

BioCoRE

A Biological Collaborative Research Environment

Investigators: Klaus Schulten*, PI

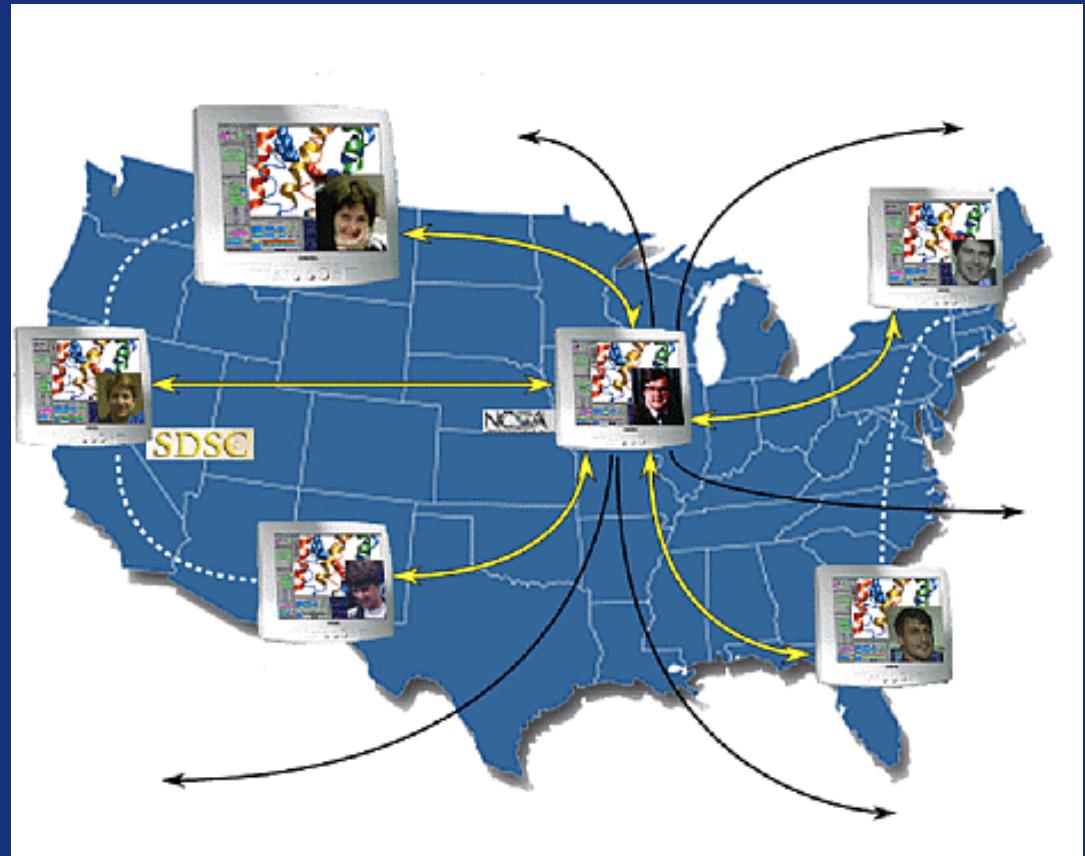
Gila Budescu, Laxmikant Kale

Developers: Mike Bach, Robert
Brunner, Kirby Vandivort, Hui
Wang

Graduate Assistants: Jay
Desouza (CS), Sameer Kumar
(CS), David Brandon (SPCOMM)

October 27-29, 2000

Pittsburgh, Pennsylvania



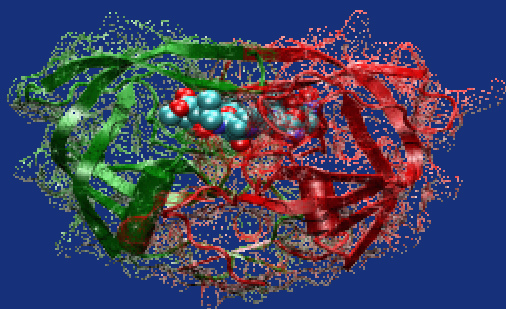
National Center for
Research Resources

NIH Resource for Biomolecular Modeling and Bioinformatics
Beckman Institute, University of Illinois at Urbana-Champaign

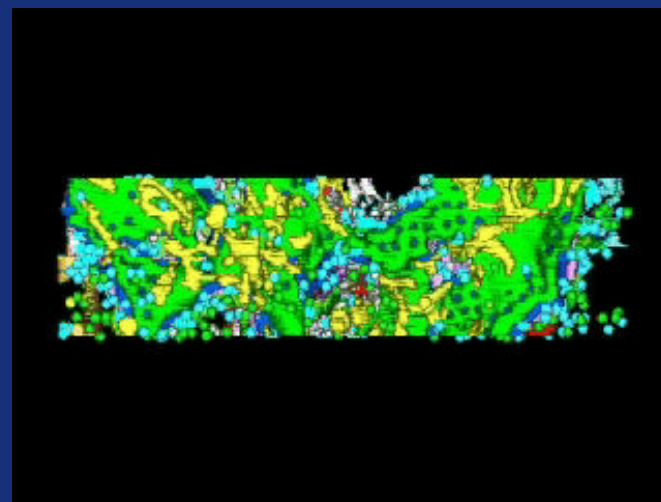
BioCoRE
Biological Collaborative Research Environment

BioCoRE Community

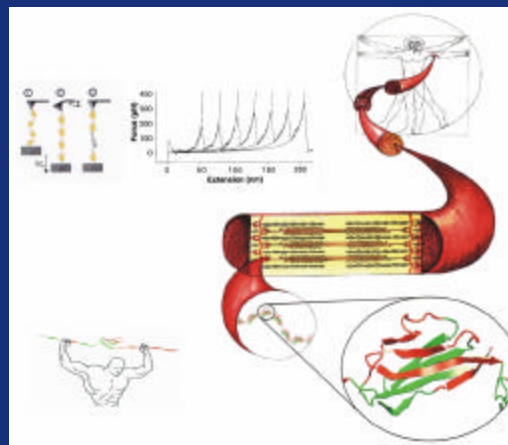
- ∞ Structural Biology
- ∞ Cellular Biology
- ∞ Structural Genomics
- ∞ Pharmacology



HIV Protease image produced by VMD



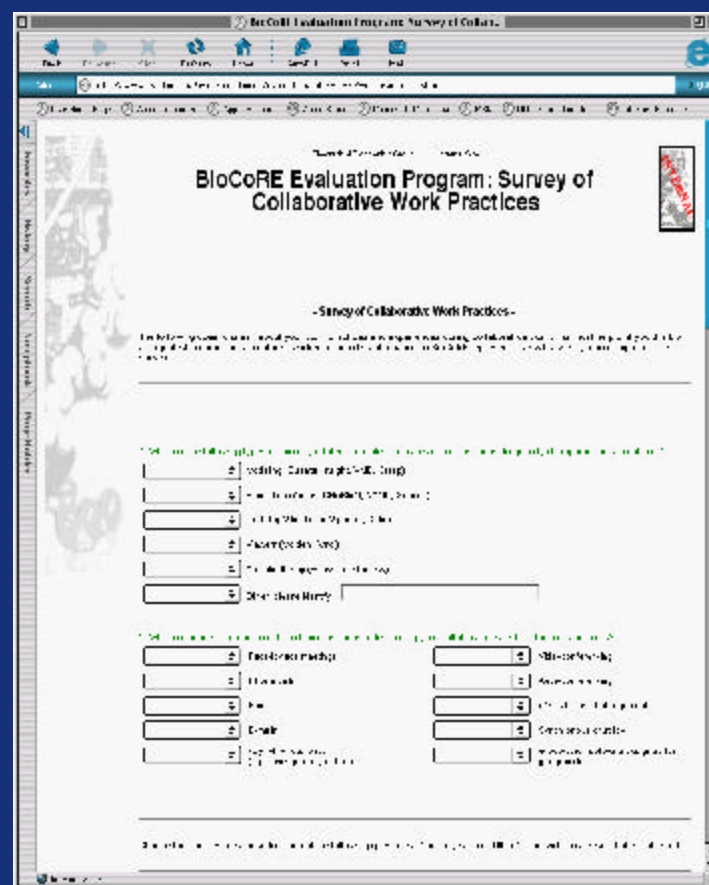
Ladinsky et. al. (1999). Golgi structure in three dimensions: Functional insights from the NRK cell. *J. Cell Biol.*, **144**: 1135-1149



W. M. Keck Center for Comparative and Functional Genomics, University of Illinois Biotechnology Center

BioCoRE Community Needs

- ∞ Access to analysis tools
- ∞ Remote simulation control
- ∞ Shared visualization sessions
- ∞ Data sharing and storage
- ∞ Joint document preparation
- ∞ Distant mentoring and training
- ∞ Multi-channel communication
(conferences, chat rooms, white boards, audio/video)



The screenshot shows a web browser window with the title "BioCoRE Evaluation Program: Survey of Collaborative Work Practices". The page content includes a header with the title and a sub-header "Survey of Collaborative Work Practices". Below the header, there is a section titled "BioCoRE Evaluation Program: Survey of Collaborative Work Practices" with a description of the survey's purpose. The main body of the form contains several sections of questions, each with a list of radio button options. The first section asks about the user's role, with options like "Leading/Coordinating/Managing", "Contributing", "Observing", and "Other (please specify)". The second section asks about the user's primary activity, with options like "Facilitating meetings", "Monitoring/Reviewing", "Providing feedback", "Assessing/evaluating", "Presenting", "Communicating", "Collaborating", and "Other (please specify)". The third section asks about the user's primary mode of communication, with options like "Text-based chat", "Voice-based chat", "Video-based chat", and "Other (please specify)".

Built-in evaluation component yields continuous data on user expectations. Current needs, as identified by interviews, registration and feedback forms, user's comments, and bug reports.

BioCoRE Toolboxes Enhance Research

Current Project: All User Test Project

BioCoRE Control Center

The monitoring tool allows you to start and monitor the progress of computational jobs on various computers. You can monitor the job from any web browser. Also more than one person can attach to and monitor the same job, so your colleagues can also monitor the simulation. And you can run VMD via BioCoRE.

Workbench

Monitoring Tool

• VMD

The ChatRoom allows you to create or join one of channels and participate in a real time text-based discussion either on public or private way. With the combination of the features of the ChatRoom and the Notebook, it provides you a variety of communication options to suit your needs.

Conference

• Chatting Room

The Notebook can be used for storing email-style discussions about the particular project. In addition, the Notebook stores permanent copies of other events that happen in the collaboratory, such as chat. And everything is searchable!

Notebook

• Notebook

Always click logout when you want to leave BioCoRE

Documents

Planned For Future

Utilities

Logout!!

The Utilities section allows you to take care of administrative functions such as changing your password or changing your current project.

asked Questions)

Need Help?

Logging into BioCoRE

- ⌚ Web-based collaborative environment
- ⌚ Platform-independent technology
- ⌚ Secure infrastructure
- ⌚ Private and confidential interactions

BioCoRE Login
You don't have a session yet. Please login!

User Name	<input type="text" value="Jdoe"/>
Password	<input type="password" value="*****"/>
<input type="button" value="Login!"/>	

Our evaluation process relies on surveys as well as usage information generated by BioCoRE users.
If you are a new user and would like to get an account on BioCoRE, [click here](#).

1. [About BioCoRE](#)
2. Please check out our [FAQ \(Frequently Asked Questions\)](#)
3. [Comments, Questions, or Feedback?](#)
4. Copyright 2000 by Board Of Trustees Of UI

Callouts:
- "Login here if you have a BioCoRE account." (points to the Login button)
- "New users can click here to create an account" (points to the "click here" link)

Note that BioCoRE screens are composed of three sections: the header, the main section and the bottom. The Bottom section for each screen usually has a [Need Help] button and a group of information about BioCoRE.

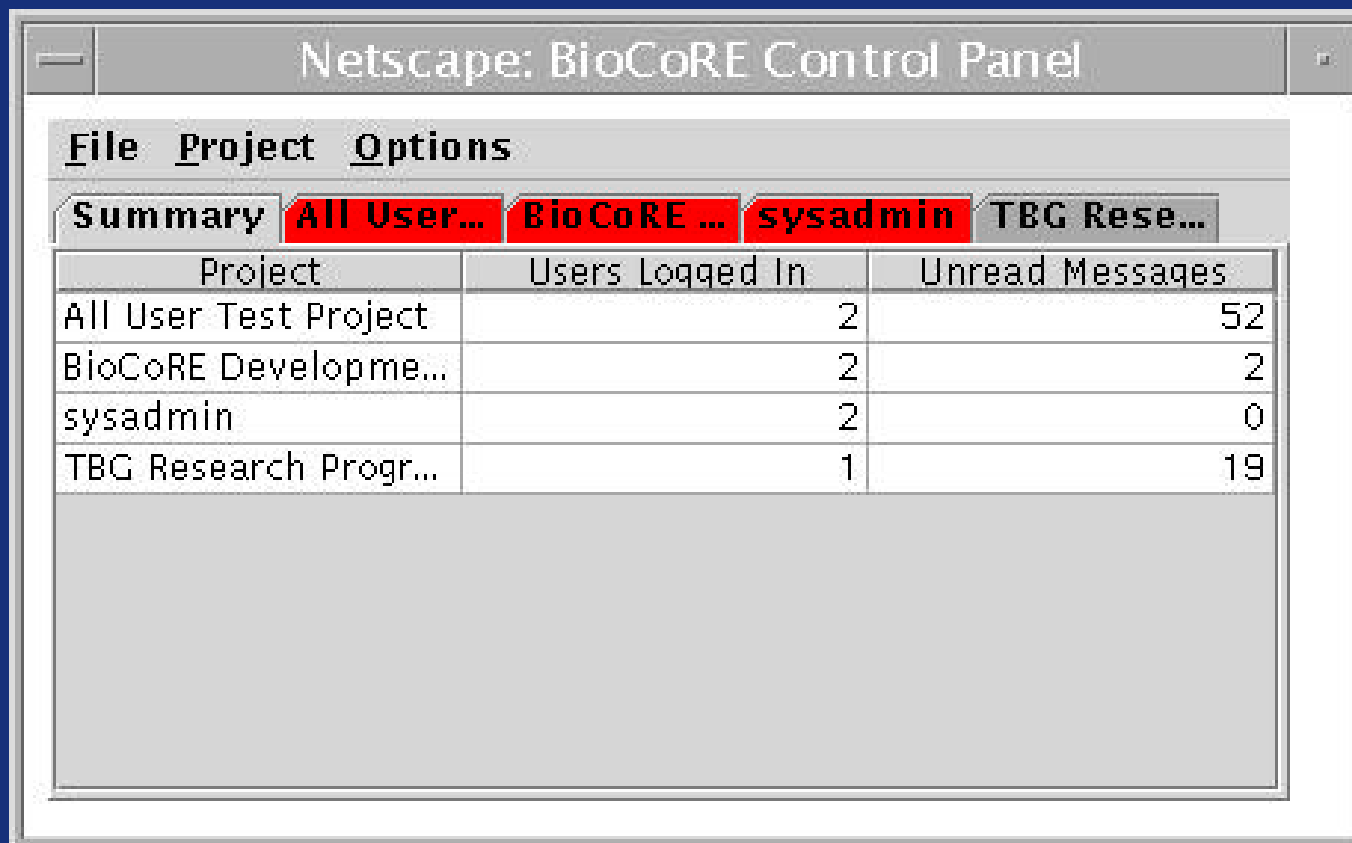
BioCoRE Project Selection

- ⌚ **Functionality:**
Activities are project-based
- ⌚ **Privacy:** Users' and projects' identities are confidential
- ⌚ **Flexibility:**
Projects are created and managed by users

```
Netscape: BioCoRE Control Panel
File Project Options
Summary All User... BioCoRE ... sysadmin TBG Rese...
Wed 14:31:johns>I just crashed the MacOS-X box hard,
had to do hardware reset, even soft power didn't
respond....
Wed 14:31:johns>All that caused it was Justin trying to
login...
Wed 14:43:rbrunner has logged in.
Wed 14:47:johns>After a reboot its working fine again
apparently...
Wed 14:56:rbrunner>You might try BioCoRE on OS-X. It
comes with a recent version of Java, so you shouldn't
need to install Swing.
Message
```

BioCoRE Control Panel

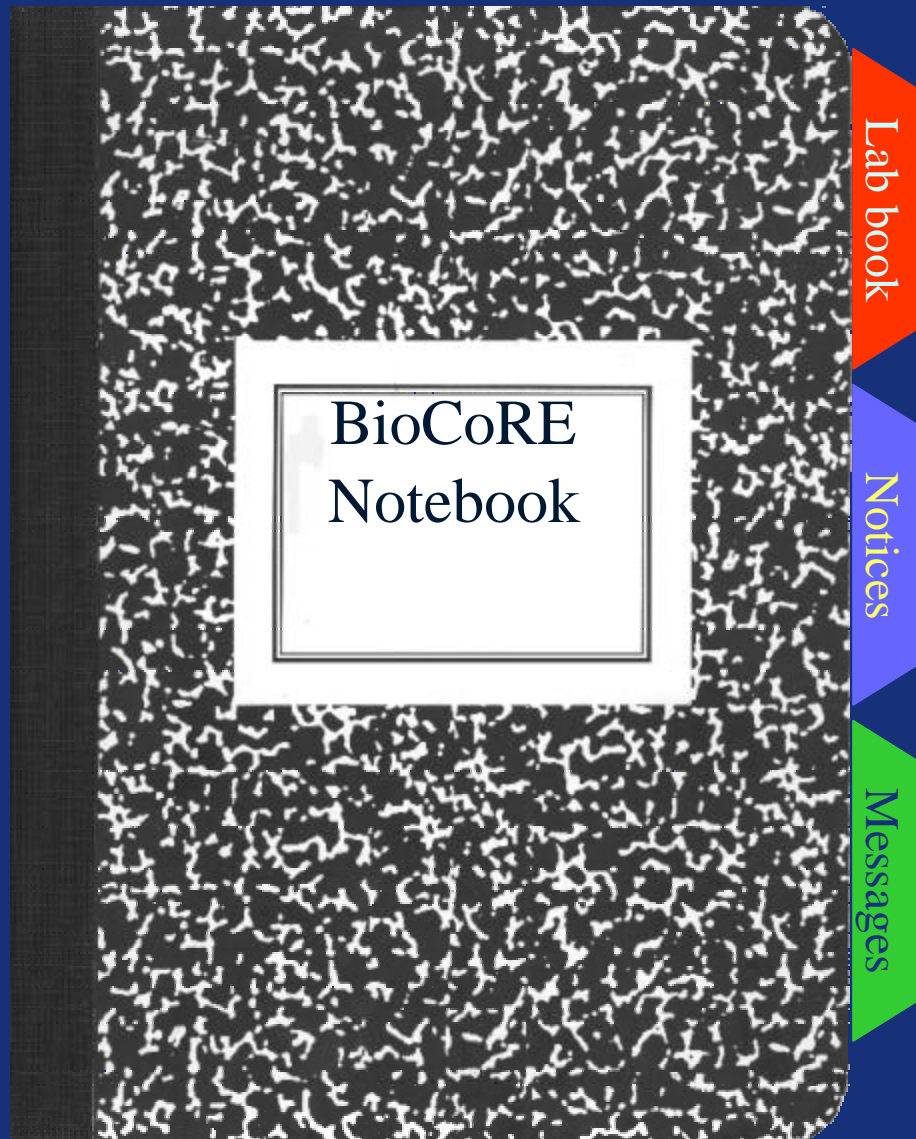
- Immediate feedback of user activity



Project	Users Logged In	Unread Messages
All User Test Project	2	52
BioCoRE Developme...	2	2
sysadmin	2	0
TBG Research Progr...	1	19

- Java applet: dynamic and portable

Notebook Toolbox



- ∞ Repository for all project data
 - Text
 - Images
 - Simulation results
 - Graphs
- ∞ Data integrity and completeness
- ∞ Searchable
- ∞ Lab book
 - Formatted, organized records
- ∞ Notice board
 - Important messages
- ∞ Message board
 - Archive of project activity
 - Sortable

Notebook → Message Board (available)

The screenshot displays a web interface for an "All User Test Project" message board. At the top, there are buttons for "Add" and "Contents", and a "Search" button. Below this is a list of messages, including "Hi (Klaus Schulten, 2000-03-02:10:47)", "Re: Hi (Dorina Kosztin, 2000-03-02:10:47)", "Graphing tools (Barry Isralewitz, 2000-03-07:14:)", "Re: Graphing tools (Barry Isralewitz, 2000-03-07:14:)", "Re: Graphing tools (James Phillips, 2000-03-09:3)", "BioCoRE runs fast now", "biocore tour (hui wang, 2000-03-09:3)", "Re: biocore tour (James Phillips, 2000-03-09:3)", "VMD 1.5a1 is available", and "very impressive (Feren, 2000-03-09:3)".

Callouts provide the following information:

- "You can add messages to the notebook" (pointing to the "Add" button).
- "You can also search all the items in the notebook for the given words." (pointing to the "Search" button).
- "The list of message pages and chat session." (pointing to the message list).
- "You can look at individual messages." (pointing to a message detail view).

The message detail view shows:

Current Project: All User Test Project

Buttons: Add, Contents, Notebook pages

Search: [] Search

From: John Stone
Date: 2000-03-17:11:2804

Hi, for anyone reading, I've just made VMD 1.5 alpha1a for download. Go to: <http://www.ks.uiuc.edu/Development/Id/download>

This version has quite a number of bug fixes and improvements over the previous version of VMD there the Windows version had to be recompiled.

[REPLY] [←] [→]

CLOSE

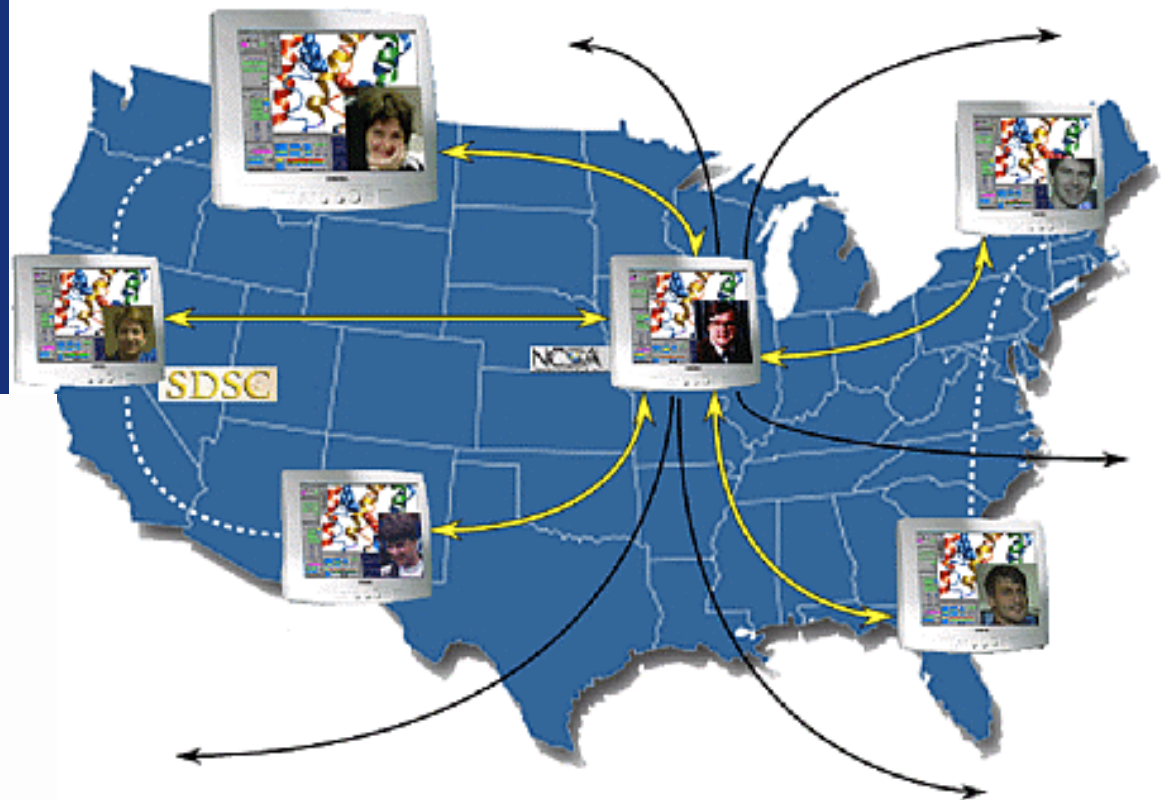
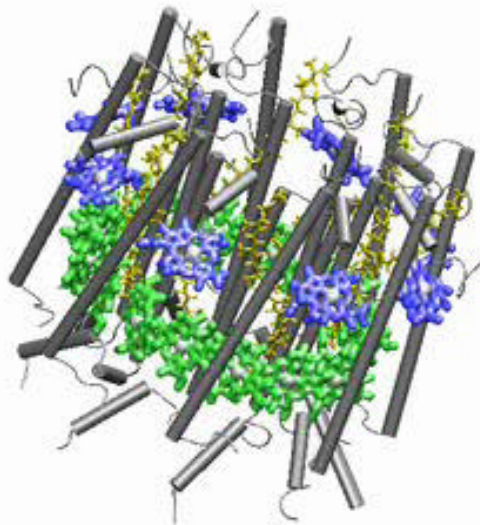
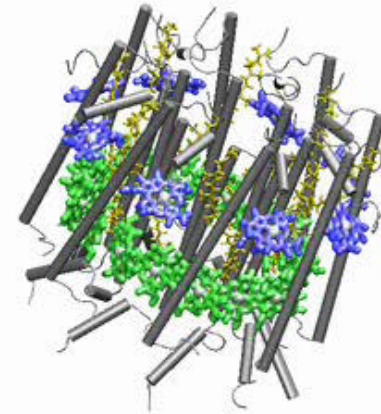
Footer: BioCoRE, Check out our FAQ/Frequently Asked Questions, Questions, or Feedback? Need Help?, © 2000 by Board of Trustees Of UIUC

Users leave messages for other project members

Chat sessions auto-archived

BioCoRE Conference Toolbox

- ∞ Real-time teleconferences: text, audio, video
- ∞ Sessions fully archived in Notebook



Conference → Chat Rooms (available)

- A project member starts a subject-specific chat session
- Project members join and leave chat session
- Transcript auto-saved in notebook

The screenshot displays the BioCoRE Chat interface. At the top, it shows the current project as 'All User Test Project'. Below this, there's a section for 'BioCoRE Chat' with a 'Choose One of Ongoing Channels' dropdown menu currently set to 'BioCoRE Chat Tour [1 user(s)]'. There's also an option to 'Or Create A New Channel' with a 'NEW' text box and a 'Submit/Enter' button. A callout points to this area, stating: 'This is the BioCoRE channel board. You can choose one of the ongoing chats OR create a new channel by typing a subject into the text box.'

The main chat area shows a list of messages. A callout at the top right explains: 'You can see how many people are in this channel before you enter it.' Another callout on the right side states: 'The public message board posts all messages on it. The user's messages such as entering, leaving and e-mail are posted also. When the board is full. The oldest line will be scrolled out and the new one will be added in.'

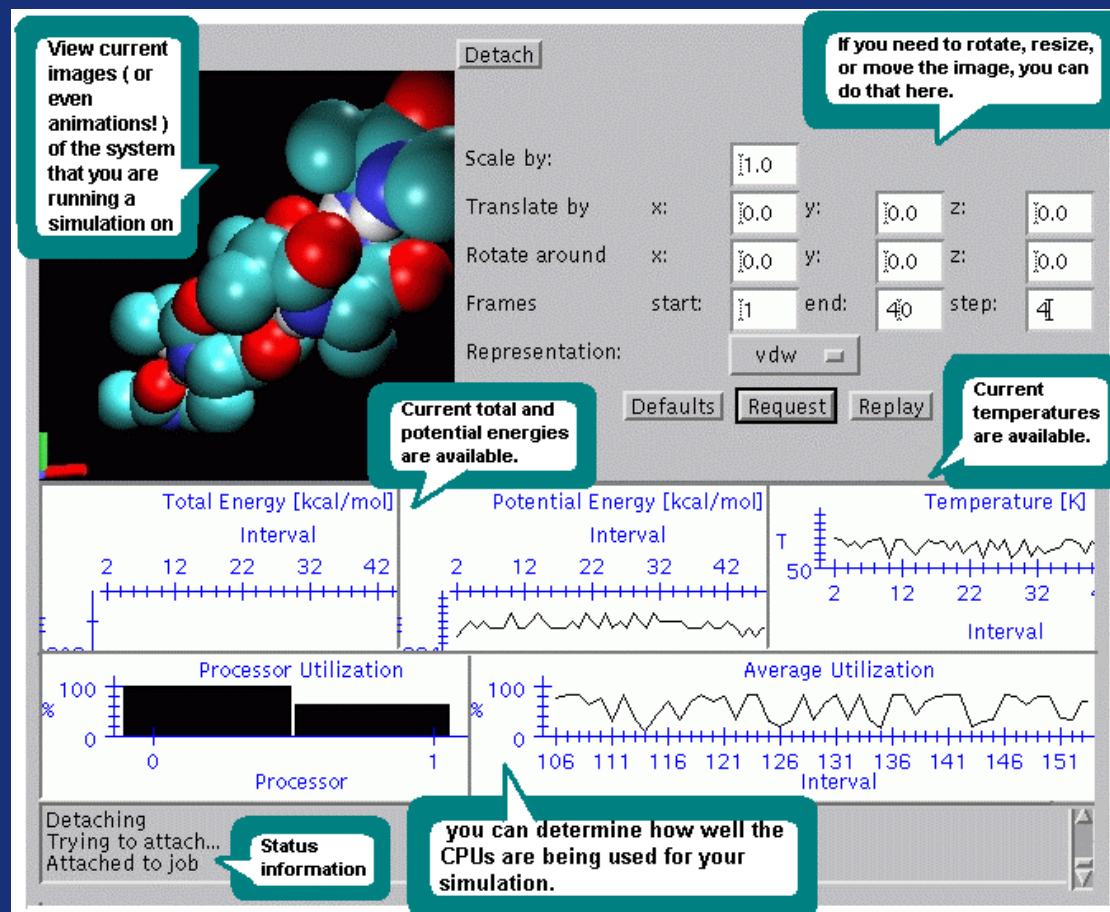
The chat messages include: Andrew Wang has entered this channel; Andrew Wang Hello every body, I just create a new channel for Chat tour. let talk about it.; John Lee has entered this channel; John Lee Hi, every one, I am a new user for BioCoRE. I found it it very interesting to join the channel to talk about the tour. And the text box allows the user to send a huge text file by just copy your file that you want to post and paste it here then click on the Sent/Refresh button. Everyone can see it; Andrew Wang I want to send a private message to Mr. first last By switching the option button from " All User to first last.

Below the main chat area is a 'Private Messages' section. A callout explains: 'A private message feature allows you to send a hidden message to a single person in the room.' The private message section shows a message from John Lee to Andrew Wang: 'Once I get the private message from Mr. hui wang. I like Wang talk something private too to him.'

At the bottom, there's a 'Control Panel: hui wang At Channel: BioCoRE Chat Tour' with a 'Your Message' text box containing 'Welcome to OnLine chatting help: 1.This [chatting started at: Fri Apr 14 11:36:44]'. There are 'Send/Refresh' and 'Leave This Channel' buttons. A callout at the bottom center states: 'The text box even allows you to paste a text file.'

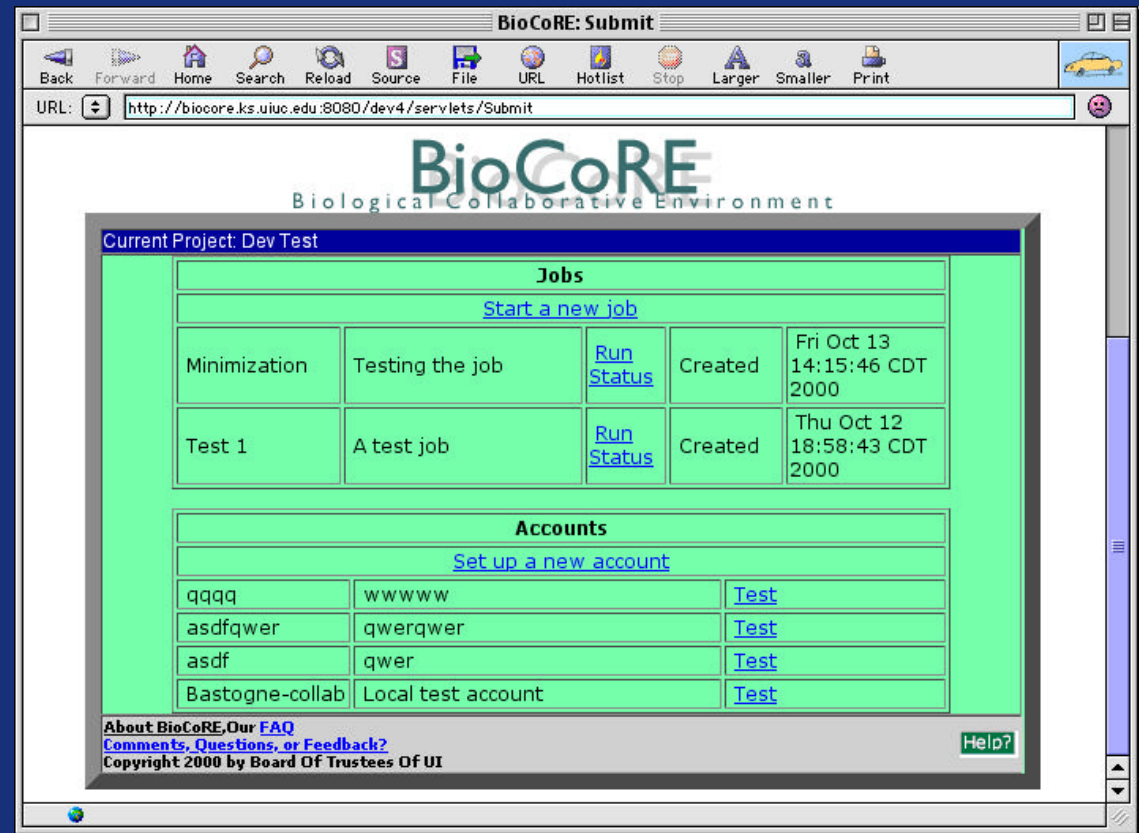
BioCoRE Workbench Toolbox

- Common interface to visualization, simulation, and analysis tools
- Collaborative visualization sessions
- Simplified job submission and monitoring
- Novel input devices



Workbench → Job submission (soon)

- ⌚ User specifies preferred computer account(s)
- ⌚ User defines job parameters
- ⌚ BioCoRE submits job following site-specific procedures
- ⌚ Results of runs accessible to project members



The screenshot shows a web browser window titled "BioCoRE: Submit" with the URL <http://biocore.ks.uiuc.edu:8080/dev4/servlets/Submit>. The page features the BioCoRE logo and the text "Biological Collaborative Environment". Below this, it indicates the "Current Project: Dev Test".

The main content area is divided into two sections: "Jobs" and "Accounts".

Jobs Section:

- A link: [Start a new job](#)
- Table of existing jobs:

Job Name	Description	Run Status	Status	Created
Minimization	Testing the job	Run Status	Created	Fri Oct 13 14:15:46 CDT 2000
Test 1	A test job	Run Status	Created	Thu Oct 12 18:58:43 CDT 2000

Accounts Section:

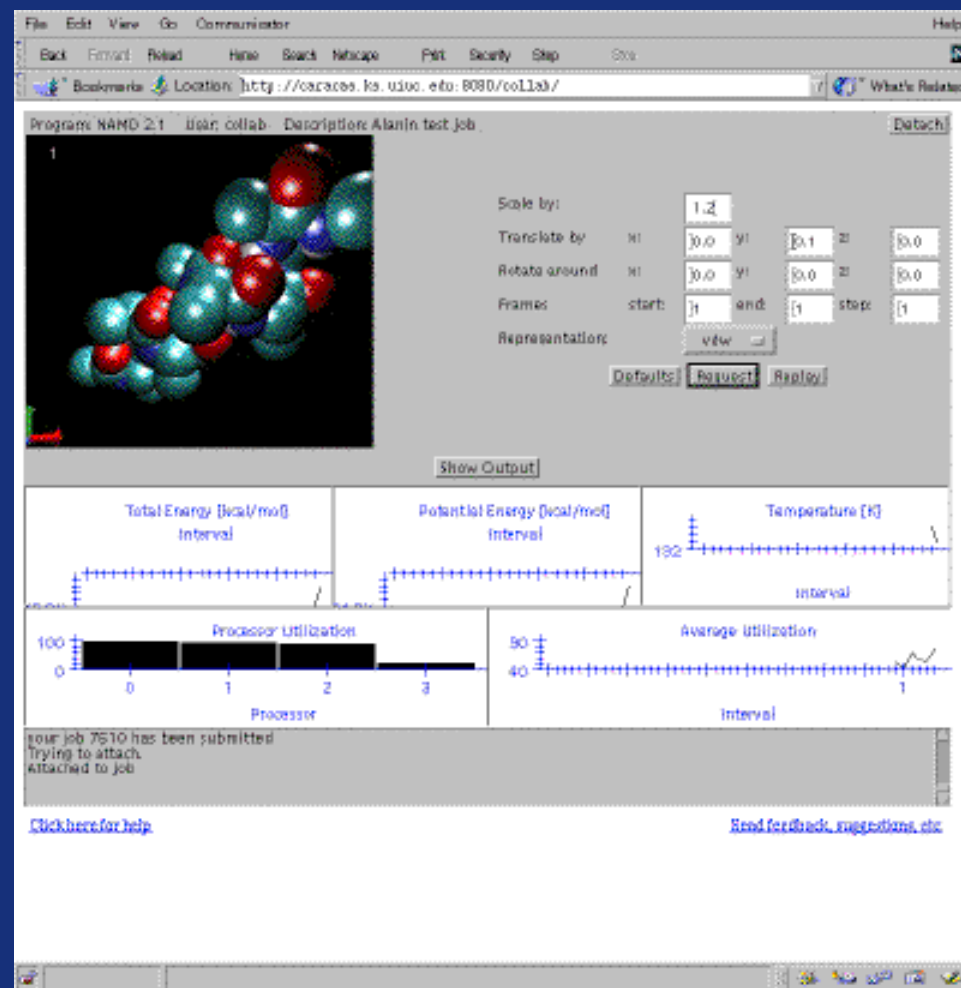
- A link: [Set up a new account](#)
- Table of existing accounts:

Account Name	Description	Action
qqqq	wwwww	Test
asdfqwer	qwerqwer	Test
asdf	qwer	Test
Bastogne-collab	Local test account	Test

At the bottom of the page, there is a footer with the text: "About BioCoRE, Our [FAQ](#), [Comments, Questions, or Feedback?](#) Copyright 2000 by Board Of Trustees Of UI" and a "Help?" button.

Workbench → Job Monitoring (available)

- ⌚ Users can gauge the health of running simulations
- ⌚ Resources are freed by stopping jobs which are not running properly
- ⌚ Job status is viewable from any web browser



Training and Mentoring in Molecular Modeling

- EMBL course, July 2000
 - Participants in Heidelberg ran MD simulations in Urbana using workbench
- Progress review of research activities

Theoretical Biophysics Group

MD Tutorial

Give each person/computer a number. The first computer can be demoC1, the next demoC2, etc. (demoC1 - demoC6 are set up).

Looking at the Input files

Using your web browser, go to:
<http://www.sbl.uiowa.edu/~demouser/>

and read the information at the top of the page and then select the link for your particular user number.

This will take you to the file directory for your user's files. You can click on any file to look at it, or you can right click on the file and download it to your local computer.

File Name	Size	Modified	Permissions
demoC1	1024	2000-07-11	rw-rw-r--
demoC2	1024	2000-07-11	rw-rw-r--
demoC3	1024	2000-07-11	rw-rw-r--
demoC4	1024	2000-07-11	rw-rw-r--
demoC5	1024	2000-07-11	rw-rw-r--
demoC6	1024	2000-07-11	rw-rw-r--

How to use:

Look up 7 - This site directory contains complete files for all of the simulations that you will be doing during this tutorial. (Something's strange happens when you go ahead and use the files in this directory, communicate with the site.)

Look up 8 - Path file for the protein.

Look up 9 - Structure file for the protein.

Look up 10 - Force field, Lagrange multiplier, reference coordinates - I'll call them "files" (they will be run in the order: minimize, equl, largevin, run).

Look up 11 - X-Box parameter file.

You can look at the NAMM configuration files at this time. You will first run the one more (a which should run quickly in about 10 minutes), then you'll run the oil-procasy case around 12.5 minutes and then you'll run the oil-procasy case around 12.5 minutes. (If there's enough time you might run the first job at the site that takes around 12.5 minutes). The process for starting each of the jobs is the same except for the configuration file name.

Logging into BioCoRE

Now, login to BioCoRE to submit your NAMM job(s). Go to:
<http://www.sbl.uiowa.edu/BioCoRE/>

and click on the link named "BioCoRE". All the login information is in the following information:

User Name: demoXX (where XX = 1, 2, ..., 15, as stated above)
User Password: demo

[Link to help/FAQs/Howto/...](#)

BioCoRE Evaluation

Upon joining the project BioCoRE users consent to be evaluated. Sources of user information include:

Process Data:

- ∩ Registration form
- ∩ User-tool interactions
- ∩ User-user interactions
- ∩ Tool-tool interactions
- ∩ Tech support logs and bug reports
- ∩ Special-purpose interviews
- ∩ Periodic surveys and a permanent feedback form



Outcome Data:

- ∩ Users' satisfaction
- ∩ Attrition
- ∩ Resulting publications
- ∩ Citations of resulting work
- ∩ Participants' professional progress
- ∩ Funding resources

BioCoRE Distribution

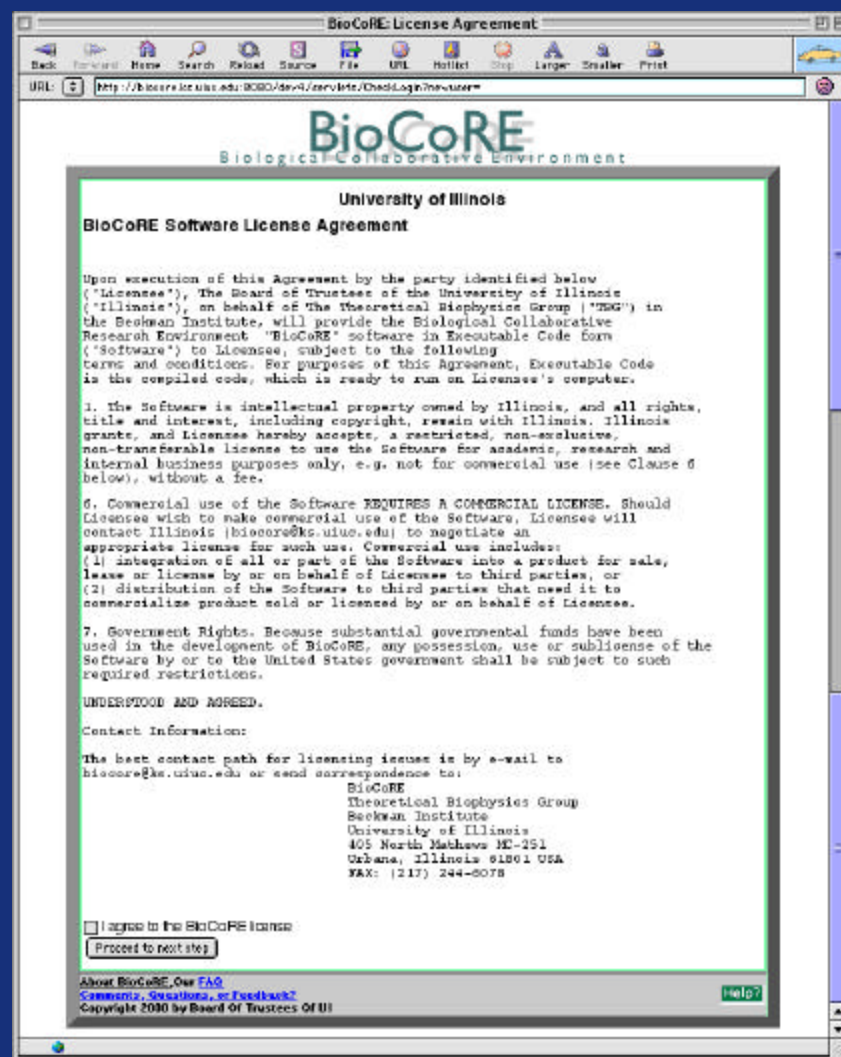
Development history

- February, 1999: BioCoRE development started
- March, 2000: Initial release
- October, 2000: First major update

171 registered users in 13 projects as of October 23; 46% projects NIH funded

Current distribution policy: users register and use our server

Soon: BioCoRE code will be available so others may set up their own servers

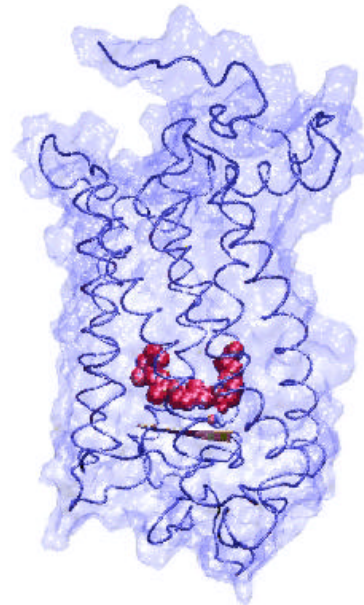


BioCoRE Case Study

- Human Frontier Science Program on Retinal Proteins
- Participating sites are in Japan, Italy, Israel, Germany, and USA

This screenshot shows the BioCoRE notebook interface. At the top, there are buttons for 'Add', 'Contents', and 'Notebook pages'. A search bar is present. Below, a list of messages is displayed, including one from Klaus Schulten and another from Dorina Kosztin. A detailed view of a message from John Stone is shown, dated 2000-03-17, discussing the VMD 1.5a1 software. Callout boxes provide instructions: 'You can add messages to the notebook', 'You can also search all the items in the notebook for the given words.', 'The list of message pages and chat session.', and 'You can look at individual messages.'

This screenshot shows the BioCoRE chat interface. On the left is a 'BioCoRE Chat' channel board with options to 'Choose One of Ongoing Channels' and 'Or Create A New Channel'. The main chat window shows a list of users (Andrew Wang, John Lee) and their messages. Callout boxes explain: 'You can see how many people are in this channel before you enter it.', 'The public message board posts all messages on it. The user's messages such as entering, leaving and e-mail are posted also. When the board is full, the oldest line will be scrolled out and the new one will be added in.', 'This is the BioCoRE channel board. You can choose one of the ongoing chats OR create a new channel by typing a subject into the text box.', 'A private message feature allows you to send a hidden message to a single person in the room.', and 'The textbox even allows you to paste a text file.'



This screenshot shows a code editor displaying a diff between two versions of a Java file. The title bar reads 'Difference for TB/collab/authorization/Check.java from version 1.49 to 1.50'. The code is color-coded to show changes, with red for deletions and blue for additions. The code includes package declarations, imports, and class definitions.