

BioCoRE : The Biological Collaborative Research Environment



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NIH Resource for Macromolecular Modeling and Bioinformatics
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana/Champaign



National Center for
Research Resources

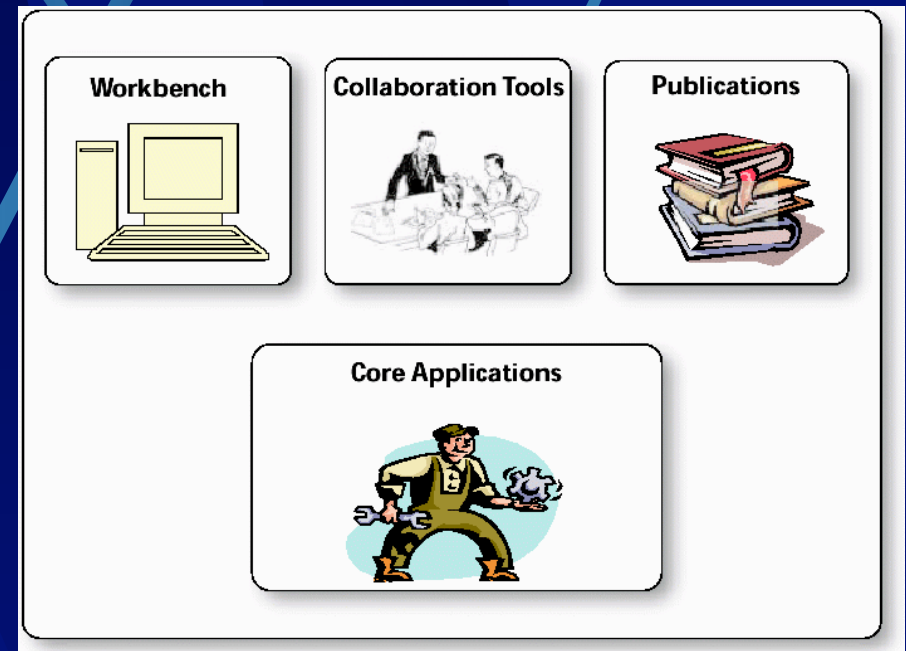
Seminar Outline

- Overview
- Live Demonstration
- Infrastructure/status

Collaboratory Overview

BioCoRE is a comprehensive environment: Workbench; Collaboration Tools; Publications; and Core applications.

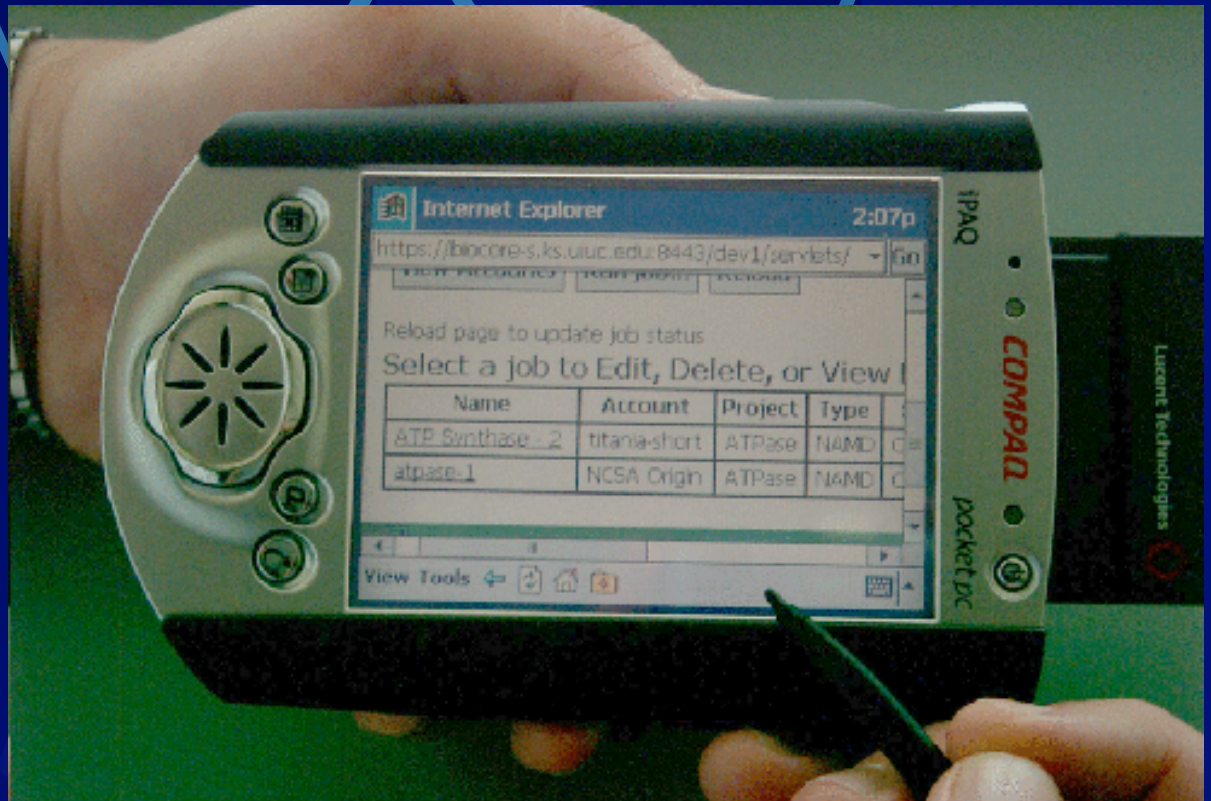
BioCoRE is enhancing the research process by increasing researcher effectiveness, improving collaborations, and providing training tools.



Accessing BioCoRE

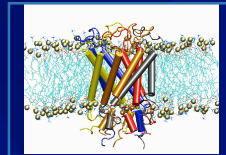
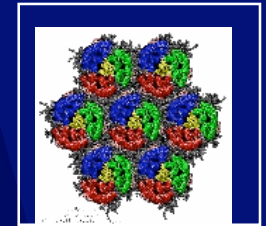
BioCoRE is a web-based collaborative environment.

- Secure browser
 - Windows
 - Unix
 - Mac OS
- Pocket PDAs
- Free!



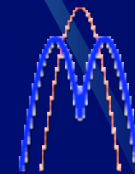
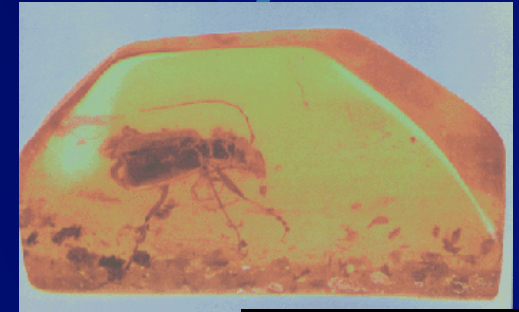
Project-Oriented Environment

- Organized around projects
- Secure (for members'-eyes only)
- Data archived by project
- Ideal for coursework



Research Tool Integration

- Seamless interface for users to tools of interest to researchers
- Planned support for AMBER, CHARMM, MOLPRO, GAMESS, Rasmol, etc.
- Enhanced support for NAMD and VMD
 - Basic analysis functions during simulation
 - VMD load/save session



GAMESS

Summary Page

- Single-view summary
- Instant status report
- Customized for each project

The screenshot displays a web browser window with the BioCoRE interface. The browser's address bar shows the URL: <http://www.ks.uiuc.edu/Research/biocore/>. The page title is "Summary: All User Test Project". The main content area includes a "Project Description" and several sections of recent activity:

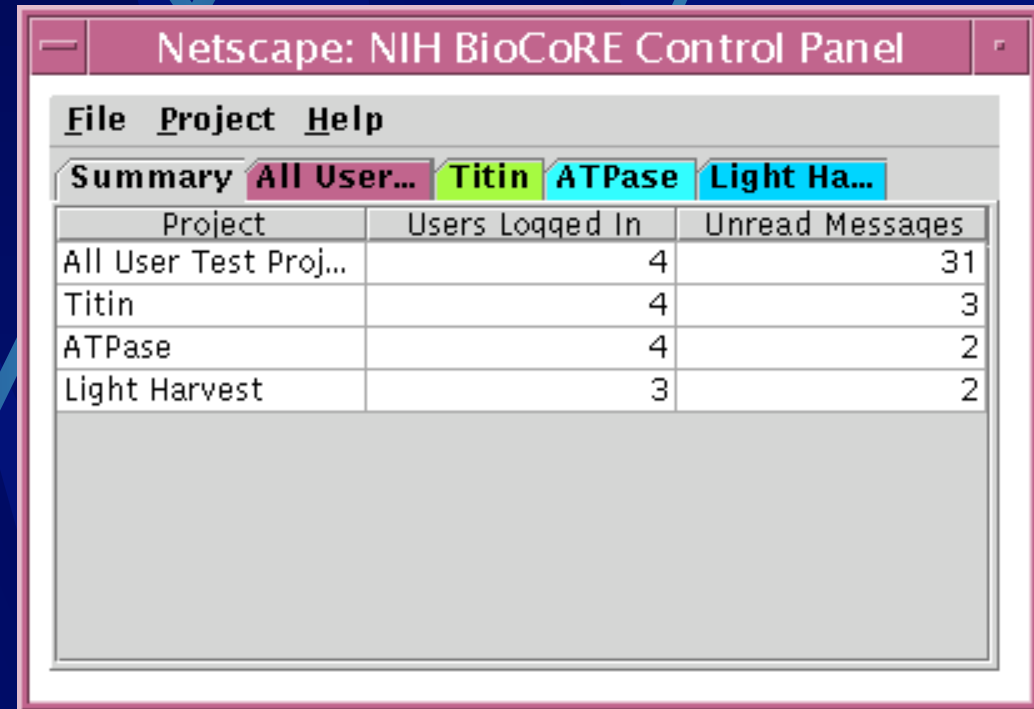
- Recent Lab Book Entries:** 1 Lab Book entry has been added in the past 7 days.
- Recent Message Board Entries:** Includes entries like "Jin Yu -- progress report Oct 19, 2002" and "Re: NAMD and WinXP: beginner question".
- Recent Link Library Entries:** Includes "Ergito - A virtual text company" and "Theoretical Biophysics Group".
- Recent BioFS Entries:** Includes file uploads like "All User Test Project/myfiles/water1.gif" and "All User Test Project/Biocomplexity/coverpage4.pdf".

The left sidebar contains navigation links for "Current Project", "Project Summary", "Workbench", "Notebook", "Documents", and "Utilities".



Control Panel

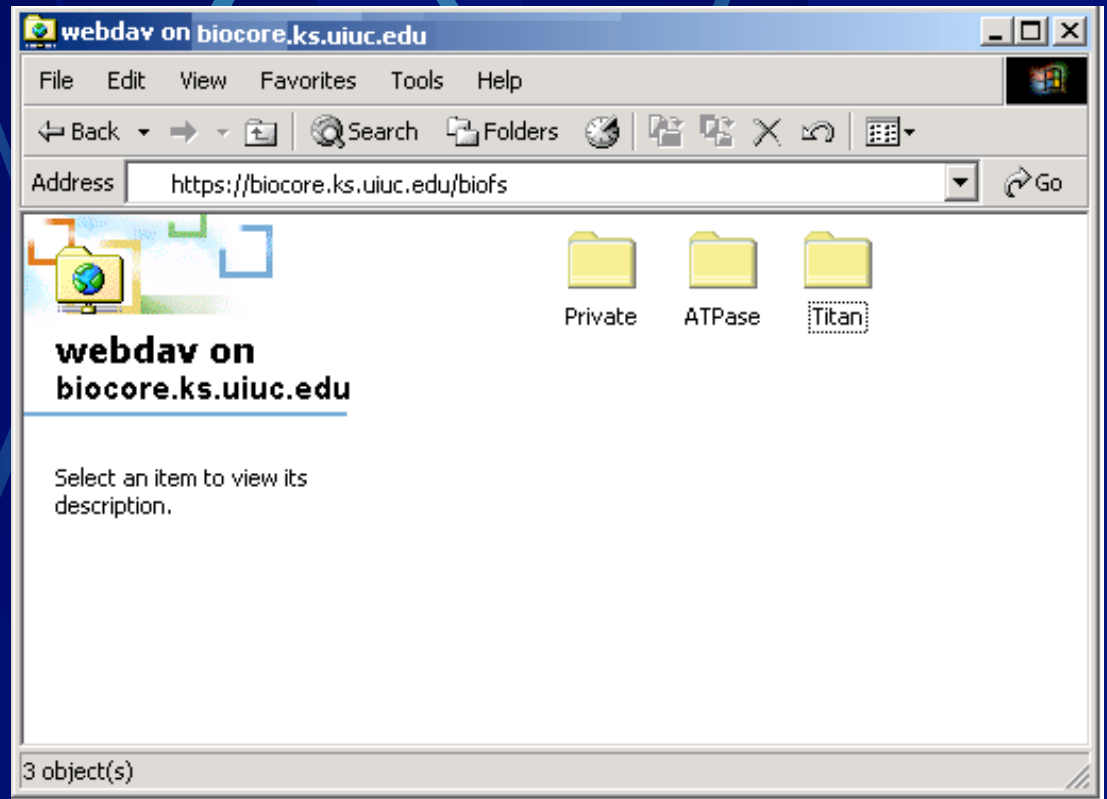
- Event notification
- Communication
- Navigation
- Web Start version
 - No browser required
 - More robust



Project	Users Logged In	Unread Messages
All User Test Proj...	4	31
Titin	4	3
ATPase	4	2
Light Harvest	3	2

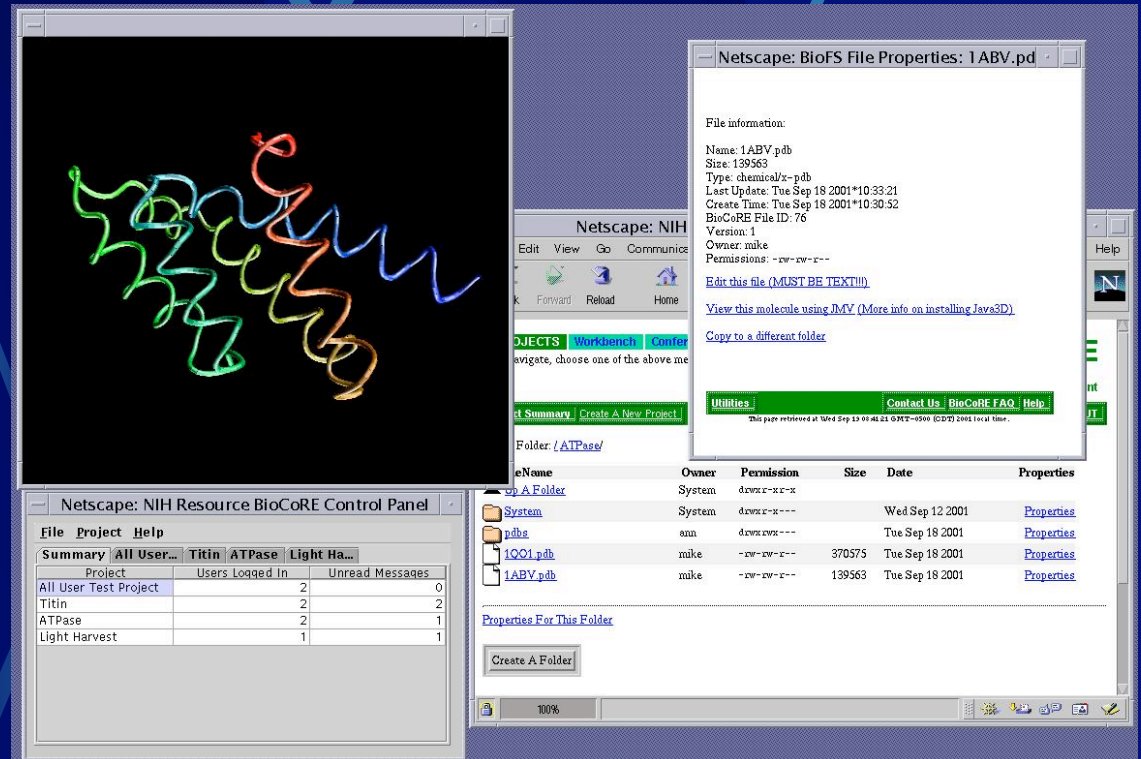
Shared Filesystem

- Web-based, project-oriented filespaces
- High bandwidth utilized
- WebDAV (beta)



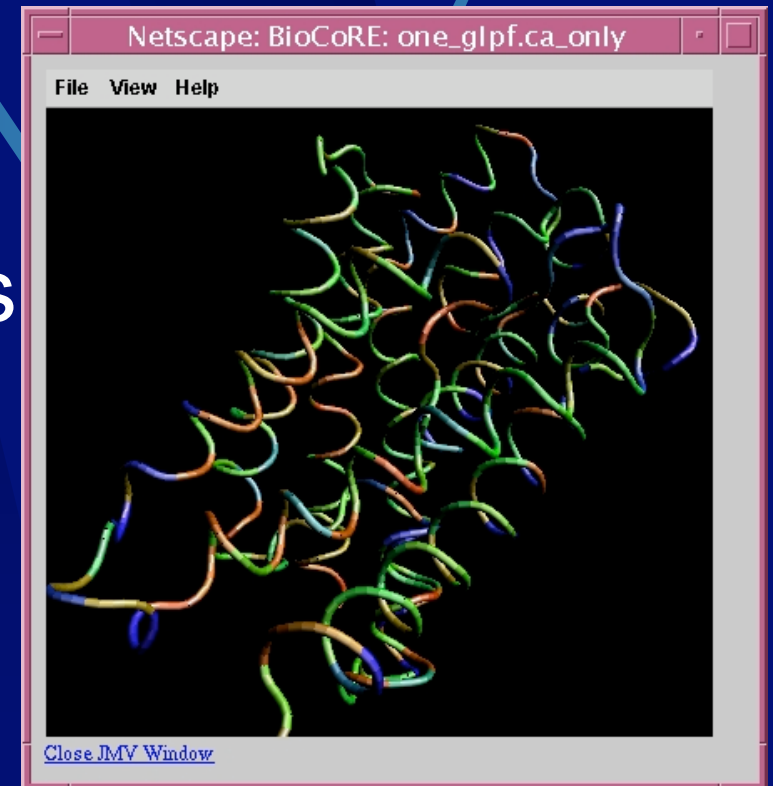
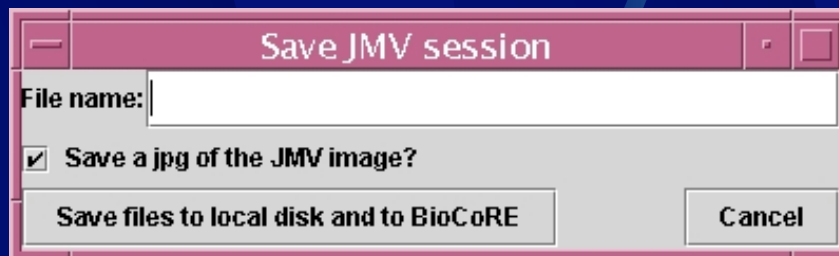
JMV – Java Molecular Viewer

- Web-based molecular viewer:
 - Integrated into BioCoRE filesystem
 - Available for web pages outside of BioCoRE and electronic textbooks.



JMV

- Rotate Views
- Change Representations
- Load/Save views from BioCoRE



Scientific Notebook

- Message Board
 - Asynchronous, Threaded
 - Project-specific
 - Email notification

The screenshot shows a web browser window displaying the BioCoRE Scientific Notebook interface. The browser's address bar shows the URL: <https://biocore-s.ks.uiuc.edu/biocore/servlet/NoteBook?>. The page features a navigation bar with links for PROJECTS, Workbench, Conference, Notebook, and Documents. The current project is identified as 'supercomputing' under the BioCoRE Biological Collaborative Research Environment. A green bar at the top contains links for Project Summary, Create A New Project, and LOGOUT. Below this, there is a 'Show:' dropdown menu set to 'Message Board Contents', a 'Create New Message' button, and a search input field with a 'Search' button. The main content area displays a message from Rosemary Braun, dated Mon Dec 10 2001*10:46:58, with the subject 'Creating a project in BioCoRE'. The message text explains the BioCoRE project structure and provides two numbered steps for creating a new project and inviting collaborators. At the bottom of the message, there are links for 'Edit This Message', 'Reply To This Message', and 'Delete This Message'. The footer of the page includes 'Utilities', 'Contact Us', 'BioCoRE FAQ', and 'Help' links, along with a timestamp: 'This page retrieved at Tue Mar 05 10:14:31 GMT -0600 (CST) 2002 local time.' and a 'Reload Control Panel, Webstart' link.

Scientific Notebook

- Message Board
 - Asynchronous, Threaded
 - Project-specific
 - Email notification
- Website Link Library
 - Project-wide *Bookmarks* file
 - Links ranked by popularity
 - Tighter integration planned with communication tools

The screenshot shows a web browser window displaying the BioCoRE website. The browser's address bar shows the URL: <https://biocore-s.ks.uiuc.edu/biocore/servlet/LinkLibrary?p=57&se>. The website has a green header with navigation tabs for 'PROJECTS', 'WorkBench', 'Conference', 'Notebook', and 'Documents'. The current project is 'supercomputing'. Below the header, there is a 'Website Library' section with an 'Add Main Topic' button. The library is divided into two main categories: 'Software' and 'Supercomputing Centers'. The 'Software' section includes links to NAMD, AMBER, CHARMM, GROMACS, and TINKER, each with a brief description and a date. The 'Supercomputing Centers' section includes links to NRAC proposal information, Alliance Allocations, and PSC Grant Information for PACI Users, also with descriptions and dates.

Lab Book

- Progress Report
- Sorted by Author

File Edit View Go Bookmarks Tools Window Help

TB-UIUC BioCoRE: Lab book Conte...

BioCoRE Change Project: [All User Test Project](#) | [BioCoRE Development](#) | [kvandivo family](#) | [sysadmin](#) | [JMV](#) | [TB Group](#) | [TBL](#) | [TB Devel](#) | [F.O.R.](#) | [biolog](#) | [VMD](#) | [BioCoRE@NCSSA](#)

HELP LOGOUT

Current Project: BioCoRE Development

Lab book: Project members can use the lab book as a place set aside for keeping journals.

Add New Entry

Sort By: [Thread] [Subject] [Author] [Date] [Mark All] [Read]

View Lab book entries from last [all] days

Kirby Vandivort

- [10/7-10/11](#) (Kirby Vandivort, Tue Oct 15 2002*09:24:08)
- [10/3-10/4](#) (Kirby Vandivort, Fri Oct 4 2002*14:33:21)
- [9/25-10/2](#) (Kirby Vandivort, Wed Oct 2 2002*15:58:25)

Mani Potnuru

- [Progress Report 10/9 - 10/16](#) (Mani Potnuru, Wed Oct 16 2002*14:33:48) UNREAD
- [Mani's Progress Report](#) (Mani Potnuru, Wed Oct 9 2002*14:23:45)

Michael Bach

- [Mike's Progress Report \(10/16/2002\)](#) (Michael Bach, Wed Oct 16 2002*13:01:36) UNREAD
- [Mike's Progress Report \(10/09/2002\)](#) (Michael Bach, Wed Oct 9 2002*10:02:15)
- [Mike's Progress Report \(10/02/2002\)](#) (Michael Bach, Wed Oct 2 2002*15:50:44)

Robert Brunner

- [17 October, 2002](#) (Robert Brunner, Fri Oct 18 2002*01:00:26) UNREAD
- [16 October, 2002](#) (Robert Brunner, Wed Oct 16 2002*13:46:42) UNREAD
- [8 October, 2002](#) (Robert Brunner, Wed Oct 9 2002*10:13:04)
- [Re: 4 October, 2002](#) (Robert Brunner, Fri Oct 4 2002*16:46:11)
- [4 October, 2002](#) (Robert Brunner, Fri Oct 4 2002*16:42:02)
- [3 October, 2002](#) (Robert Brunner, Fri Oct 4 2002*09:29:08)
- [1 October, 2002](#) (Robert Brunner, Wed Oct 2 2002*10:03:29)

Sameer Kumar

- [Progress Report OCT 9-16](#) (Sameer Kumar, Wed Oct 16 2002*13:45:34)
- [Sameer's Progress Report](#) (Sameer Kumar, Wed Oct 9 2002*12:45:28)

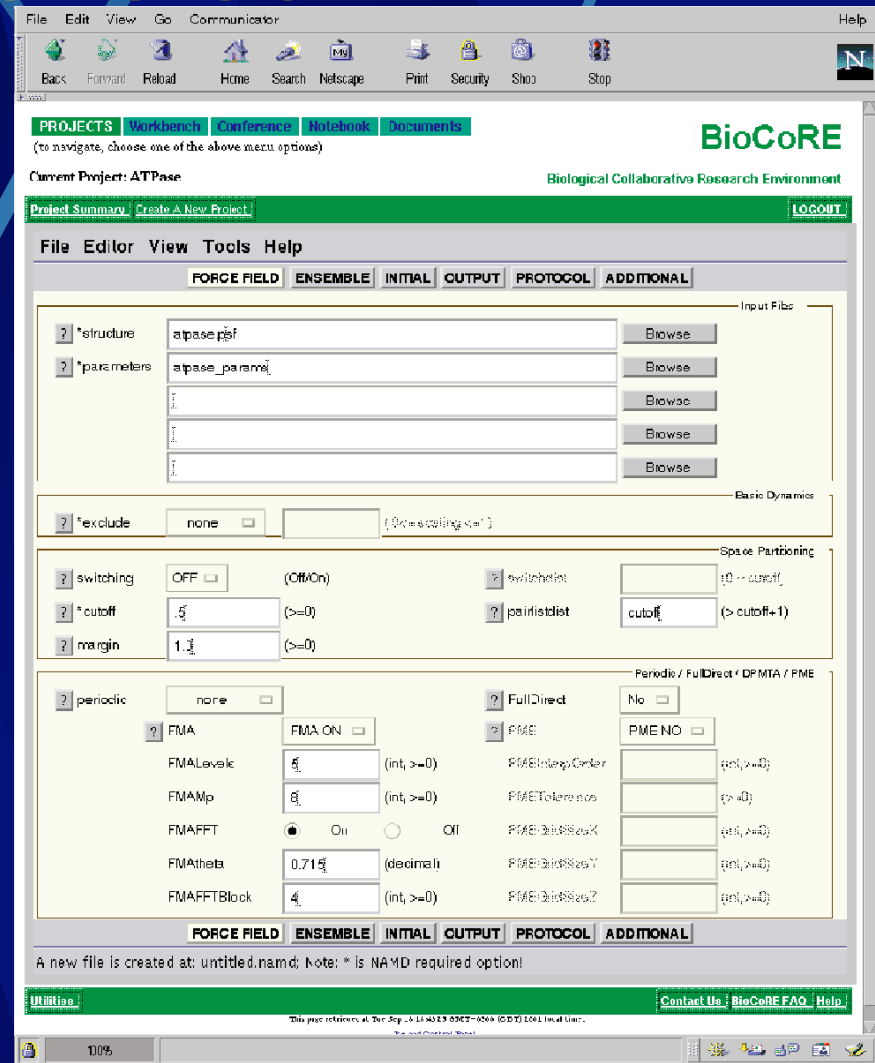
[View previously deleted Lab book entries](#)

This page retrieved at Mon Oct 21 2002 15:05:30 GMT-0500 (CDT) local time.
Control Panel: [Applet](#), [Webstart](#) ([more info](#))

Document: Done (1.139 secs)

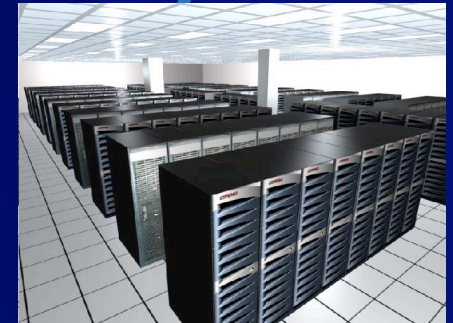
Simulation Configuration File Generator

- Simplifies creation of NAMD/HYDRA simulation input files
- Checks for common input errors
- Offers context-sensitive help
- Coming soon: Support for other configuration file-driven programs (e.g. CHARMM)

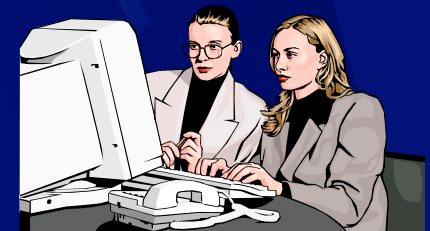


Supercomputer Job Management

- User submits/monitors supercomputer jobs
- User accesses multiple supercomputers from a single BioCoRE page
- Handles system-specific aspects (queues, etc) automatically
- Acts as front-end to Globus

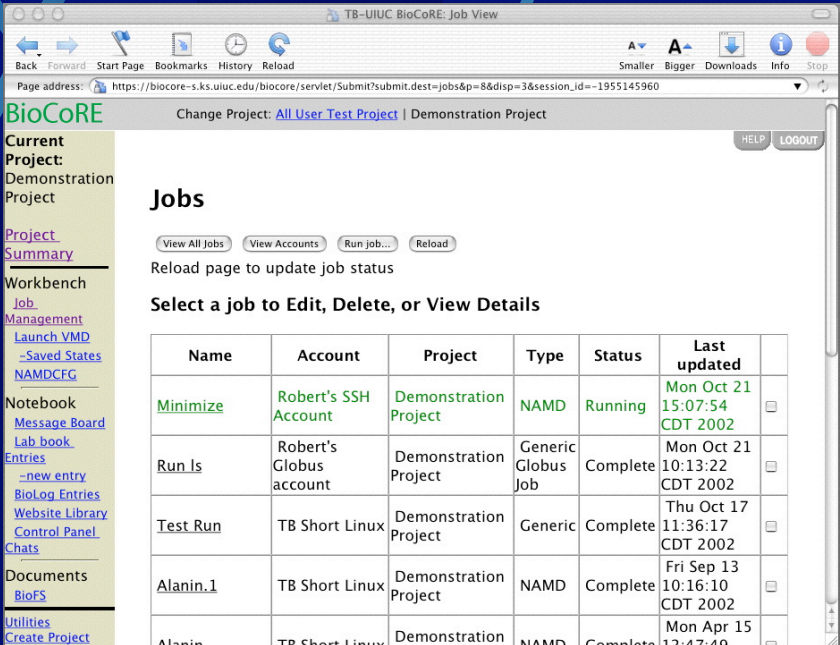


BioCoRE
Biological Collaborative Environment



What Job Management Does For You

- Submits jobs to supercomputers or local machines
- Keeps track of accounts and jobs
- Provides a simplified form-based interface
- Sends input files from BioCoRE to remote resource
- Retrieves and archives output files
- Monitors job status



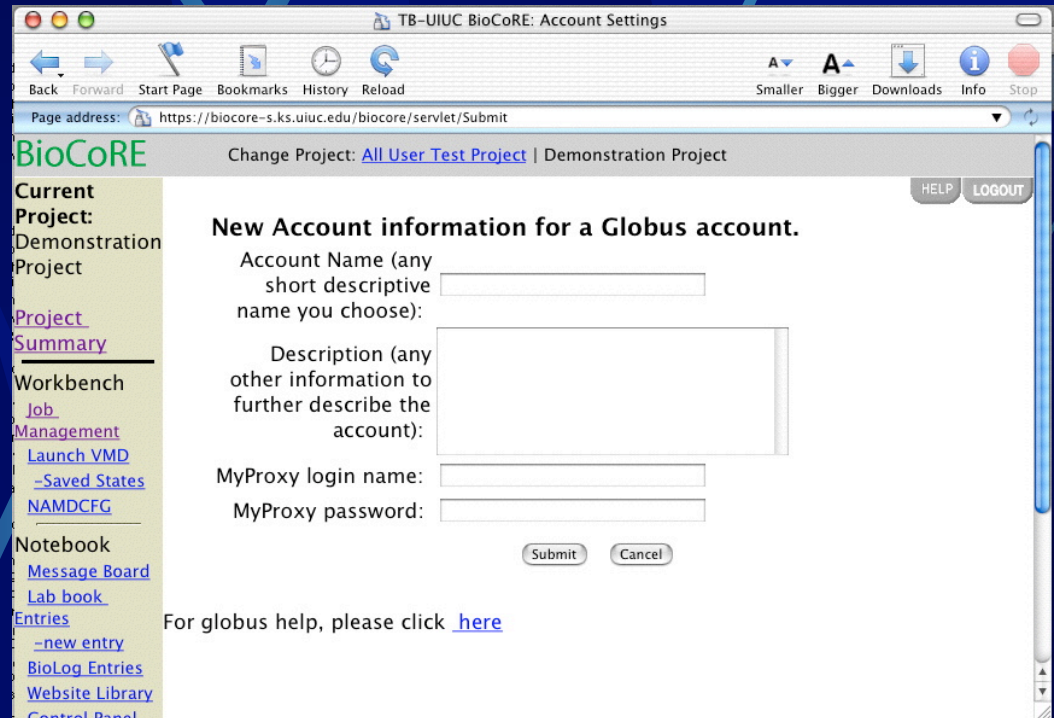
The screenshot shows the BioCoRE Job View web interface. The browser address bar displays the URL: https://biocore-s.ks.uiuc.edu/biocore/servlet/Submit?submit.dest=jobs&p=8&disp=3&session_id=-1955145960. The page title is "BioCoRE" and the current project is "Demonstration Project". The interface includes a sidebar with navigation links such as "Project Summary", "Workbench", "Notebook", "Documents", and "Utilities". The main content area displays a table of jobs with columns for Name, Account, Project, Type, Status, and Last updated. The table contains the following data:

Name	Account	Project	Type	Status	Last updated
Minimize	Robert's SSH Account	Demonstration Project	NAMD	Running	Mon Oct 21 15:07:54 CDT 2002
Run ls	Robert's Globus account	Demonstration Project	Generic Globus Job	Complete	Mon Oct 21 10:13:22 CDT 2002
Test Run	TB Short Linux	Demonstration Project	Generic	Complete	Thu Oct 17 11:36:17 CDT 2002
Alanin.1	TB Short Linux	Demonstration Project	NAMD	Complete	Fri Sep 13 10:16:10 CDT 2002
Alapin	TB Short Linux	Demonstration Project	NAMD	Complete	Mon Apr 15 12:47:49

Supports NCSA Origin 2000 and Platinum, and PSC T3E and TCS, and is easily extended for other platforms

How It Works

- Users create an Account, which tells BioCoRE how to access a remote system
 - Uses SSH or Globus/MyProxy
 - BioCoRE sets up temporary credentials or an SSH private/public key pair
 - User password not stored



The screenshot shows a web browser window titled "TB-UIUC BioCoRE: Account Settings". The address bar shows the URL "https://biocore-s.ks.uiuc.edu/biocore/servlet/Submit". The page content includes a navigation menu on the left with links for "Project Summary", "Workbench Job Management", "Notebook Message Board", and "Entries". The main content area is titled "New Account information for a Globus account." and contains the following fields:

- Account Name (any short descriptive name you choose):
- Description (any other information to further describe the account):
- MyProxy login name:
- MyProxy password:

There are "Submit" and "Cancel" buttons at the bottom of the form. Below the form, there is a link: "For globus help, please click [here](#)".

Running Jobs

- User selects a Job type
 - Generic jobs: Any command line or script
 - Applications (e.g. NAMD)
- User selects an account
- Form-interface provides prompts for filling in job details

The screenshot shows a web browser window titled "TB-UIUC BioCoRE: Job Settings". The address bar shows the URL "https://biocore-s.ks.uiuc.edu/biocore/servlet/Submit". The page content includes a sidebar with navigation links such as "Current Project: Demonstration Project", "Project Summary", "Workbench", "Notebook", "Documents", and "Utilities". The main content area is titled "Required information for application NAMD running on account Robert's SSH Account". It contains several form fields: "Job Name (any short descriptive name you choose)" with a text input field containing "Minimize"; "Description (any other information to further describe the job)" with a text area containing "Minimize BPTI"; "Working directory on remote machine; absolute path, or relative to home directory (no ~):" with a text input field containing "tstrun"; "Application information:" section with "NAMD Executable Path:" (input: "/usr/local/bin/namd2"), "NAMD input filename:" (input: "minimize.namd"), and "Standard output file (optional, if file exists std. output will be appended):" (input: empty).

Completing Job Request

- User provides name and description for job
- User fills in work directory and application parameters
- User selects input files from the BioFS to be staged to the work directory
- Job console output automatically retrieved. Other output files may also be specified

Required information for application NAMD running on account Robert's SSH Account

Job Name (any short descriptive name you choose):

Description (any other information to further describe the job):

BioCoRE does not yet stage files to the remote machine, so you have to put your files there manually.

Working directory on remote machine; absolute path, or relative to home directory (no ~):

Application information:

NAMD Executable Path: :

NAMD input filename:

Standard output file (optional, if file exists std. output will be appended):

Submitting the Job

- BioCoRE submits the job
 - creates a job script
 - stages it (and other input files) to the remote system
 - Monitors the job status

Name	Account	Project	Type	Status	Last updated
Minimize	Robert's SSH Account	Demonstration Project	NAMD	Running	Mon Oct 21 15:07:54 CDT 2002
Run ls	Robert's Globus account	Demonstration Project	Generic Globus Job	Complete	Mon Oct 21 10:13:22 CDT 2002
Test Run	TB Short Linux	Demonstration Project	Generic	Complete	Thu Oct 17 11:36:17 CDT 2002
Alanin.1	TB Short Linux	Demonstration Project	NAMD	Complete	Fri Sep 13 10:16:10 CDT 2002
Alanin	TB Short Linux	Demonstration Project	NAMD	Complete	Mon Apr 15 12:47:49 CDT 2002

Job Monitoring

- BioCoRE monitors and reports job status (Submitted, Running, Complete, etc.)
- Upon completion, BioCoRE retrieves job output
- User can view console output of the job as its running
- Files are accessible upon job completion

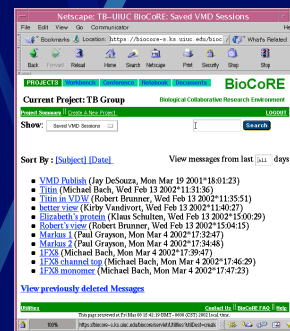
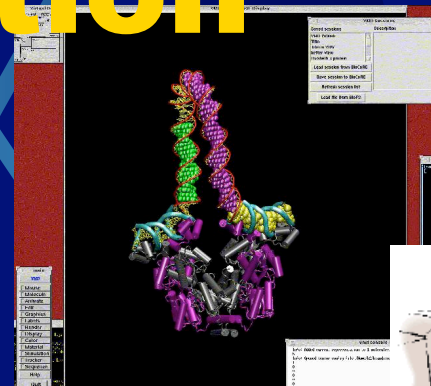
```
Change Project: All User Test Project | Demonstration Project

Current Project: Back
Demonstration Project Go to bottom...
Project Summary
Workbench
  Job Management
  Launch VMD
  -Saved States
  NAMDCFG
Notebook
  Message Board
  Lab book
Entries
  -new entry
  BioLog Entries
  Website Library
  Control Panel
Chats
Documents
  BioFS

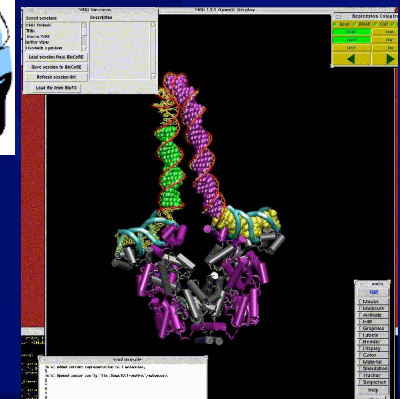
BIOCORESTART:3504.2002.10.21.15.07.41.
Info: NAMD 2.5b1 for Linux-i686-Scyld
Info:
Info: Please visit http://www.ks.uiuc.edu/Research/namd/
Info: and send feedback or bug reports to namd@ks.uiuc.edu
Info:
Info: Please cite Kale et al., J. Comp. Phys. 151:283-312 (1999)
Info: in all publications reporting results obtained with NAMD.
Info:
Info: Sending usage information to NAMD developers via UDP.
Info: Sent data is: 1 NAMD 2.5b1 Linux-i686-Scyld 16 titania.ks
Info: Running on 16 processors.
Info: 4327 kB of memory in use.
Measuring processor speeds... Done.
Info: Configuration file is minimize.namd
TCL: Suspending until startup complete.
Info: SIMULATION PARAMETERS:
Info: TIMESTEP 2
Info: NUMBER OF STEPS 500
Info: STEPS PER CYCLE 10
Info: LOAD BALANCE STRATEGY Other
Info: LDB PERIOD 2000 steps
Info: FIRST LDB TIMESTEP 50
```

Collaborative Visualization

- Loads VMD visualization sessions
- Saves visualization sessions in Scientific Notebook
- Will offer similar support for other visualization programs
- Training



BioCoRE
Biological Collaborative Environment



Accessing Shared Visualizations

- Researchers start VMD sessions from BioCoRE
- Views are stored into the notebook

Netscape: NIH BioCoRE: Saved VMD States

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Bookmarks Location: <https://ostia.ks.uiuc.edu:8443/biocore/serv1> What's Related

BioCoRE Change Project: [All User Test Project](#) | [ATPase](#) | [Titin](#) | [Glycerol](#)

Current Project: ATPase HELP LOGOUT

Project Summary **VMD States:** This page shows a listing of all of the VMD states that have been saved in this project. These states can be saved to BioCoRE directly from VMD by clicking on Launch VMD in the lefthand column.

Workbench
[Job Management](#)
[Launch VMD](#)
[-Saved States](#)
[NAMDCFG](#)

Notebook
[Message Board](#)
[Lab book Entries](#)
[-new entry](#)
[BioLog Entries](#)
[Website Library](#)
[Control Panel Chats](#)
[NEW Notebook Editor](#)

Documents
[BioFS](#)

Utilities
[Create Project](#)
[Contact Us](#)
[BioCoRE FAQ](#)

Sort By : [\[Subject\]](#) [\[Date\]](#) View VMD saved states from last days

- [GLPF](#) (Bob McAlister, Wed Oct 16 2002*13:44:22)
- [Glycerol Channel](#) (Bob McAlister, Wed Oct 16 2002*13:45:12)

[View previously deleted VMD saved states](#)

Control Panel [Applet](#) [Webstart](#) (more info)

Document: Done.

Selecting a View

- Stored View contains a snapshot and annotation

Netscape: NIH BioCoRE: Saved VMD Session

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Bookmarks Location: <https://ostia.ks.uiuc.edu:8443/biocore/servlet/Not> What's Related

BioCoRE Change Project: [All User Test Project](#) | [ATPase](#) | [Titin](#) | [Glycerol](#)

Current Project: ATPase

[Project Summary](#)

Workbench
[Job Management](#)
[Launch VMD](#)
[- Saved States](#)
[NAMDCFG](#)

Notebook
[Message Board](#)
[Lab book Entries](#)
[- new entry](#)
[BioLog Entries](#)
[Website Library](#)
[Control Panel Chats](#)
[NEW Notebook Editor](#)

Documents
[BioFS](#)

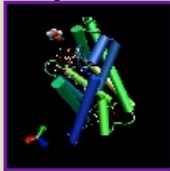
Utilities
[Create Project](#)
[Contact Us](#)
[BioCoRE FAQ](#)

START VMD SESSION

▪ Next message: [Glycerol Channel](#)

From: Bob McAlister
Date: Wed Oct 16 2002*13:44:22
Subject: GLPF

Image:

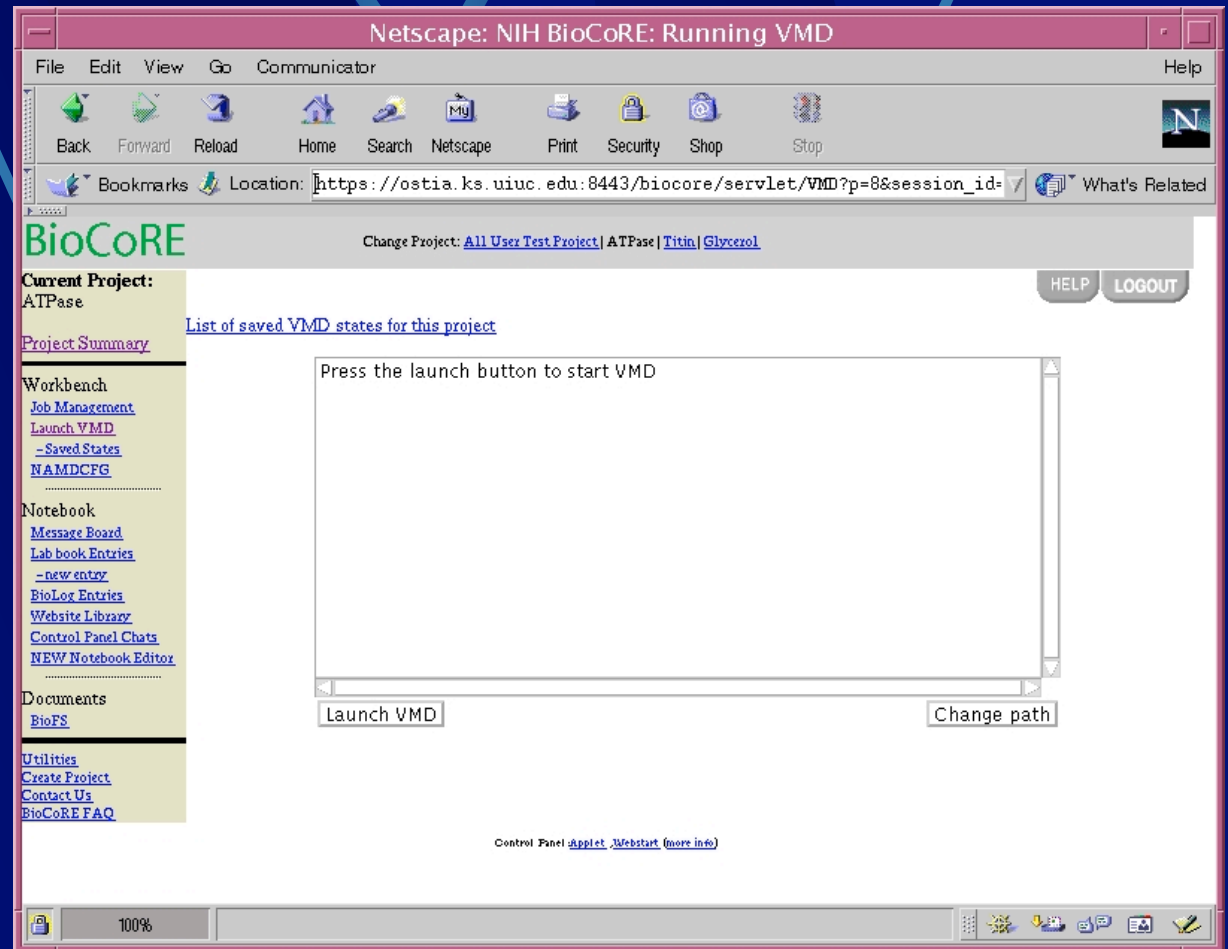


VMD version: 1.8a27
Pub/synch version: .70
Description: Published on: Wed oct 16 13:30:56 CDT 2002
Description: For E. Coli to absorb glycerol (a simple sugar), and use it for energy, the glyco
Description:
Description:
#! /usr/local/bin/vmd

100%

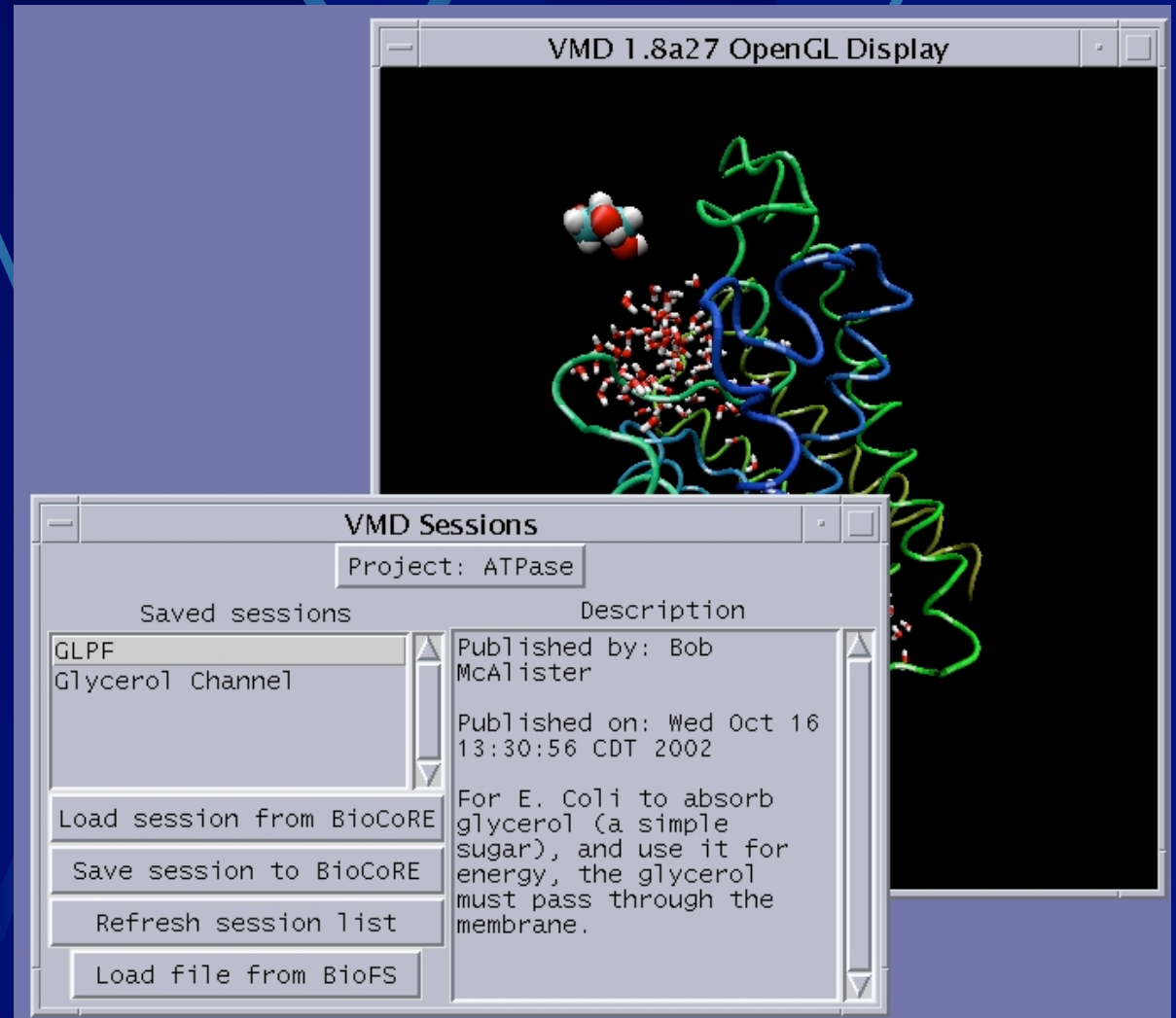
Loading the View

- A Java applet loads VMD, which is installed on the local machine



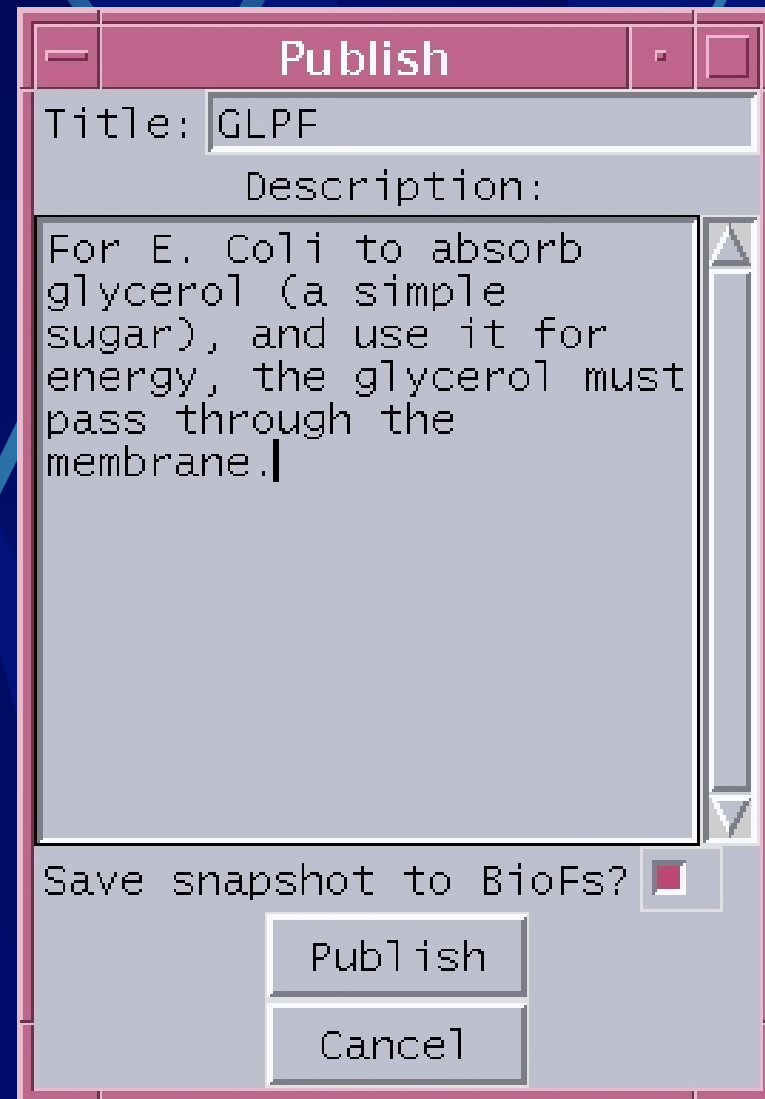
Loading the View

- VMD launches with a VMD Sessions window that lets users load and save states



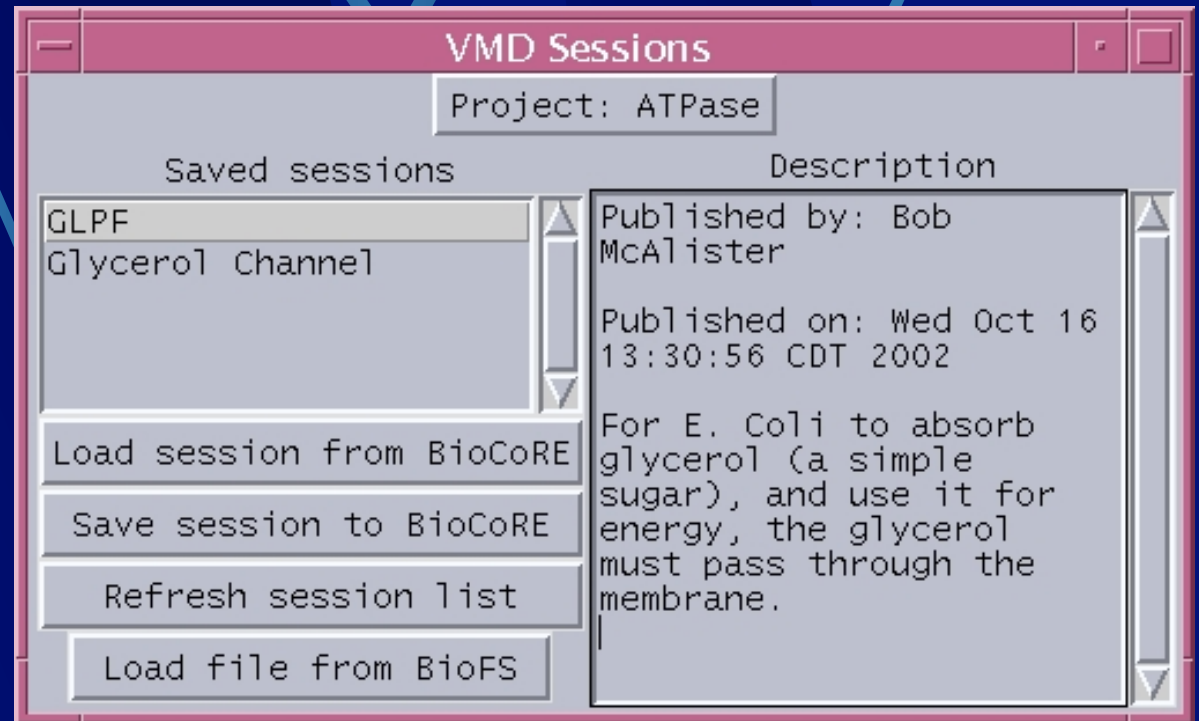
Saving a View

- Clicking the “Save Session to BioFS” button brings up the Publish box



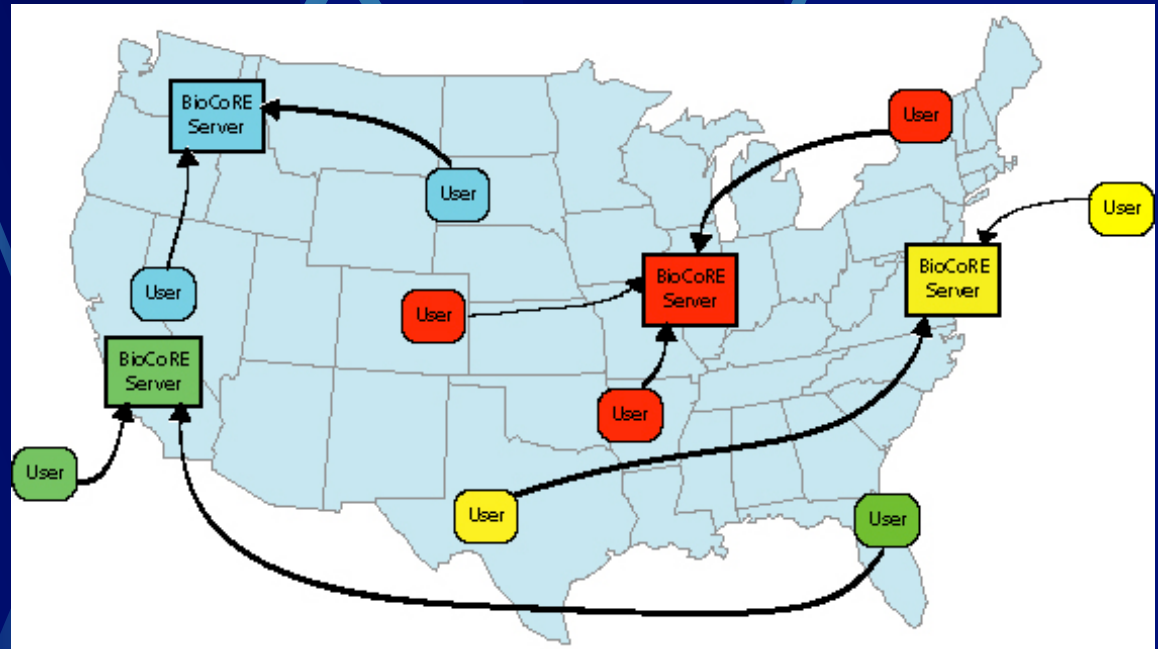
Sharing a View

- The Control Panel notifies others that a new Session has been published
- The Sessions window shows the new session



BioCoRE Server Community

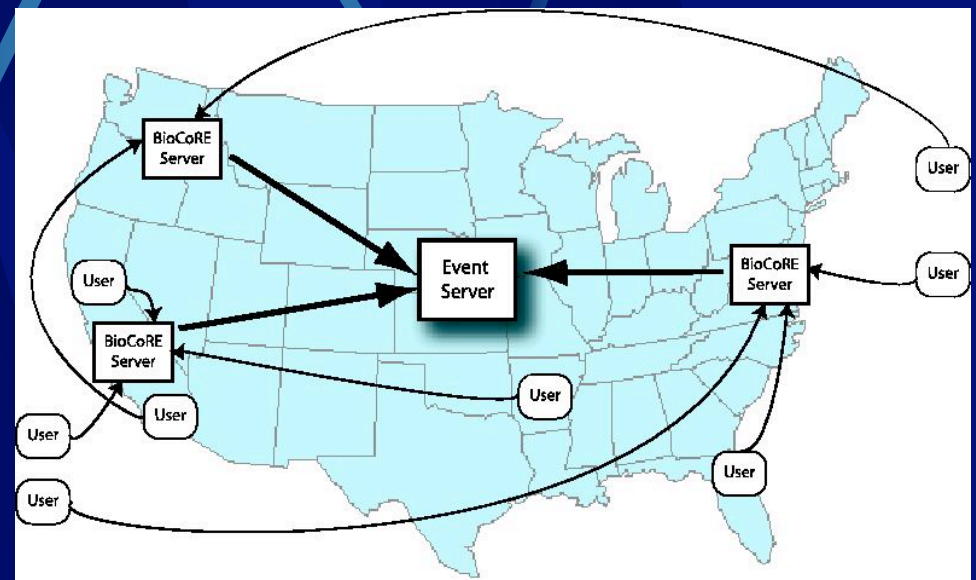
- Parent server at Illinois
- Server software at other academic locations, super-computer centers, and industry
 - Faster access
 - More customizability
 - Privacy



Evaluation

BioCoRE's built-in evaluation component provides continuous user data and feedback.

- External servers report usage patterns to the Illinois server
- Usage information helps guide development



Status

- 500 registrants, 100+ projects after 2.5 years of operation
- BioCoRE server software released
 - NCSA, PSC, and industry are deploying servers
- BioCoRE in meetings, workshops, newsgroups, e-mail lists, web, press releases (SC2001, BPS 2002, PSC 2000, on-site demos)
- BioCoRE in training (NCSA NAMD 2002, EMBL, PSC, U. Western Australia)

The End

<http://www.ks.uiuc.edu/Research/biocore/>



Don't Go Past This Slide

