

BioCoRE

Submits, Runs, and Visualizes Your Simulation From Afar

Presenter: Kirby Vandivort

K. Schulten (PI), G. Budescu, L. Kalé

Development Team: M. Bach, D. Brandon, R. Brunner, J. DeSouza, S. Kumar,
K. Vandivort, H. Wang

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



BioCoRE Overview

BioCoRE is a collection of web-based tools that:

- Forms a complete environment for biomedical research
- Allows single password login
- Is freely available

BioCoRE consists of Java servlets accessed through secure Apache with a database back end

BioCoRE Goals

(**B**iological **C**ollaborative **R**esearch **E**nvironment)

- Enhance the research process
- Increase researcher effectiveness
- Improve collaborations

Netscape: BioCoRE: A Tool-Oriented Collaboratory for Structural Biology

File Edit View Go Window Help

Theoretical Biophysics Group | Section: Development

BioCoRE

Biological Collaborative Environment
University of Illinois

BioCoRE is a tool-oriented collaboratory for structural biology. With BioCoRE researchers can visualize information, share resources and interact with each other and with structural biology tools via a common infrastructure ([more details...](#)).

Secure BioCoRE Login

New Users: [Open An Account](#)

Existing Users: User Name:

Password:

[Forgot your password?](#)

Announcements

- [BioCoRE Now Supports PDAs](#)
- [Change Log/Development Status](#)
- [Previous Announcements](#)

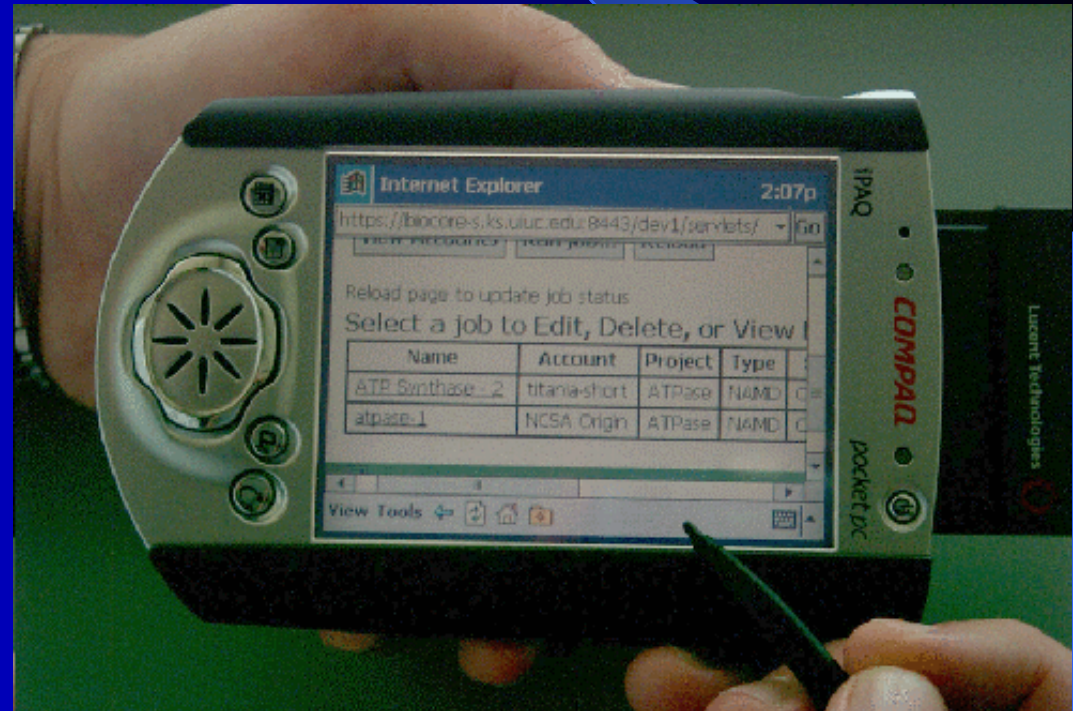
Overview

- [Take Our Online Tour!](#)
- [Entering BioCoRE](#)

100%

Accessing BioCoRE

- Standard web browser
 - BioCoRE applets require Java support
- Windows
- Unix
- Mac OS
- PocketPC PDAs



BioCoRE Projects

- Organized around *Projects*
- Projects are secure (only project members can see project data)

Netscape: NIH BioCoRE: Create New Project

File Edit View Go Window Help

Project Summary Create A New Project LOGOUT

The real power of BioCoRE lies in creating "projects" for the topics you are currently researching. You can create a project for each topic and this can help you organize your work into pieces that are relevant to each of those research topics. Create a project by filling out the form below, add other researchers to it, and you and your fellow researchers are the only people that can view what is done in that project.

NOTE: Projects that are inactive (no logins) for more than six months are subject to deletion.

BioCoRE Project Data Form

Project Title:

Password:

Re-enter password:

Project purpose:

Project goals:

Why are you using BioCoRE for this particular project? Select all that apply.

- To save time lost in a standard face-to-face collaboration
- Interface provides easier access to needed tools
- My collaborator elected to use this tool
- Need to share information with a number of persons
- Other reason

If you are working with a peer or peers why did you choose to collaborate on this project? Select all that apply.

- Needed peer's expertise to complete study
- Trusted colleague or peer I have worked with on other projects
- Met peer informally/socially, decided to collaborate
- Needed resources peer has access to to complete study

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BioCoRE Tool Areas

- Workbench
- Conferences
- Notebook
- Documents

Netscape: NIH BioCoRE: Toolboxes

File Edit View Go Window Help

PROJECTS Workbench Conference Notebook Documents

(to navigate, choose one of the above menu options)

BioCoRE

Biological Collaborative Research Environment

Project Summary Create A New Project **LOGOUT!**

Summary: ATPase

Project Description: Testing

Users currently logged in: 1

Login	Inactive time	Current Task
ann	less than a minute	Currently working on an ATPase simulation (Change user info)

Job Management status

Name	Account	Type	Status	Last updated
ATP Synthase - 2	titania-short	NAMD	Complete	Tue Sep 18 11:44:15 CDT 2001
atpase-1	NCSA Origin	NAMD	Complete	Tue Sep 18 11:40:32 CDT 2001

Recent Message Board Entries: 1 unread message

- [Equilibration in ATPase](#) (Bob McAlister, Tue Sep 18 2001*14:03:56) **UNREAD**
- [Re: Re: Delta subunit](#) (Jeff Fannigan, Tue Sep 18 2001*11:14:01)
- [Re: Delta subunit](#) (Bob McAlister, Tue Sep 18 2001*11:04:41)
- [Re: Delta subunit](#) (Mike Jones, Tue Sep 18 2001*11:04:16)
- [Delta subunit](#) (Jeff Fannigan, Tue Sep 18 2001*11:03:35)

Recent Additions to Link Library: 0 links have been added in the past 7 days.

- [NBCI](#) - Biophysics: National Center for Biotechnology Information
- [PDB \(Protein Data Bank\)](#) - Biophysics: Collection of many pdb files
- [Membrane proteins and lipids](#) - References / Membranes: Many articles on Membrane proteins and lipids. Very informative.
- [ATP synthase: two motors, two fuels \[Minireview\]](#) - References: From the Oster group
- [Yoshida Group movies](#) - Figures: Direct Observation of Rotation of F1-ATPase by Yoshida Group

Recent Additions to BioPS: 0 files have been added in the past 7 days.

- [/ATPase/1ABV.pdb](#) (Mike Jones, Tue Sep 18 2001*10:30:52)
- [/ATPase/1QO1.pdb](#) (Mike Jones, Tue Sep 18 2001*09:32:48)
- [/ATPase/pdbs/1QO1.pdb](#) (Ann Lessing, Mon Sep 17 2001*22:26:10)

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Workbench Tools

- Simulation Configuration File Generator
- Supercomputer Job Management
- VMD* Save/Load state
- JMV** – Java Molecular Viewer – Java3D applet

*<http://www.ks.uiuc.edu/Research/vmd/>

**<http://www.ks.uiuc.edu/Development/jmv/>



Configuration File Generator

- Simplifies creation of NAMD* input files
- Checks for common input errors
- Java applet

The screenshot shows the 'NAMD Configuration File Generator' window. It has a menu bar with 'New', 'Open...', 'Save', 'Save As...', 'View Text', and 'Exit'. Below the menu bar are tabs for 'FORCE FIELD', 'ENSEMBLE', 'INITIAL', 'OUTPUT', 'PROTOCOL', and 'ADDITIONAL'. The main area is divided into sections: 'Input Files', 'Basic Dynamics', 'Space Partitioning', and 'Periodic / FullDirect / DPMTA / PME'. Each section contains various configuration options with input fields and checkboxes.

Input Files

- paraFormat: X-Plor CHARMM
- *structure: /home/brunner/systems/ApoA1/apoa1.psf [Browse]
- *parameters: /home/brunner/systems/ApoA1/par_all22_popcexplor0 [Browse]
- /h/home/brunner/systems/ApoA1/par_all22_popcexplor1 [Browse]
- /home/brunner/systems/ApoA1/par_all22_popcexplor2 [Browse]

Basic Dynamics

- exclude: scaled1-4 [] 1.0 [] (0<= scaling <=1)

Space Partitioning

- switching: ON [] (Off/On)
- *cutoff: 10 [] (>=0)
- margin: 0 [] (>=0)
- switchdist: 8 [] (0 ~ cutoff)
- pairlistdist: 12 [] (> cutoff+1)

Periodic / FullDirect / DPMTA / PME

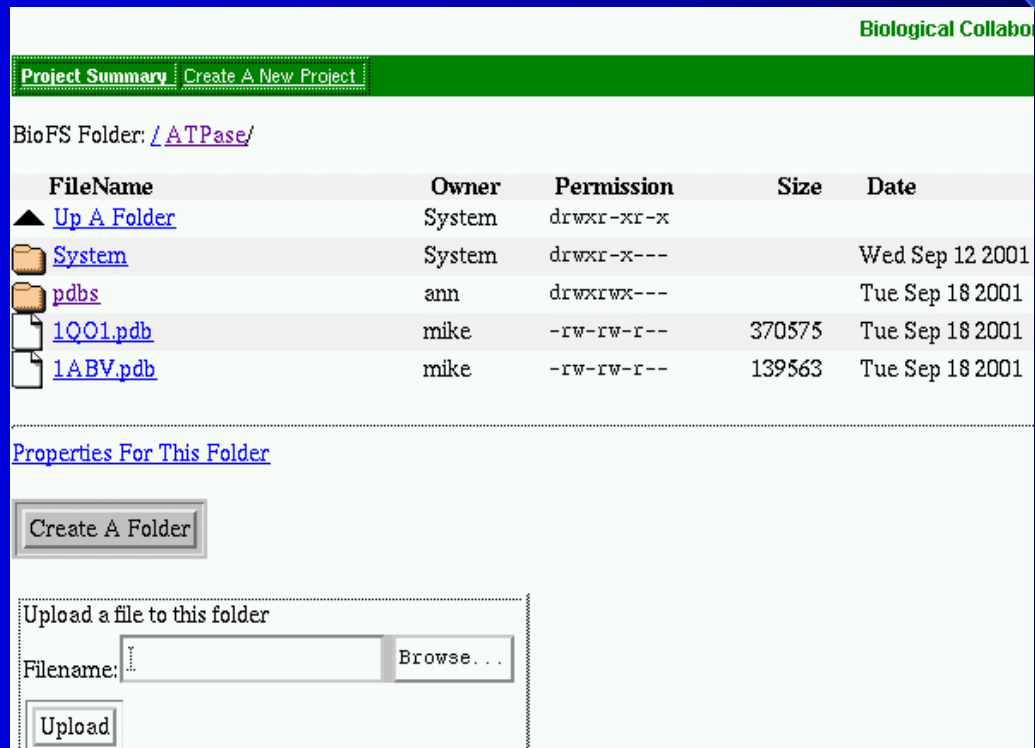
- periodic: 3 dimensions []
- FMA: FMA OFF []
- FMALevels: [] (int, >=0)
- FMAhp: [] (int, >=0)
- FMAFFT: On Off
- FMAtheta: [] (decimal)
- FMAFFThold: [] (int, >=0)
- FullDirect: No []
- PME: PME YES []
- PMEInterpOrder: 2 [] (int, >=0)
- PMEtolerance: 4 [] (>=0)
- PMEGridSizeX: 3 [] (int, >=0)
- PMEGridSizeY: 7 [] (int, >=0)
- PMEGridSizeZ: 8 [] (int, >=0)

*<http://www.ks.uiuc.edu/Research/namd/>



BioFS File System






- Web-based File system
- High bandwidth utilized
- WebDAV support



Biological Collabor

[Project Summary](#) [Create A New Project](#)

BioFS Folder: [/ATPase/](#)

FileName	Owner	Permission	Size	Date
 Up A Folder	System	drwxr-xr-x		
 System	System	drwxr-x---		Wed Sep 12 2001
 pdbs	ann	drwxrwx---		Tue Sep 18 2001
 1QQ1.pdb	mike	-rw-rw-r--	370575	Tue Sep 18 2001
 1ABV.pdb	mike	-rw-rw-r--	139563	Tue Sep 18 2001

[Properties For This Folder](#)

Upload a file to this folder

Filename:

Supercomputer Job Management

- Submits and monitors supercomputer jobs
- Accesses multiple supercomputers from a single web page
- Handles system-specific aspects (queues, file directories, etc.) automatically

Supercomputer Job Management

- Single-screen summary of jobs

Current Project: ATPase Biological Collaborative Research E

[Job Summary](#) [Create A New Project](#)

Jobs

Reload page to update job status

Select a job to Edit, Delete, or View Details

Name	Account	Project	Type	Status	Last updated
ATP Synthase - 2	titania-short	ATPase	NAMD	Complete	Tue Sep 18 11:44:15 CDT 200
atpase-1	NCSA Origin	ATPase	NAMD	Complete	Tue Sep 18 11:40:32 CDT 200

[Contact Us](#) [BioCoR](#)

This page retrieved at Sun Oct 28 12:44:00 GMT-0600 (CST) 2001 local time.
[Reload Control Panel](#)

Registering Supercomputer Accounts with BioCoRE

- User needs account on desired supercomputer
- No need to remember supercomputer passwords

Current Project: ATPase Biological Coll

[Project Summary](#) [Create A New Project](#)

Accounts

[View Project Jobs](#) [Make account...](#)

Select an account to edit or view details

Account name	Account type
titania-short	UIUC TBDQS
NCSA Origin	NCSA Origin 2000

For job help, please click [here](#)

ES

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[Reload Control Panel](#)

BioCoRE Account Registration

- User selects supercomputer
- SC account accessed via Globus or SSH

PROJECTS | **Workbench** | Conference | Notebook | Documents

(to navigate, choose one of the above menu options)

Current Project: ATPase Biological Collaborative Res

[Project Summary](#) | [Create A New Project](#)

You may select one of the following account types:

- ◆ NCSA Origin 2000
- ◆ Globus
- ◆ PSC T3E: jaromir.psc.edu
- ◆ PSC TCS: tcsini.psc.edu
- ◆ UIUC TB DQS

For globus help, please click [here](#)

[Utilities](#) [Contact Us](#)

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[Reload Control Panel](#)

Globus Support

- Uses standard BioCoRE user interface
- Supports Alliance machines
- Certificates set up by users
- BioCoRE obtains user certificates via the MyProxy credential server

Account Details (Globus)

Netscape: NIH BioCoRE: Account Settings

File Edit View Go Window Help

PROJECTS Workbench Conference Notebook Documents

(to navigate, choose one of the above menu options)

BioCoRE

Current Project: ATPase Biological Collaborative Research Environment

Project Summary Create A New Project LOGOUT

New Account information for a Globus account.

Account Name (any short descriptive name you choose):

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

MyProxy login name:

MyProxy password:

Submit Cancel

Utilities Contact Us BioCoRE FAQ Help

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100%

Account Details (SSH)

Netscape: NIH BioCoRE: Account Settings

File Edit View Go Window Help

PROJECTS Workbench Conference Notebook Documents

(to navigate, choose one of the above menu options)

BioCoRE

Current Project: ATPase Biological Collaborative Research Environment

Project Summary Create A New Project LOGOUT

New Account information for a NCSA Origin 2000 account.

Account Name (any short descriptive name you choose):

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

Login name:

This account will use SSH to allow BioCoRE to log in and monitor your job. To do this, BioCoRE will set a public key in the .ssh/authorized_keys file in your home directory on the front-end machine. To do this, BioCoRE will log in using your password now, and then destroy your password.

Password:

Utilities Contact Us BioCoRE FAQ Help

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100%

Job Submission via BioCoRE

- Submit a new job based on previous job parameters

Netscape: NIH BioCoRE: New Job Type

File Edit View Go Window Help

PROJECTS Workbench Conference Notebook Documents

(to navigate, choose one of the above menu options)

BioCoRE

Current Project: ATPase Biological Collaborative Research Environment

Project Summary Create A New Project LOGOUT

Create a job based on a previous job:

ATP Synthase - 2 (titania-short)
atpase-1 (NCSA Origin)

Or:

You may select one of the following job types: (not applicable if a previous Job is chosen)

NAMD
 Generic
 Generic Globus Job

Submit Cancel

Utilities Contact Us BioCoRE FAQ Help

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Job Submission via BioCoRE

- Submit a new job based on previous job parameters
- (or create a new one)

The screenshot shows a Netscape browser window titled "NIH BioCoRE: New Job Type". The interface includes a navigation menu with "PROJECTS", "Workbench", "Conference", "Notebook", and "Documents". The current project is "ATPase". A green bar contains "Project Summary", "Create A New Project", and "LOGOUT". The main content area has a section "Create a job based on a previous job:" with a dropdown menu and a "Submit" button. Below this is an "Or:" section with the text "You may select one of the following job types: (not applicable if a previous Job is chosen)". Three radio buttons are listed: "NAMD", "Generic", and "Generic Globus Job". At the bottom of this section are "Submit" and "Cancel" buttons. A green bar at the bottom contains "Utilities", "Contact Us", "BioCoRE FAQ", and "Help". A footer message states "This page retrieved at Sun Oct 28 12:13:27 GMT-0600 (CST) 2001 local time." with a "Reload Control Panel" link. The browser status bar shows "100%" zoom.

Job Submission via BioCoRE

- Select account
- Check queue status

PROJECTS | Workbench | Conference | Notebook | Documents

Navigate, choose one of the above menu options)

Current Project: ATPase Biological Collaborativ

Summary | Create A New Project

Select an account to run this job:

- ◆ titania-short
Type: UIUC TB DQS Login: mbach Host: anzio.ks.uiuc.edu [Queue Status](#)
- ◆ NCSA Origin
Type: NCSA Origin 2000 Login: rbrunner Host: modi4.ncsa.uiuc.edu [Queue Status](#)

This page retrieved at Sun Oct 28 12:22:04 GMT-0600 (CST) 2001 local time.
[Reload Control Panel](#)

Job Submission via BioCoRE

- Set the job parameters

The screenshot shows a Netscape browser window titled "NIH BioCoRE: Job Settings". The browser's address bar shows "Current Project: Airase" and the page title is "Biological Collaborative Research Environment". A green navigation bar contains "Project Summary", "Create A New Project", and "LOGOUT".

The main content area is titled "Required information for application NAMD running on account titania-short". It contains the following fields:

- Job Name** (any short descriptive name you choose): A single-line text input field.
- Description** (any other information to further describe the job): A multi-line text area.
- Working directory on remote machine**; absolute path, or relative to home directory (no ~): A single-line text input field.
- Application information:**
 - NAMD Executable Path**: A single-line text input field containing "/usr/local/bin/namd2".
 - NAMD input filename**: A single-line text input field.
 - Standard output file** (optional, if file exists std. output will be appended): A single-line text input field.
 - Standard error File** (optional, if file exists std. error will be appended): A single-line text input field.
 - Enable applet view** (experimental feature, see Help at the bottom of this page for more info): A checkbox that is currently unchecked.

At the bottom of the form are "Submit" and "Cancel" buttons. The browser status bar at the bottom shows "100%".

Job Submission via BioCoRE

- Set the job parameters
- Submit job

The screenshot shows a Netscape browser window titled "Netscape: NIH BioCoRE: Job Settings". The browser's address bar shows "Current Project: ATRase" and the page title is "Biological Collaborative Research Environment". The interface includes a green navigation bar with "Project Summary" and "Create A New Project" links, and a "LOGOUT" button. The main content area is titled "Required information for application NAMD running on account titania-short". It contains several form fields: "Job Name (any short descriptive name you choose):" with the value "BPTI Langevin"; "Description (any other information to further describe the job):" with a text area containing "Langevin Dynamics on BPTI"; "Working directory on remote machine; absolute path, or relative to home directory (no ~):" with the value "s/collaboratory/collab/demo/bpti"; and "Application information:" section with fields for "NAMD Executable Path:" (value: "/usr/local/bin/namd2"), "NAMD input filename:" (value: "langevin.namd"), "Standard output file (optional, if file exists std. output will be appended):", and "Standard error File (optional, if file exists std. error will be appended):". There is also a checkbox for "Enable applet view (experimental feature, see Help at the bottom of this page for more info):" which is unchecked. At the bottom of the form are "Submit" and "Cancel" buttons. The browser status bar at the bottom shows "100%".

Monitor Running Jobs

- The new job has been submitted

Netscape: NIH BioCoRE: Job View

File Edit View Go Window Help

PROJECTS [Workbench](#) [Conference](#) [Notebook](#) [Documents](#)

(to navigate, choose one of the above menu options)

BioCoRE

Current Project: ATPase Biological Collaborative Research Environment

[Project Summary](#) [Create A New Project](#) [LOGOUT](#)

Jobs

[View All Jobs](#) [View Accounts](#) [Run job...](#) [Reload](#)

Reload page to update job status

Select a job to Edit, Delete, or View Details

Name	Account	Project	Type	Status	Last updated
BPTI Langevin	titania-short	ATPase	NAMD	Submitted	Sun Oct 28 12:28:35 CST 2001 <input type="checkbox"/>
ATP Synthase - 2	titania-short	ATPase	NAMD	Complete	Tue Sep 18 11:44:15 CDT 2001 <input type="checkbox"/>
atpase-1	NCSA Origin	ATPase	NAMD	Complete	Tue Sep 18 11:40:32 CDT 2001 <input type="checkbox"/>

[Select all](#) [Forget selected jobs](#)

[Utilities](#) [Contact Us](#) [BioCoRE FAQ](#) [Help](#)

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[Reload Control Panel](#)

100%

BioCoRE Job Details

- Details of running jobs can be displayed

The screenshot shows a Netscape browser window titled "NIH BioCoRE: View Job: ATP Synthase - 2". The interface includes a navigation menu with "PROJECTS", "Workbench", "Conference", "Notebook", and "Documents". The current project is "ATPase". A green bar contains "Project Summary" and "Create A New Project" links, along with a "LOGOUT" button. Below this are buttons for "View Project Jobs", "View Accounts", "View Output", "View Submission Output", "Forget Job", and "Back". The main content area is titled "Information for job ATP Synthase - 2" and contains the following text: "Running on account: [titania-short](#)", "Project: ATPase", "Description: ATP synthase simulation" (in a text box), "Work directory: atpase", "State: Complete: Tue Sep 18 11:44:15 CDT 2001", "ENERGY: 1000 11.1358 81.5656 89.9502 16.6031 -2000.4678 -332.0344 0.0000 0.0000 -2133.2474 58.1096", "Will retrieve output files and deposit in BioFS" with a link "View files in BioFS", and "Input file name: minimize.namd". The browser status bar shows "100%".

BioCoRE Job Details

- Standard output of the job

```
Netscape: NIH BioCoRE: View Output of BPTI Langevin
File Edit View Go Window Help
PROJECTS Workbench Conference Notebook Documents
(to navigate, choose one of the above menu options)
BioCoRE
Current Project: ATPase Biological Collaborative Research Environment
Project Summary Create A New Project LOGOUT
Back
Go to bottom...
Info: NAMD 2.3 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 2.3 Linux-i686-Scyld 32 oberon mbach
Info: Running on 32 processors.
Info: 1092 kB of memory in use.
Measuring processor speeds... Done.
Info: Configuration file is langevin.namd
TCL: Suspending until startup complete.
Info: SIMULATION PARAMETERS:
Info: TIMESTEP 2
Info: NUMBER OF STEPS 50000
Info: STEPS PER CYCLE 10
Info: MAX SELF PARTITIONS 100
Info: MAX PAIR PARTITIONS 10
Info: LOAD BALANCE STRATEGY Other
Info: LDB PERIOD 2000 steps
Info: FIRST LDB TIMESTEP 50
Info: INITIAL TEMPERATURE 350
Info: CENTER OF MASS MOVING? NO
Info: DIELECTRIC 1
Info: EXCLUDE SCALED ONE-FOUR
Info: 1-4 SCALE FACTOR 0.4
Info: DCD FILENAME bpti_lang.dcd
Info: DCD FREQUENCY 500
Info: NO EXTENDED SYSTEM TRAJECTORY OUTPUT
100%
```







Job Details Saved To BioFS

- Accessible to all project members

Biological Collaborative Rese

Project Summary [Create A New Project](#)

BioFS Folder: [/ATPase/System/Jobs/ann/ATP_Synthase_-_2/](#)

FileName	Owner	Permission	Size	Date
 Up A Folder	ann	drwxrwx---		Tue Sep 18 2001
 ATP_Synthase_-_2.38403596000.out	ann	-rw-r-----	207861	Tue Sep 18 2001
 ATP_Synthase_-_2.38403596000.err	ann	-rw-r-----	0	Tue Sep 18 2001
 ATP_Synthase_-_2.html	ann	-rw-r-----	965	Tue Sep 18 2001

[Properties For This Folder](#)

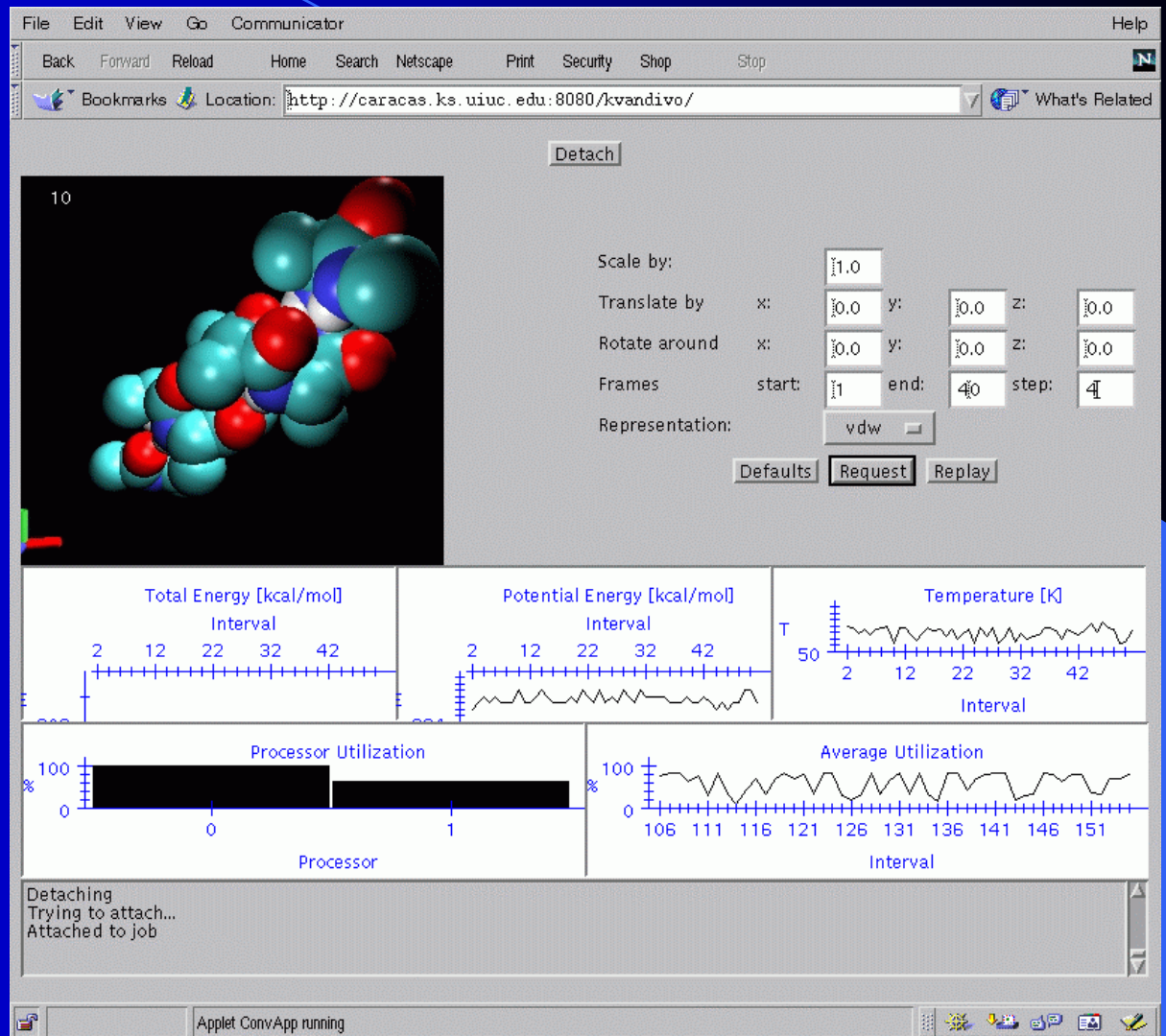
Upload a file to this folder

Filename:

Utilities [Contact Us](#)

BioCoRE Job Details

- Graphical capabilities when running NAMD



Launching VMD

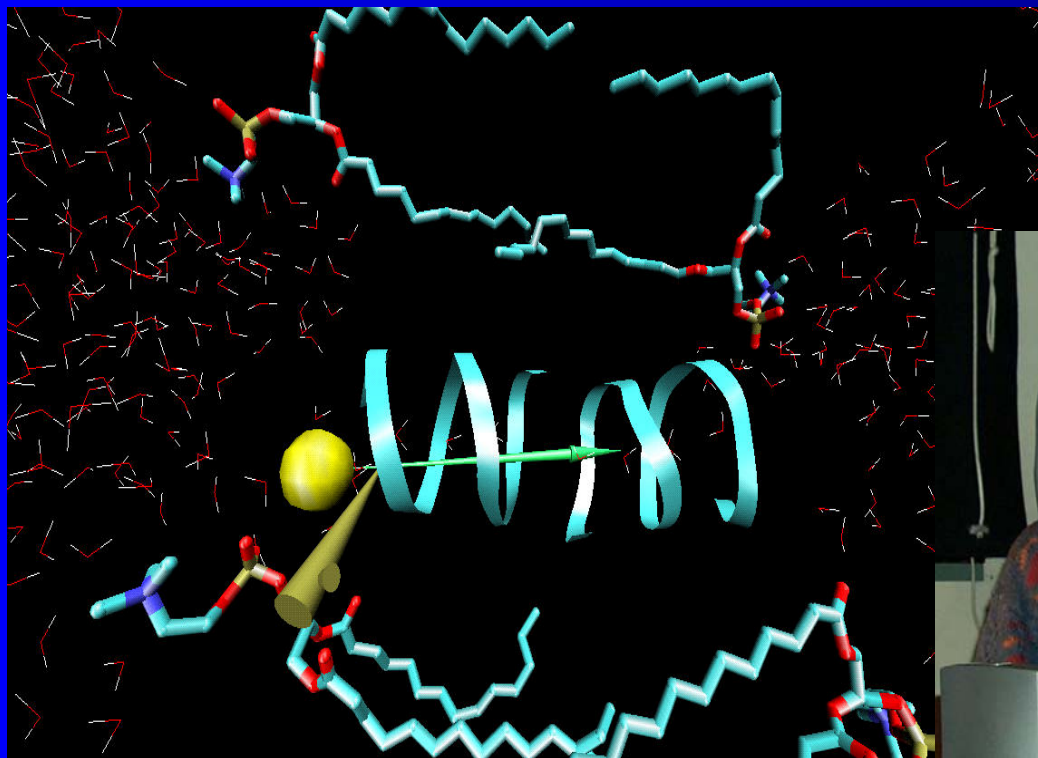
The screenshot displays a web browser window titled "Netscape: NIH Resource BioCoRE: Running VMD". The browser shows a navigation menu with options like "PROJECTS", "Workbench", "Conference", "Notebook", and "Documents". The current project is "ATPase" under the "Biological Collaborative Research Environment". A "VMD States" dialog box is open, showing a list of saved states: "Delta structure", "ATP Synthase (new view)", and "ATPase". The description for the selected state is "Representation: Tube" and "Colored by: Chain". The VMD window itself shows a 3D ribbon model of a protein structure, colored by chain. A control panel on the right includes buttons for "main", "VMD", "Mouse", "Molecule", "Animate", "Edit", "Graphics", "Labels", "Render", "Display", "Color", "Material", "Simulation", "Tracker", "Sequence", "Help", and "Quit". The "vmd console" at the bottom shows the following output:

```
Info) Opened sensor config file /usr/local/lib/vmd.171a1/.vmdsensors
Info) Added current representation to 1 molecules.
Info) Opened sensor config file /usr/local/lib/vmd.171a1/.vmdsensors
```



Interactive MD

- Real-time interaction between VMD/NAMD



JMV Support Within BioCoRE

- JMV: Web-based Java3D molecular viewer
- Can view PDB files straight from the BioFS

The screenshot displays a Netscape browser window with two main panes. The left pane shows a 3D molecular model of a protein structure, rendered in various colors (green, blue, orange, red) against a black background. The right pane shows the 'BioFS File Properties' for the file '1ABV.pdb'. Below the file information, there is a table listing files in the folder '/ATPase/'.

File information:

- Name: 1ABV.pdb
- Size: 139563
- Type: chemical/x-pdb
- Last Update: Tue Sep 18 2001*10:33:21
- Create Time: Tue Sep 18 2001*10:30:52
- BioCoRE File ID: 76
- Version: 1
- Owner: mike
- Permissions: -rw-rw-r--

[Edit this file \(MUST BE TEXT!!!\)](#)

[View this molecule using JMV \(More info on installing Java3D\)](#)

[Copy to a different folder](#)

[Utilities](#) | [Contact Us](#) | [BioCoRE FAQ](#) | [Help](#)

This page retrieved at Wed Sep 19 09:45:21 GMT-0500 (CDT) 2001 local time.

Folder: /ATPase/

File Name	Owner	Permission	Size	Date	Properties
ATPase Folder	System	drwxr-xr-x			
System	System	drwxr-xr-x		Wed Sep 12 2001	Properties
pdbs	ann	drwxrwxr-x		Tue Sep 18 2001	Properties
1QQ1.pdb	mike	-rw-rw-r--	370575	Tue Sep 18 2001	Properties
1ABV.pdb	mike	-rw-rw-r--	139563	Tue Sep 18 2001	Properties

Properties For This Folder

[Create A Folder](#)

Netscape: NIH Resource BioCoRE Control Panel

File Project Help

Summary All User... Titin ATPase Light Ha...

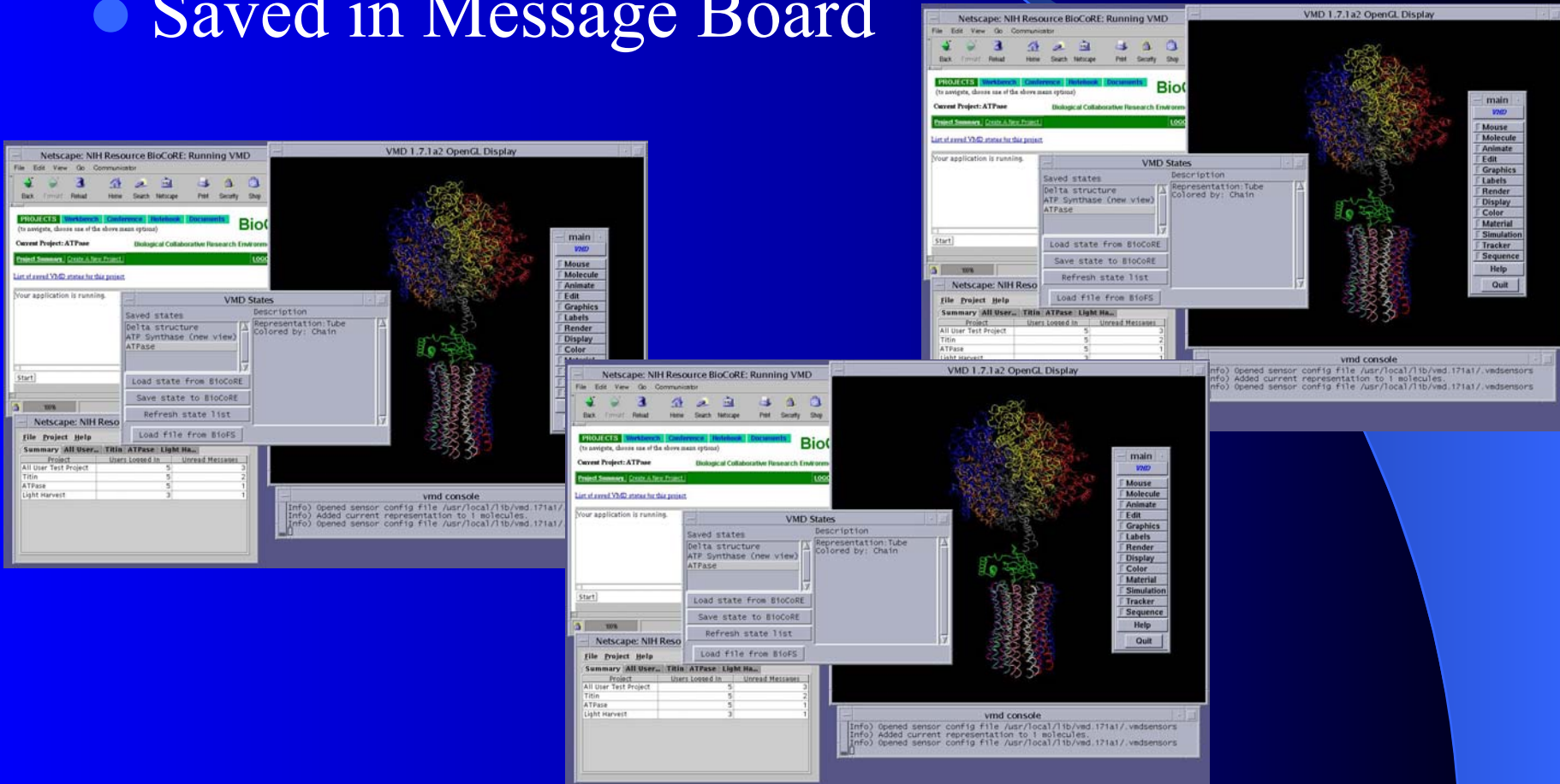
Project	Users Logged In	Unread Messages
All User Test Project	2	0
Titin	2	2
ATPase	2	1
Light Harvest	1	1

Collaboration Tools

- Collaborative VMD
- Message Board
- Project-wide *Bookmarks* file
- Control Panel

Collaborative VMD

- Load/save visualization states
- Saved in Message Board



BioCoRE Message Board

- Asynchronous
- Threaded
- Sortable
- Searchable

The screenshot shows a Netscape browser window displaying the BioCoRE Message Board. The browser's address bar shows the URL: https://biocore-s.ks.uiuc.edu:8443/dev1/servlets/NoteBook?p=8&session_id=. The page features a navigation menu with links for [PROJECTS](#), [Workbench](#), [Conference](#), [Notebook](#), and [Documents](#). The current project is identified as **ATPase**, part of the **Biological Collaborative Research Environment**. A green header bar 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 'Sort By:' options include [\[Thread\]](#), [\[Subject\]](#), [\[Author\]](#), and [\[Date\]](#), along with a [\[Mark All Read\]](#) button. A 'View messages from last' dropdown is set to 'all' days. The message list includes:

- [Walker's crystal](#) (Mike Jones, Mon Sep 17 2001*22:03:50)
 - [Re: Walker's crystal](#) (Ann Lessing, Mon Sep 17 2001*22:08:10)
- [Delta subunit](#) (Jeff Fannigan, Tue Sep 18 2001*11:03:35)
 - [Re: Delta subunit](#) (Mike Jones, Tue Sep 18 2001*11:04:16)
 - [Re: Delta subunit](#) (Bob McAlister, Tue Sep 18 2001*11:04:41)
 - [Re: Re: Delta subunit](#) (Jeff Fannigan, Tue Sep 18 2001*11:14:01)
- [Equilibration in ATPase](#) (Bob McAlister, Tue Sep 18 2001*14:03:56) **UNREAD**

Below the message list is a link for [View previously deleted Messages](#). At the bottom, a green bar contains [Utilities](#), [Contact Us](#), [BioCoRE FAQ](#), and [Help](#). A footer note states: 'This page retrieved at Mon Oct 29 14:25:17 GMT -0600 (CST) 2001 local time.' and a [Reload Control Panel](#) link is provided.

Website Link Library

- Project-wide *Bookmarks* file
- Ranked by popularity

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Bookmarks Location: <https://biocore-s.ks.uiuc.edu:8443/dev1/servlets/LinkLibrary?p=8&> What's Related

Project Summary Create A New Project LOGOUT

Website Library

Add Main Topic

Biophysics [\[Add Subtopic/ Add Link\]](#)

Useful Biophysics links – Ann Lessing, Mon Sep 17 2001*22:33:58 [\[edit\]](#)

- [PDB \(Protein Data Bank\) \(http://www.pdb.org/ \)](http://www.pdb.org/)
Collection of many pdb files – Ann Lessing, Mon Sep 17 2001*22:34:28 [\[edit/delete\]](#)
- [NBCI \(http://www.ncbi.nlm.nih.gov/ \)](http://www.ncbi.nlm.nih.gov/)
National Center for Biotechnology Information – Wanda Smith, Tue Sep 18 2001*16:35:06

References [\[Add Subtopic/ Add Link\]](#)

Articles related to ATP synthase and related topics – Ann Lessing, Mon Sep 17 2001*22:10:16 [\[edit\]](#)

- [ATP synthase: two motors, two fuels \[Minireview\] \(http://reviews.bmn.com/browse/areas/record?uid=JSTR.st7411&rendertype= \)](http://reviews.bmn.com/browse/areas/record?uid=JSTR.st7411&rendertype=)
From the Oster group – Ann Lessing, Mon Sep 17 2001*22:13:49 [\[edit/delete\]](#)

Membranes [\[Add Subtopic/ Add Link\]](#)

Membrane and membrane protein simulations – Ann Lessing, Mon Sep 17 2001*22:15:01 [\[edit\]](#)

- [Membrane proteins and lipids \(http://journals.bmn.com/journals/list/latest?jcode=jstb&node=TOC@@@ISTB@10@04@10_0 \)](http://journals.bmn.com/journals/list/latest?jcode=jstb&node=TOC@@@ISTB@10@04@10_0)
Many articles on Membrane proteins and lipids. Very informative. – Ann Lessing, Mon Sep 17 2001*22:15:57 [\[edit/delete\]](#)

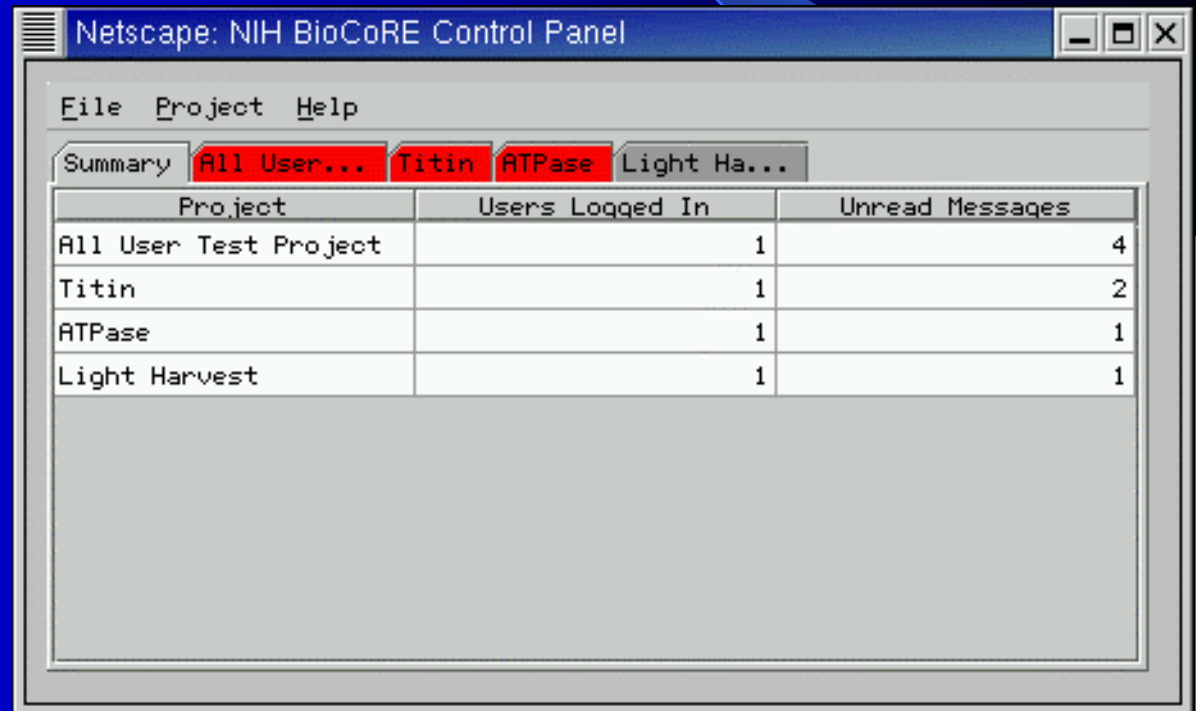
Figures [\[Add Subtopic/ Add Link\]](#)

Figures and movies – Mike Jones, Mon Sep 17 2001*21:58:41

100%

BioCoRE Control Panel

- “Always-on”
- Automatic event notification
- Java Swing

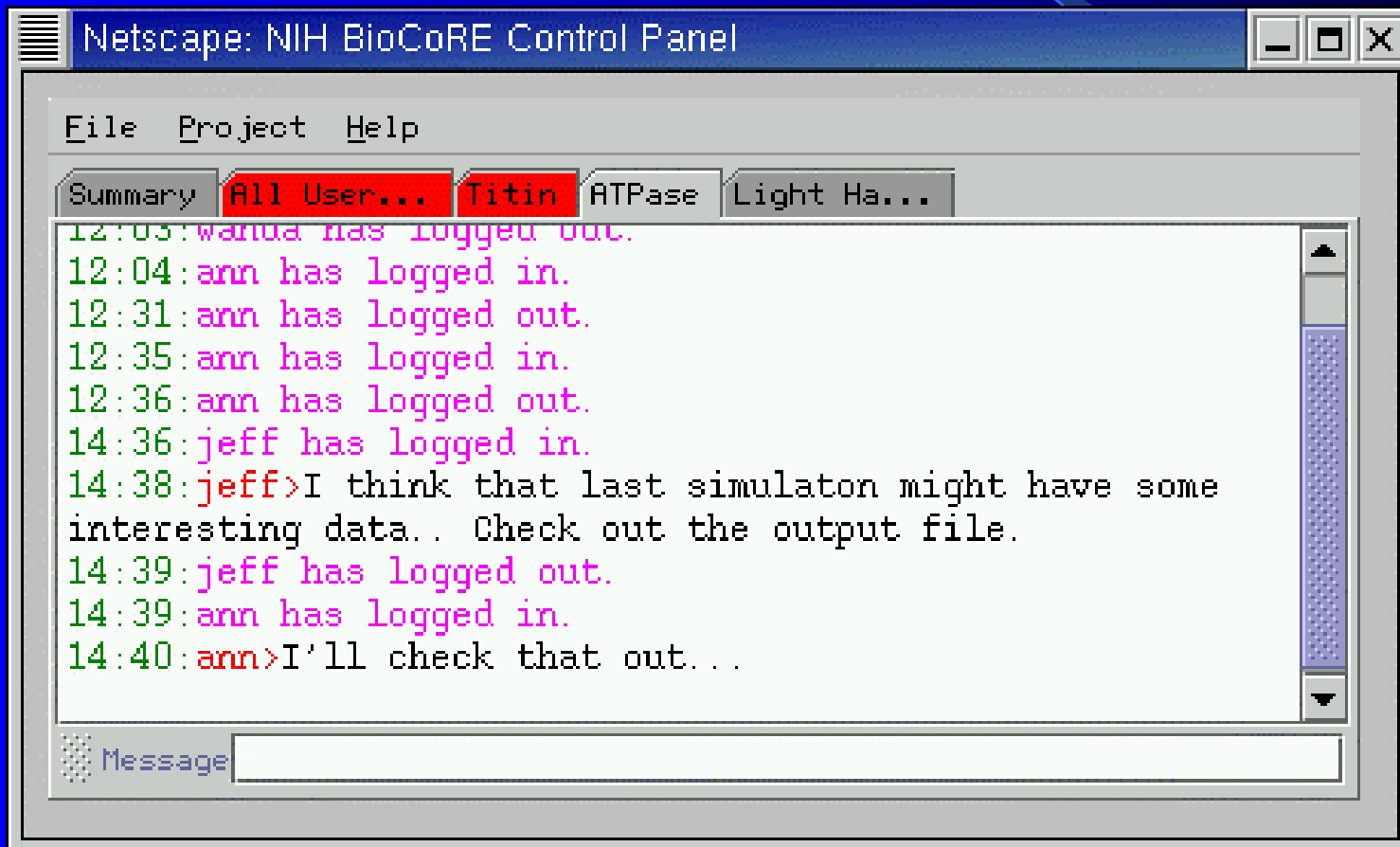


The screenshot shows a Netscape browser window titled "Netscape: NIH BioCoRE Control Panel". The browser's menu bar includes "File", "Project", and "Help". Below the menu bar is a tabbed interface with four tabs: "Summary", "All User...", "Titin", and "ATPase". The "Summary" tab is active, displaying a table with the following data:

Project	Users Logged In	Unread Messages
All User Test Project	1	4
Titin	1	2
ATPase	1	1
Light Harvest	1	1

Control Panel Chat

- Saved to Message Board



Publication Tools

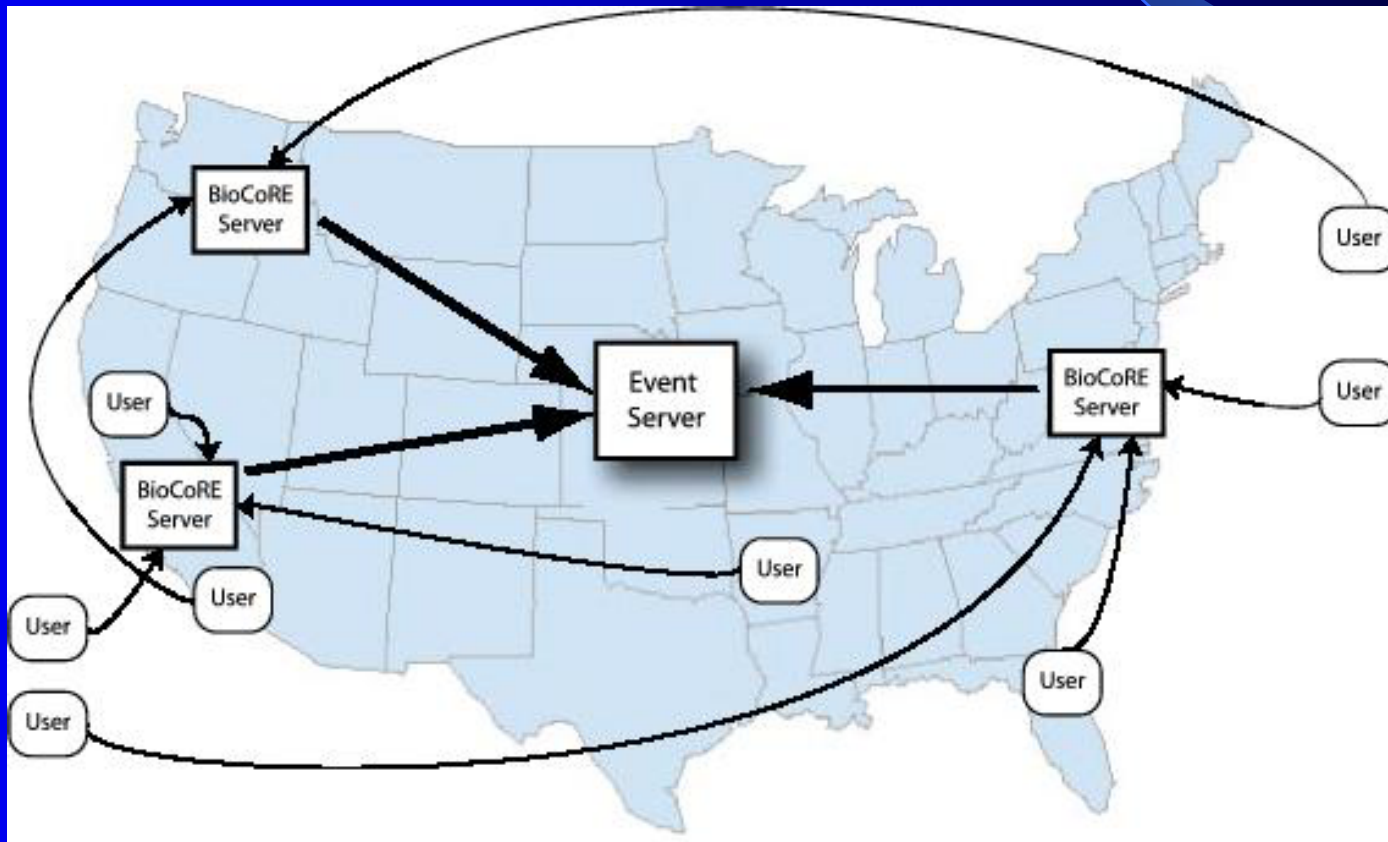
- BioFS support for seamless file transport across platforms
- File conversions planned (Word→TeX, TeX →Word, etc.)
- WebDAV for easy access

Evaluation

- Tracking BioCoRE usage patterns, analysis of BioCoRE users' feedback and needs
- Support of development process (product design, integration of user preferences and input)
- Assessment of BioCoRE impact and benefits to research efforts and outcomes

Local BioCoRE Servers

- Research groups can install own server
- Tracking data sent to central server



User Statistics

- Initial release : March 2000
- Registered Users: 299
- Logins: 2,553
- Registered Projects: 50
- Job Submissions (since March 2001): 1,114

Questions?

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

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