes of Health
National Center for Research Resources
Funding Period
02/01/1999 – 07/31/2002

Klaus Schulten, PI
Gila Budescu, CO-PI
Laxmikant V. Kale, CO-PI

NIH Resource for Macromolecular Modeling and Bioinformatics
The Beckman Institute for Advanced Science and Technology
The University of Illinois at Urbana-Champaign
http://www.ks.uiuc.edu/Research/BioCoRE

BioCoRE Final Report

PI: K. Schulten, Co-PIs: G. Budescu, L. Kale
Lead Programmers: R. Brunner, K. Vandivort

Overview

BioCoRE, a unified web-based biological collaborative environment for research practice and management, is developed by the NIH Resource for Macromolecular Modeling and Bioinformatics at UIUC. Resting on a simple yet powerful concept of platform-independence, BioCoRE takes full advantage of the very latest and most effective offerings in computer hardware, software, and communication technologies. BioCoRE features an integrated, tool-oriented computing and communication system, incorporating in-house and third-party tools. A dynamic evaluation component contributes continuous user data and feedback. Researchers can use the BioCoRE server operated by the Resource, or download and install their own local server. BioCoRE is freely available from the Resource web site[1].

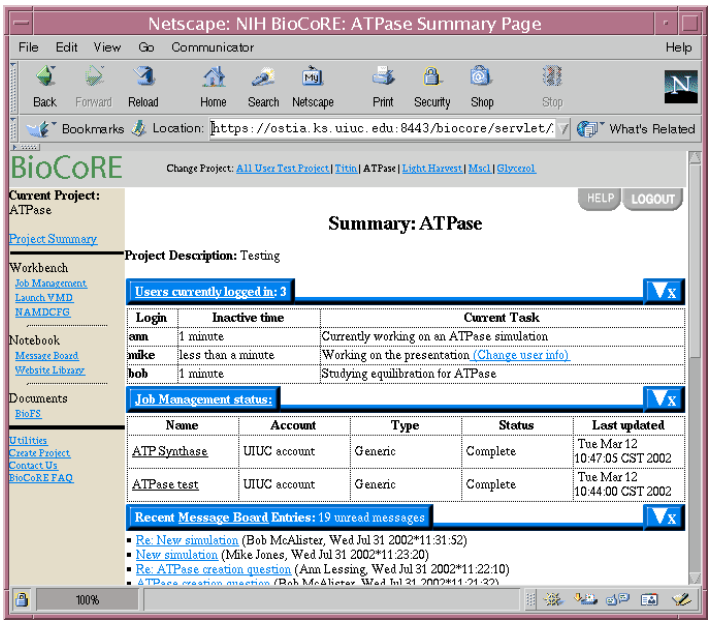
BioCoRE supports the biomedical research process to fruition—from performing computer simulations, through analysis and visualization of biomolecular structures, to preparing publications and other documents. While at present BioCoRE is mostly biomedicine-oriented, in the future general-purpose tools will also be considered for integration, depending on needs and availability of resources. Unique and clearly unlike most collaboratories, BioCoRE is *not* strictly designed as a fixed access point for costly scientific instruments (such as a microscope, telescope, or particle accelerator). Rather, BioCoRE offers seamless access to a broad range of local and remote resources (i.e. the PDB and other databases, supercomputers, and more). Driven by rapidly shifting research needs, BioCoRE is flexible and extensible, and capitalizing on technological opportunities, it is essentially a wide-open speedway to scientific, technological and human capital, regardless of either the users' or resources' location. Thus, BioCoRE is a virtual environment particularly opportunity-laden, training-relevant, and exceptionally far-reaching.

The funds for BioCoRE development were awarded in February 1999, and following extensive staffing efforts, actual work began in late spring of that year. BioCoRE was first released to the public in March 2000, and the server software has been available for download since February 2002. BioCoRE currently boasts 463 registrants and 106 projects; several off-site servers are about to be installed.

[1] http://www.ks.uiuc.edu/Research/biocore/localServer/

BioCoRE Aims

The overarching goal driving BioCoRE development is to enhance the collaborative research process through a comprehensive and secure online environment. BioCoRE does just that by streamlining and improving the collaborative capacity between biomedical researchers located at either the same or at geographically distant places, and by facilitating the transparent use of and communication between technological resources (hardware and software) and databases. Scientists within BioCoRE interact in both synchronous and asynchronous fashion with each other or with the research tools via a common infrastructure. A built-in evaluation component in BioCoRE guarantees the systematic assessment of usage and acceptance of the BioCoRE environment. For evaluation purposes, BioCoRE has been planned with a built-in event tracker of user actions (such as when a user accesses a particular tool). The tracker, which has greatly influenced the design of BioCoRE, provides this information to the Resource evaluators. The tracking is done via a single "event" logger running on a Resource computer and connected to all other BioCoRE servers. Each installed BioCoRE server (on- and off-site) tracks user actions (or events), caches these events, and sends them to the event logger regularly.



The BioCoRE Project Summary Screen

Organized around the concept of a "project", BioCoRE members create a separate project for any research topic they work on. BioCoRE project-team leaders can add or remove members from the project as required, and researchers can join more than one project. Information entered into a given project is fully shared among project members. As security is an obvious concern, users are only permitted to access projects of which they are members.

BioCoRE manages four fundamental groups of activities pertinent to the research enterprise: utilization of a wide range of computational tools; record keeping;

collaborative communication (visual and otherwise); and document preparation (papers, reports, etc.). The required functionality is implemented in four areas of BioCoRE: *Workbench, Notebook, Conferences*, and *Documents*, respectively. Many of these same activities also pertain to the training arena that is essentially collaborative in nature, making BioCoRE a useful educational venue.

The BioCoRE *Workbench* includes a web-based interface for submitting and monitoring supercomputer jobs and shared access to visualization programs. The *Notebook* furnishes tools for logging, locating, and reviewing methodology, data, results, and annotations related to ongoing projects. Investigators are able to discuss their research in real-time or time-delayed sessions via the *Conferences* interface. The BioCoRE *Documents* interface features access to a common file system that benefits all areas of BioCoRE and enables collaborators to easily save, retrieve, and exchange data. This makes BioCoRE a valuable multi-purpose tool for, among other uses, assisting in communication of raw data, preparing multi-author documents for publication, and for managing projects. Built-in evaluation yields ongoing and immediate assessment of users' needs, pattern of use, effectiveness of tools, and more. Evaluation findings help to guide the development efforts.

BioCoRE, as a research and training platform, presents an ideal environment to cultivate and nurture collaborative work. It could also be instrumental in supervising and mentoring within one's department/unit/institution and between facilities and organizations across any distance, exploiting readily available fast (and ever-faster) communication networks.

Accomplishments

BioCoRE is geared towards meeting essential needs of cutting-edge biomedical research and addressing capabilities lacking in older software packages. As such, BioCoRE has numerous features and functionalities, the most salient and representative of which are outlined below:

Core Environment

The tools within BioCoRE form a coherent core environment that furnishes a simple, flexible, secure, and intuitive setting suitable for users with various levels of expertise, working in a variety of disciplines. The main interface to BioCoRE is through a standard web browser (with Java servelets) that makes BioCoRE a simple and affordable platform-independent framework. By classifying data into projects BioCoRE establishes security and hides data from those researchers not involved in a given project. In practice, this means that researchers who are not members of a particular project are not even aware of the existence of other projects. Furthermore, all network communication in BioCoRE uses secure (HTTPS) sockets. The basic look and feel of the user interfaces are consistent and uncomplicated, providing intuitive access to all of the BioCoRE tools. A web-based environment of this nature calls for powerful server-side tools. BioCoRE uses Sun's Java Servlet technology and the Apache Tomcat Servlet Engine as the server-side programming environment. Achieving the wide range of functions

that are expected of BioCoRE depends on efficient access to a large amount of data. BioCoRE accomplishes this by using an SQL database, handled by the MySQL data management software. In addition to being the best solutions for meeting BioCoRE's needs, these software tools are freely-available, allowing off-site user groups/organizations to operate their own BioCoRE servers with little expense.

File System

Since collaborative research often demands exchange of large data files, part of the BioCoRE core environment is BioFS, a shared online file system. BioFS provides an area for the exchange of data such as large datasets, or documents in preparation. The BioFS is accessible via a web browser (in the *Documents* area) as a workspace where users can upload files to their projects. Once uploaded, the files are accessible to other researchers in their project. Moreover, the file system is an elementary piece of the core environment since other components use it as an underlying mechanism to deposit and share larger amounts of data not conveniently stored in the database. For example, when a researcher runs a simulation using his/her supercomputer account, BioCoRE will automatically send simulation input files from the BioFS to the supercomputer, and will retrieve output from the simulation back into the BioFS at the conclusion of the simulation. The BioFS is also accessible through WebDAV, an emerging standard for internet-based file system access. By using WebDAV, BioCoRE's file system can be accessed by any application running on several popular computing platforms (including recent versions of Windows and Mac OS X) as if it were a local disk. This permits basic integration of a large number of applications on those platforms with the BioCoRE file system.

Job Management

Within the *Workbench* area, the BioCoRE Job Management tool has a simplified interface for computational job submissions to supercomputer centers (including NCSA, PSC and SDSC), local computational resources, or even to the workstation on researchers' own desk. BioCoRE uses Globus, the emerging standard for Grid-based computing, as well as the ubiquitous SSH protocol, to submit and monitor simulations and other computational jobs. Through a common web interface, researchers can monitor all of their running simulations from a single web page. Researchers specify which files to transfer from the BioCoRE file system to the supercomputer before the job begins, and BioCoRE automatically brings back output files upon completion of the job. BioCoRE trivializes the task of monitoring the output from the run during the course of the simulation, saving both researchers' time and computational resources by allowing early detection of problems and the termination and restarting of the simulation.

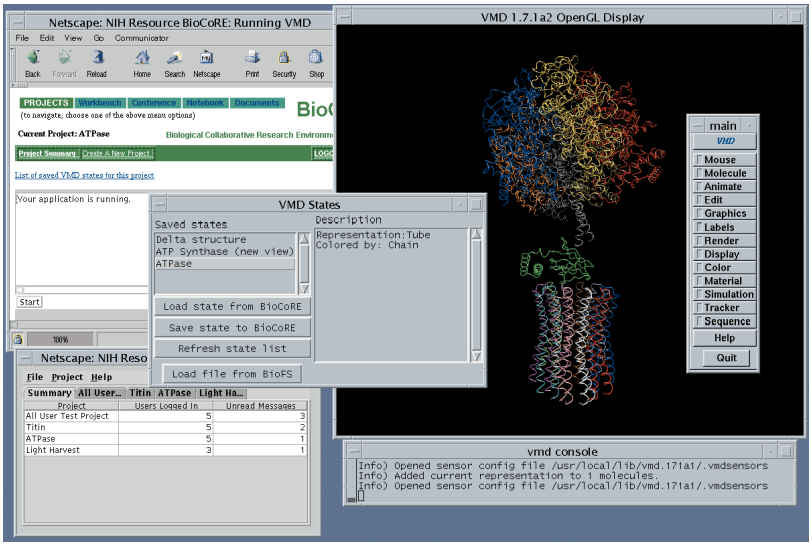
Simulation Configuration File Generator

The Simulation Configuration File Generator applet within the *Workbench* provides a graphical user interface for creating configuration files for the

Resource's molecular dynamics simulation program, NAMD[2]. This tool supplies online help and built-in error checking, making it easier for novices to set up simulations and helps experienced users to catch simple errors.

Collaborative Visualization

Another component of the *Workbench* area of BioCoRE is collaborative visualization. Using this tool, a researcher can load a molecular structure from the BioFS into the Resource's visualization software, VMD[3]. The researcher can manipulate a particularly insightful view, and deposit it back into BioCoRE. Other researchers may later load that same view, manipulate it further, and deposit the result back to BioCoRE. Archiving and exchanging visual project data is invaluable and enables an unusually systematic and detailed study of the structure under investigation. Since it takes only seconds to save and retrieve a view, it is also an efficient way of running interactive visualization sessions by convenient back-and-forth exchange of molecular views between widely-separated sites/researchers.



The Collaborative Visualization Tool in Use

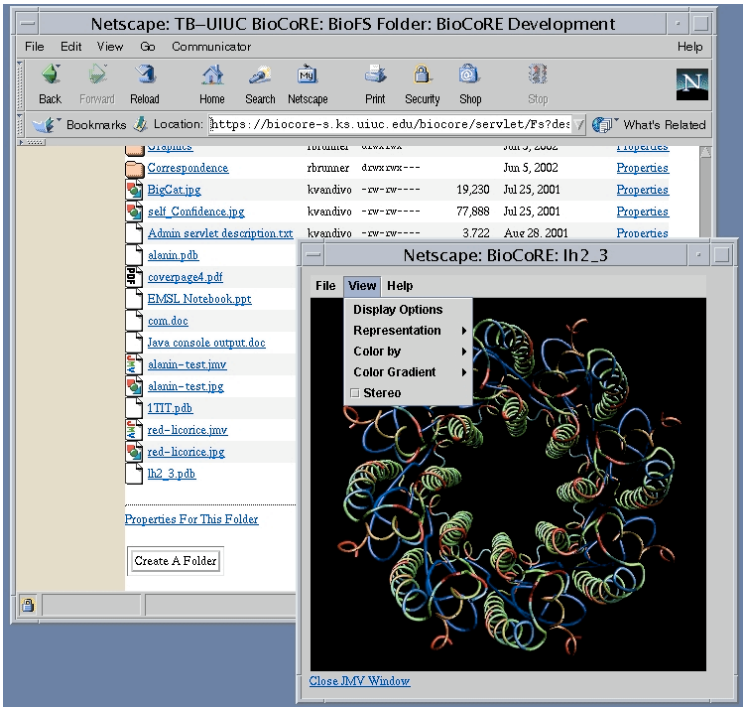
JMV[4]

The Java Molecular Viewer JMV has been written utilizing Java3D, and is available as a BioCoRE tool and as a stand-alone product. It is a small, easy-to-use tool that displays views of molecular files stored within the BioCoRE filesystem or retrieved directly from the Protein Data Bank. These views can be manipulated in 3-D on a variety of computer platforms, providing a means of sharing the visual data that is critically important in molecular biology research,

[2] http://www.ks.uiuc.edu/Research/namd/
[3] http://www.ks.uiuc.edu/Research/vmd/
[4] http://www.ks.uiuc.edu/Development/jmv/

especially in those cases where installing a full-scale molecular visualization tool (such as the Resource's own VMD or other graphics programs) is not practical. JMV is user-customizable thanks to the use of Java Beans technology. JMV, which was only recently released, promises to be advantageous as both a BioCoRE component, and a simple stand-alone molecular viewer for applications such as electronic textbooks.

As a novel collaborative tool par excellence, JMV has the potential for immense reward in diverse disciplines and environments. Remarkably suited for web-based presentation and dissemination of biomolecular information, JMV can be downloaded and run on-the-fly on commodity computers with Java and Java3D support. While the biomedical research world is desperate to replace older tools such as MDL's Chime, currently the most widely used method for displaying 3D structures on the web, JMV is on the verge of supplying a superior and much needed alternative.



A File Loaded from the Shared File System into JMV

Message Board

The *Notebook* area of BioCoRE contains a Message Board, a threaded discussion area, where researchers exchange messages with each other. Discussions are stored in the BioCoRE database for later review as needed.

Scientific Data Archive

Serving as a data warehouse, the BioCoRE *Notebook* stores textual data from internal and external applications. Data from external applications can be archived

within BioCoRE via a tool for capturing text output from any command-line program and programming interfaces in several computer languages.

Link Library
Researchers often wish to share web links with their collaborators, and the BioCoRE *Notebook* is equipped to create a library of web site links for each BioCoRE project by topic. Researchers maintain a link library for their project by adding, removing, annotating, and organizing useful links they find in the course of their research.

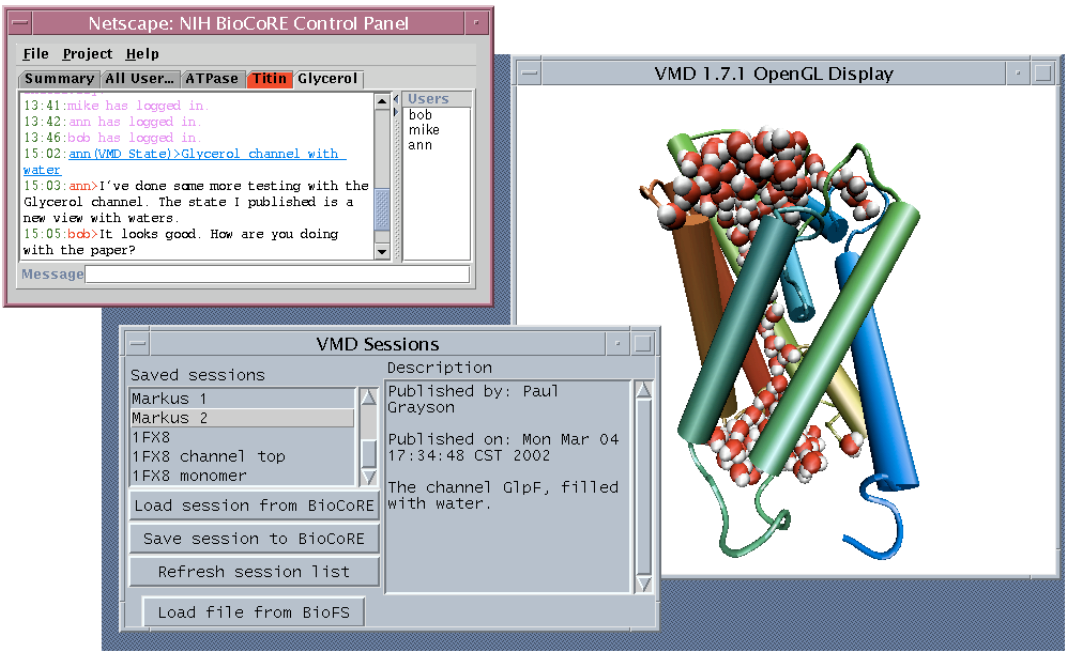
Control Panel
The Control Panel notifies researchers of important events occurring in BioCoRE, such as when a researcher deposits new project data. As a component of the BioCoRE *Conferences* area, the Control Panel's most important function is a text-based chat tool, allowing researchers in different locations to practically converse with each other online and have the conversation archived. Namely, unlike many popular internet-chat systems, all BioCoRE Control Panel chat contents are stored, so that researchers may go back to past chats, whether or not they participated in the real-time discussion. The Control Panel is written as a Java applet, and can run within the user's browser, or as a stand-alone application, independent of the user's web browser.

BioCoRE User Perspective
Productive research relies on extensive and intensive interactions at different levels and content among scientists, and the ability to easily and rapidly exchange both textual and visual information is vital. This is particularly critical in the biomedical sciences, where discussions of molecular graphics images and the transfer of extremely large data files are a daily routine. To facilitate effective communication among project members, BioCoRE offers tools such as the message board (described above), allowing for easy exchange of textual information. For visual communication scientists can use JMV and VMD to view, manipulate and store molecular graphics images. The storage capability enables a researcher to depict a specifically interesting view of a given biological system, store it; later other project members, whenever and wherever they are, can virtually share, modify, and review the system with their colleagues. Eventually, selected images can be easily incorporated into resulting papers and documents.

Ongoing research projects create sizable datasets, with trajectory files of biomolecular simulations easily reaching sizes of several gigabytes, precluding easy exchange via email. This demands the ability to deposit and share information and accessibility of all project-related data at any time. BioCoRE meets the challenge by allocating each project its own file space, thereby creating a central hub where all project-data, e.g. structure files, simulation data, and analysis results of files associated with a joint publication can be stored.

Joint research is typically performed by project members at different places. Each collaborating scientist, in his/her lab, would need an environment with expert assistance

tools to harness their work productivity and quality. Accordingly, BioCoRE provides, among other features, tools to set up computer simulations, submit scientists' jobs to Globus or supercomputer sites and to perform run time job monitoring. BioCoRE also supplies a unified environment in which researchers can manage their multiple accounts at multiple computer sites. BioCoRE's archiving features make it particularly beneficial for scientists who join the project after its inception, as well as for those who are at times unavailable and inaccessible. Since everything within the BioCoRE project directory is saved, new and/or temporarily absent project members can easily retrieve data and (re)acquaint themselves with the project from its initiation.



A Collaborative Visualization Discussion Session

Generally, projects involving scientists across physical and temporal barriers require a comprehensive work environment that empowers and facilitates research and communication. BioCoRE is a uniquely optimal solution to overcome those barriers and bring researchers together.

Evaluation

As a problem-solving environment, BioCoRE relies on computer-mediated rather than in-person interaction; the speed and breadth of communication within the collaboratory and with the outside world is of a different magnitude; and the ever-changing collaboratory boundaries are conceptual rather than physical. To assess the effectiveness of BioCoRE, the evaluation team has focused on aspects that are germane to the structural biology community. Participants' feedback and collaboratory interactions while designing, implementing, and using the BioCoRE tools constituted the bulk of the raw data.

The evaluation studies emphasize several inter-related factors:

1. Selection of new features and functionalities (based on users' needs and preferences as well as technological developments);
2. Evaluation of newly implemented features;
3. Measurement of user satisfaction (by feature, by component, global environment);
4. Assessment of BioCoRE effectiveness and impact on quality of research process and outcomes.

Progress

In the past funding period the BioCoRE evaluation team has supported BioCoRE development by anchoring the development efforts in a relevant context representing the typical work environment of structural biologists. All four factors above have been addressed, but naturally, due to the project's young age, the first three have been most investigated. BioCoRE effectiveness and impact will become the focus of the evaluation activities in the upcoming funding period. Thus, the evaluation team studied scientists' work habits and provided the development team with data on user needs and preferences. The evaluation activities included usability tests on BioCoRE components, reliability and validity analyses of BioCoRE scales designed to measure self efficacy and satisfaction in BioCoRE users, and the design and administration of user surveys to evaluate in-house software products to be incorporated into BioCoRE.

To appraise developers of user needs and preferences, BioCoRE components are subjected to usability tests while they are being developed. Initially, the developers and evaluation team conduct a usability analysis of pre-released components; then the components are put before users for further evaluation. For example, developers with the evaluation team tested the BioCoRE Job Management tool by first using paper-based, iterative rapid-prototyping to refine it, and later scientist input was gathered employing a cognitive walk-through of the new component. Heuristic analysis was performed on the development team, and then on scientists/users, to evaluate the Simulation Configuration File Generator. Other tools such as VMD Load/Save State, JMV and others were subjected to similarly careful evaluation.

Recent efforts have encompassed interviews with local Resource members focusing on time management during collaborative projects and their preferences concerning the BioCoRE *Workbench*, Collaborative Tools, Publications, and Core Application components. The resulting data were used in a functional analysis of scientists' work behavior during collaborative projects. Drawn from the fields of industrial/personnel psychology and job analysis, functional analysis translates work behavior into tasks, functions within a task, and smaller behavior units within functions. The analysis yielded a detailed look at tasks common to scientific collaborative work. Additionally, to improve the BioCoRE registration form and the definition of users' disciplinary affiliation, a card-sort procedure of fields of study listed by BioCoRE registrants was conducted. As VMD and

NAMD were the first to be launched from within BioCoRE, the BioCoRE evaluation team has conducted the recent VMD[5] and NAMD[6] user surveys.

When suitable measures are not available, the evaluation team develops new instruments to apply to the BioCoRE environment. Two such measures developed for BioCoRE, the Collaboration Technology Self-Efficacy Scale (CTSE)[7] and the Satisfaction with Collaboration Scale (SATCO)[8], were assessed for reliability and validity using BioCoRE registration data. Results indicated satisfactory reliability for the CTSE, but suggested revision for the SATCO. A modified version of the SATCO was subsequently placed on the BioCoRE registration form.

During the past years the evaluation team has been grappling with the need to identify a relevant theoretical approach to frame the evaluation program. Theory applied to groupware typically emphasizes a single topic (e.g. communication channels or a particular feature) or has been ill fit due to assumptions about the state or context of a product (e.g. adaptive structuration and diffusion of innovations). The best option for the BioCoRE evaluation program appears to be a fusion of two complementary models used for technology evaluation: the Triandis model of the antecedents of action, and the Technology Acceptance Model (TAM). The Triandis model is more comprehensive in identifying factors that influence technology acceptance, and the TAM is more specific in identifying perceptions of software. When combined, the two models promise to complement each other and explain overall patterns of BioCoRE use by scientists.

Finally, a summary of the recent BioCoRE survey results indicates that the majority of BioCoRE users are affiliated with academic institutions, and use BioCoRE for research. Most respondents reported to be funded, at least partially, by NIH. The majority of users find BioCoRE easy to learn and use, and are satisfied with BioCoRE support and impact on the quality of their work. Survey response rate was 37% and most users expressed global satisfaction with BioCoRE. The full report[9] is posted on the Resource web site.

Academic users	93%
Use for research	90%
NIH funded	60%
Use local computational resources	86%
Easy to learn	80%
Easy to use	72%
Support team is responsive	86%

[5] http://www.ks.uiuc.edu/Research/vmd/survey/
[6] http://www.ks.uiuc.edu/Research/namd/survey/
[7] http://www.ks.uiuc.edu/Research/biocore/evaluation/NewScales/BioCoRE_CTSE_Scale_Report.pdf
[8] http://www.ks.uiuc.edu/Research/biocore/evaluation/NewScales/BioCoRE_SATCO_Scale_Report.pdf
[9] http://www.ks.uiuc.edu/Research/biocore/survey/

Quality of own work satisfaction	57%
Satisfied overall	66%

Summary of 2002 BioCoRE Survey Findings

Future

In coming years the evaluation program will treat several domains:

First, the definition of the target user population will be refined further through registration data, feedback survey, project data, literature reviews, surveys, and structured interviews. Dynamic determination of target groups, and statistics of BioCoRE usage patterns will draw from data recorded by the built-in evaluation and supporting research. Demographics obtained at registration time will be used to characterize the BioCoRE user population, to identify and project future needs, and to reach new target groups. The resulting profiles will ground the collaboratory in a broader research context, drive expansion goals, help to boost BioCoRE's appeal, and will ultimately increase the visibility and usability of BioCoRE. This analysis will also offer a more reliable basis for conclusions regarding the effectiveness of the BioCoRE collaboratory environment in general and in comparison to traditional research settings and other collaboratories.

Second, three levels of evaluation will be established to accommodate external sites that limit on-line monitoring. Researchers often deal with restrictive policies that prevent the BioCoRE evaluation component from working in full capacity. Moreover, many researchers must comply with company reluctance to cooperate with evaluation paradigms such as BioCoRE‘s. To deal with these constraints, the Resource will distribute versions of the BioCoRE server with three different levels of evaluation. The institution of these levels of data collection will increase the flexibility to users and will prepare the anticipated release of BioCoRE server for easier reception by sectors that practice varying degrees of confidentiality. The levels formulated are:

1. A default level that requests detailed information about who is using BioCoRE, and their usage activities.
2. In cases where no usage data may be released for evaluation purposes, an intermediate level would monitor tool usage, and no information regarding what is being done with each tool would be made available for evaluation.
3. Where only minimal level of monitoring is possible, sites could request that no information at all be returned to the Resource, except for the number of users and their NIH funding status.

Third, the Resource will continue to select third-party tools for integration within BioCoRE based on transparent and clear criteria. The selection and prioritization criteria for new BioCoRE tools will ensure that only high-quality tools will be added to BioCoRE, thereby advancing and sustaining a powerful and coherent computing environment, truly beneficial to biomedical research. The selection process will involve feasibility studies in order to reach reliable and sound

decisions regarding any specific tool considered for integration. The team will use for this purpose surveys, interviews, published reports, literature and trade reviews. The selection criteria are listed below and address matters of content, nature, integration considerations and more:

Applicability and Content
- Relevance to intended research fields and target audience
- Scope and purpose and the fit between the two
- Functionality: does the tool do what it claims to, is the tool general/specific
- Currency: release and update history of the tool, up-to-date concepts underlying the tool, programming language

Nature
- Collaborative value of tool, its popularity, quality of code
- Distribution and availability of tool, accessibility, commercial or not, licensing terms

Technical Aspects
- Stability of tool and ease-of-use
- Potential level of integration: will be determined by source availability, etc.
- Coupling with other tools
- Support of tool's users: availability, accessibility, documentation

The BioCoRE selection criteria will be modified and updated as the collection of tools grows, research needs and priorities change, communication networks become faster and new technological solutions make their way to the market. The process will produce well-structured reports on the tools under consideration and will ensure well-informed and timely development progress.

Last but not least, the Resource will increasingly study BioCoRE's impact on the research process and outcomes. The evaluation efforts will include further usability assessments and prototyping of newly released features and/or integrated tools. Where needed, more inquiry into scientists' work habits will occur. Data generated by the BioCoRE feedback form, available from the BioCoRE front page with real-time tallying of results, will be correlated in the near future with the periodic survey results and will be used to validate ongoing assessments. New reports describing BioCoRE registrant data, BioCoRE user profile, and the theoretical architecture of the BioCoRE evaluation program will be completed.

Challenges

Until now, the greatest challenge for the evaluation team has been developing meaningful indicators of the unobtrusive data. In the coming years the evaluation team will collect, analyze, and interpret systematic information on the attitudes, expectations and needs of users and developers. Interactions among members and between members and technologies will supply another significant data source. Data on the extent of tool usage will be generated through periodic interviews,

content analysis of BioCoRE interactions over time (i.e. patterns of communication), type and frequency of interactions, and of records retrieved from the BioCoRE archive, relying on BioCoRE data mining capabilities.

As BioCoRE is becoming a more mature environment, other significant challenges are anticipated in the near future. Indicators of emerging BioCoRE work culture (shared work values and identity, shared goals), attitude measurements (motivation, commitment, satisfaction), and code of conduct practiced by members will be surveyed. Studying the nature of participants' working relationships and access to resources (clarity of collaborative policies, nature of collaborative relationship and structure, local/national/global-specific emphases) will illuminate additional aspects of BioCoRE climate. Data on potential users and other relevant groups will be gathered when a specific need for comparative analyses arises. The collection of outcome data (resulting publications in refereed journals, references to published work, professional progress of participants, funding resources, and other established indicators) will intensify. Data on factors such as popularity of the new environment, commitment and loyalty to a given technology or a collaboratory tool, success of dissemination efforts and accessibility, will also be assessed. Bug reports and suggestions for improvements will be used in a similar fashion.

We clearly recognize the critical value of evaluating BioCoRE and fully appreciate the complexity of doing it right. This is particularly true in the case of BioCoRE and of collaboratories in general, as these novel work environments are young and, consequently, have not been studied much. The literature, therefore, provides very few evaluation tools that can be safely applied as is to collaboratories' structure, processes, research experience and outcomes. While our commitment to the comprehensive and systematic evaluation of BioCoRE is relentless, with the limited resources allocated for evaluation, analyzing the expected huge and rich unobtrusive datasets, conducting impact studies, and publishing meaningful, reliable and valid assessments will be an equally exciting and demanding undertaking.

Server Distribution

BioCoRE is designed to have multiple local BioCoRE servers running at any given time. This improves response time for the user and allows local sites to customize their own BioCoRE servers. In addition, this redistributes the workload from the Resource's own servers to many local BioCoRE servers around the world. Currently, each local server controls the entire BioCoRE session for its users and no server-to-server communication occurs. In the near future, we expect to have server-to-server communication, so that users can log into the BioCoRE server nearest to them and achieve full functionality in a completely transparent manner, regardless of where and on which of the various BioCoRE servers their project data are stored.

At present, a remote server is available in the Chemistry Department at UIUC and several locations have applied to install remote servers, including NCSA, PSC, BASF (Industry), and CLAN BioTech.

Service, Training and Dissemination

Since February 2002 the unique visits' monthly average to the BioCoRE site has been 13,297, representing a 48% increase in traffic over the past six months. Presently BioCoRE has 106 projects and 463 registrants, and BioCoRE servers are about to be installed in several off-site locations. Dissemination efforts have been extensive and included participation in meetings, workshops, and other events. The BioCoRE brochure[10] and poster[11] are available in printed and electronic formats.

BioCoRE Website and Online Tutorials

Since its very beginning, the BioCoRE team has maintained extensive public and private web sites and BioCoRE is practically being developed online. The public site is by design the Resource's principal BioCoRE dissemination/distribution/communication vehicle and contains general and technical information, as well as direct access to the BioCoRE environment and links to its sister software sites (VMD, NAMD). Deliberately keeping very close to the user community, BioCoRE public site is used first and foremost to communicate with users; share updates on new features; highlight key developments; provide support and bug reports; announce BioCoRE news, events and publications; and train users and prospective members. As a multiple-way communication channel, the public site supplies users with a friendly means to easily contact the BioCoRE team for help, concerns and quick structured feedback. An online BioCoRE tour offers a visual overview of BioCoRE capabilities. Other documentation on the web site describes BioCoRE in more detail, and explains how users may set up an account on the Resource's server for their own research, how interested researchers may choose to download and install their own servers, and more. The internal BioCoRE page supplements the BioCoRE project within BioCoRE itself, providing interfaces to continuously-updated event tracking data, the BioCoRE software bug-tracking system, and other internal documents such as development roadmaps, regular meeting agendas and minutes, work journals and more.

Since BioCoRE is web-based and there is no need for researchers to install new versions, the software is easily updated, and the Resource is able to release updates frequently. The Resource's own server is updated with the most recent improvements approximately every week. The local server code available for downloading is updated whenever significant new features are added, approximately once a month. About every six months, announcements of new BioCoRE features are sent to a number of relevant mailing lists and Usenet news groups. New key features (such as JMV) are announced to the public as they become available and off the regular schedule.

[10] http://www.ks.uiuc.edu/Publications/TB_Brochures/BioCoRE_Brochure/
[11] http://www.ks.uiuc.edu/Research/biocore/presentations/bps2002/

Resulting Papers

BioCoRE: A collaboratory for structural biology. Milind Bhandarkar, Gila Budescu, William F. Humphrey, Jesus A. Izaguirre, Sergei Izrailev, Laxmikant V. Kale, Dorina Kosztin, Ferenc Molnar, James C. Phillips, and Klaus Schulten. 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.

BioCoRE Citations

Quasicontinuum representations of atomic-scale mechanics: From proteins to dislocations. Rob Phillips, Markus Dittrich, and Klaus Schulten. *Annual Review of Materials Research*, 32:219-233, 2002.

BioCoRE Talks, Posters, and Presentations

October, 2002: BioCoRE: A Biological Collaborative Research Environment *Access Grid seminar*, NCSA and other Access Grid nodes. Urbana, IL (K. Vandivort)

August, 2002: BioCoRE: A Biological Collaborative Research Environment Software demonstration, *10th International Conference on Intelligent Systems for Molecular Biology*. Edmonton, Canada. (K. Vandivort; 25-30 attendees)

August, 2002: BioCoRE as a training tool software demonstration. *WEB02 Special Interest Group, 10th International Conference on Intelligent Systems for Molecular Biology*. Edmonton, Canada. (K. Vandivort; 60 attendees)

May 8, 2002: BioCoRE: A Biological Collaborative Research Environment, 2002 *National Computational Science Alliance All-Hands Meeting* (Poster). Urbana, IL. (R. Brunner and K. Vandivort)

February 23-27, 2002: BioCoRE: A Biological Collaborative Research Environment, *2002 Biophysical Society Meeting* (Poster), San Francisco, CA. (B. Isralewitz)

November 15, 2001: BioCoRE - Submits, Runs and Visualizes your Simulation from Afar, *2001 SC Global event.* (Access Grid presentation) Urbana, IL. (K. Vandivort)

March 2, 3, 2001: *2001 College of Engineering Open House*, BioCoRE Demonstration (120 visitors). Urbana, IL. (R. Brunner) http://www.ks.uiuc.edu/Research/biocore/presentations/COEOpenHouse2001/

October 27-29, 2000: *NCRR Biomedical Collaboratories Workshop* Pittsburgh Supercomputer Center. Pittsburgh, PA. (G. Budescu, K. Schulten, K. Vandivort)

May 1, 2000: Demonstration of BioCoRE/Haptic, *HICS Conference*, Beckman Institute, Urbana, IL. (R. Brunner, K. Vandivort)
http://www.ks.uiuc.edu/Research/biocore/presentations/HICS_2000/ (20 visitors)

April 27, 2000: BioCoRE: A Collaboratory for Structural Biology, *Imaging Technology Group Forum*, Beckman Institute. Urbana, IL. (K. Vandivort)

March 3, 4, 2000: *2000 College of Engineering Open House*, BioCoRE Demonstration (294 visitors). Urbana, IL. (K. Vandivort)
http://www.ks.uiuc.edu/Research/biocore/presentations/openHouse/

November 1999: BioCoRE and Interactive Molecular Dynamics (IMD), *SuperComputing 99 Conference*, Portland, Oregon. (K. Vandivort)
http://www.ks.uiuc.edu/Research/biocore/presentations/sc99.shtml

Workshops Supported by BioCoRE
April 17-19, 2002, *NCSA NAMD Workshop 2002*, Biomedical Applications of Molecular Dynamics on the TeraGrid, Champaign, Illinois (32 on-site participants, 60 off-site, http://www.ncsa.uiuc.edu/Divisions/eot/training/NAMD/)

August 15-18, 2001, *PSC NAMD Workshop 2001*, Methods and Applications of Molecular Dynamics to Biopolymers, Pittsburgh, Pennsylvania (20 participants, http://www.psc.edu/biomed/training/workshops/2001/mamd/)

July 10, 2000, EMBL Practical Course on Biomolecular Simulation, Heidelberg, Germany (50 participants)

April 21-May 1, 2000, *Master Classes in Molecular Biophysics*, Perth, Australia (30 participants)

On-Site BioCoRE Demos and Tutorials
July 17, 2002: BioCoRE demonstration, Beckman Institute (Illinos Science Teachers Association: Building A Presence for Science Institute attendees)

April 15, 2002: BioCoRE demonstration and discussion (Ferenc Molnar, BASF Germany)

April 15, 2002: BioCoRE demonstration (Vijay Pande, Stanford University, Nicolae-Viorel Buchete, Boston University)

November 29, 2001: BioCoRE demonstration (Director Pierre Wiltzius, Beckman Institute, Dean David Daniel, College of Engineering, Director John Parks, Research Park and Incubator)

April 6, 2001: BioCoRE Job Submission/Monitoring demonstration, Beckman Institute (NCSA visitors)

March 22, 2001: BioCoRE demonstration, Beckman Institute (Scyld Computing Corporation staff)

July 17, 2000: BioCoRE demonstration, Beckman Institute (Ernest Retzel, Director of the Computational Biology Centers, U of Minnesota)

May 11, 2000: BioCoRE demonstration, Beckman Institute (Olaf Kuebler, President, ETH Zurich; Thomas Eichenberger, Assistant to the President; Computer Science Professors: Moira Norrie, Peter Windmayer, Walter Gander)

Leading Sites Linking to BioCoRE
Search engines yielded 27 links from outside of our domain and key links include:
Biomolecular Modeling:
http://restools.sdsc.edu/biotools/biotools6.html

Computational Chemistry at OSC:
http://oscinfo.osc.edu/chemistry/description/biocore.html

bioinformatics.de link index:
http://www.bioinformatik.de/cgi-bin/browse/Catalog/Software

Collaboratory for Research on Electronic Work:
http://www.crew.umich.edu/resources.htm

European Molecular Biology Network:
http://www.es.embnet.org/links/molmod.html

NCSA news story, Seeing the Light:
http://www.ncsa.uiuc.edu/News/Access/Stories/MolPhotodynamics/light3.html

SC99 Research Exhibits:
http://www.ngi.gov/sc99/demo_contacts.html

Tel Aviv University Bioinformatics unit:
http://www.tau.ac.il/lifesci/bioinfo/sites/sites.html

Department of Chemistry, Technion-Israel Institute of Technology:
http://www.technion.ac.il/technion/chemistry/links/computing.html

Pasteur Institute:
http://www.pasteur.fr/cgi-bin/biology/bnb_s.pl?bool=et&rsc=logiciel

UTHSCSA briefing on bioinformatics developments:
http://bioc09.uthscsa.edu/~hs_lab/bioinfo2.html

NCRR Biomedical Collaboratories Workshop Report:
http://www.ncrr.nih.gov/biotech/btcollabwrkshprpt10-2000.pdf

elegansNet: Organism Bioinformatics and Research Menu Hubsite:
*http://members.tripod.com/C.elegans/index.htm*l