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

National Center for Research Resources

BioCoRE Overview

BioCoRE is a collection of web-based tools that:

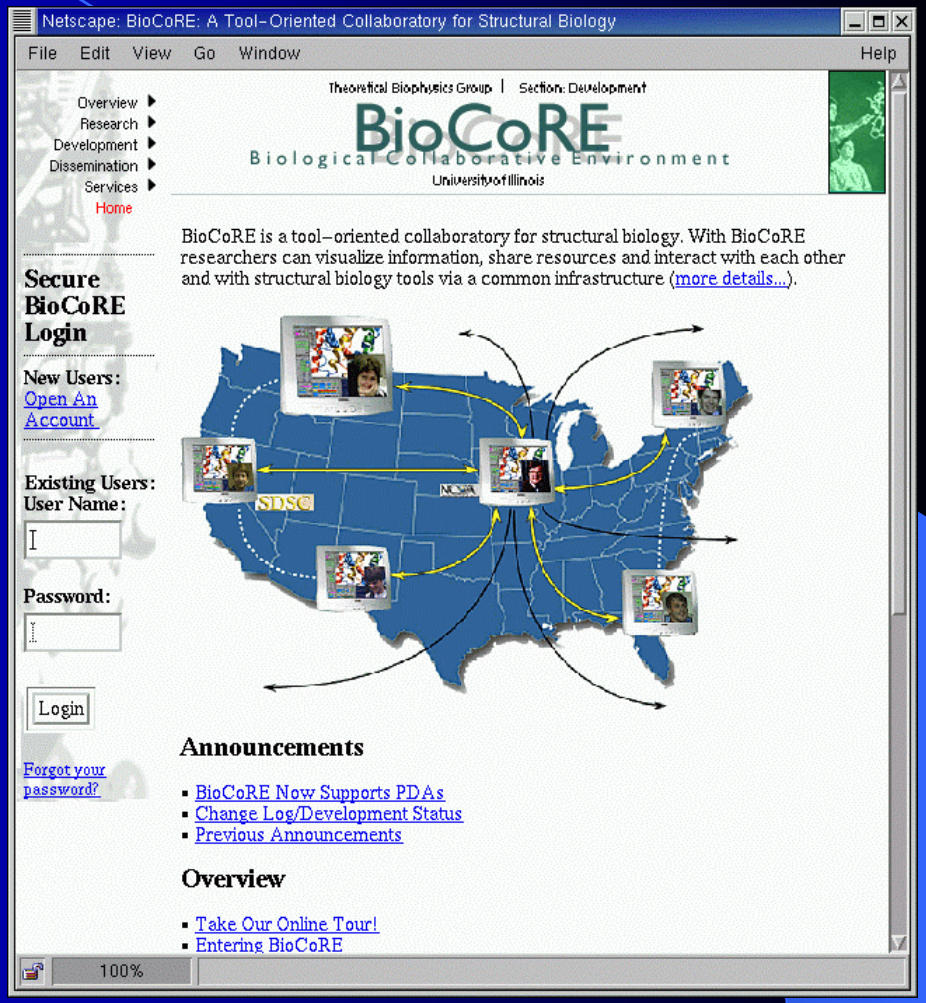
- Forms a complete environment for biomedical research
- Allows single password login
- Is freely available

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

BioCoRE Goals

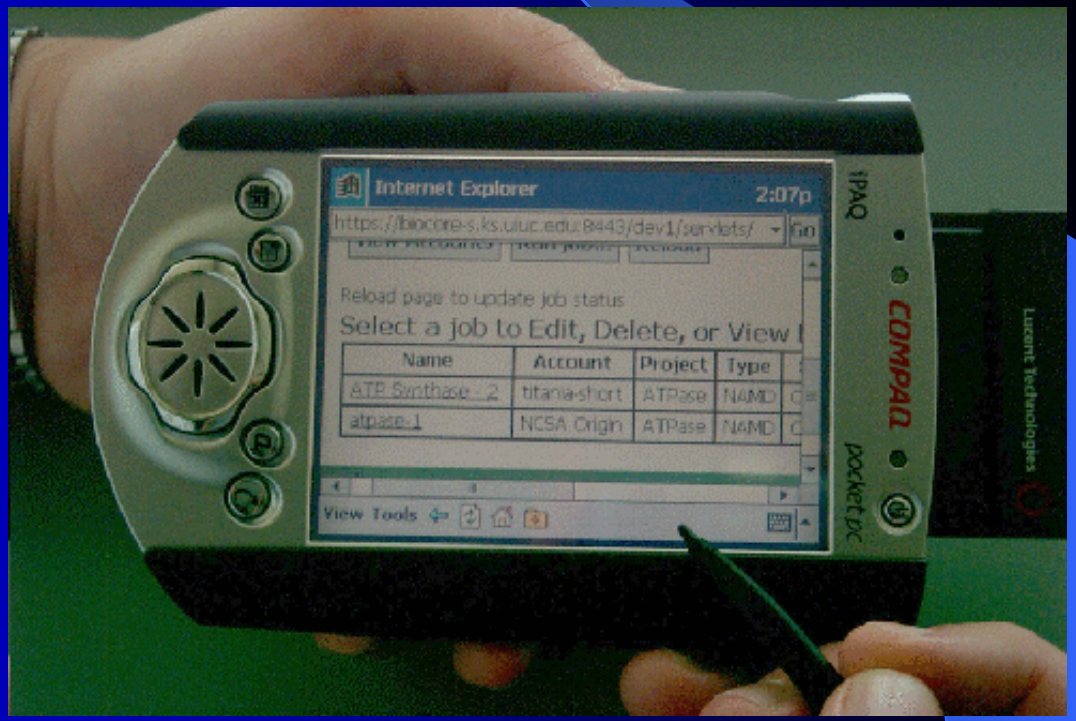
(**Bio**logical **Co**llaborative **R**esearch **E**nvironment)

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



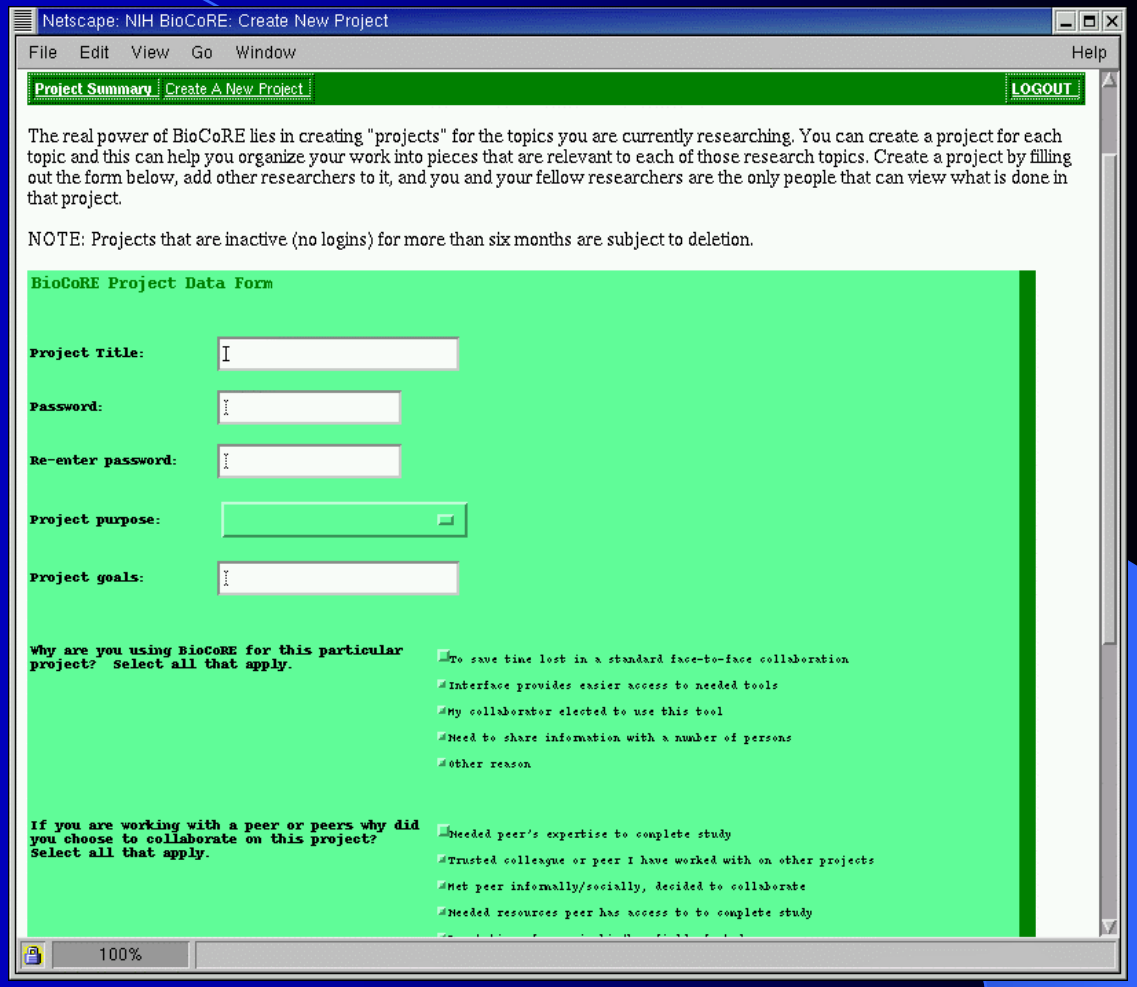
Accessing BioCoRE

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



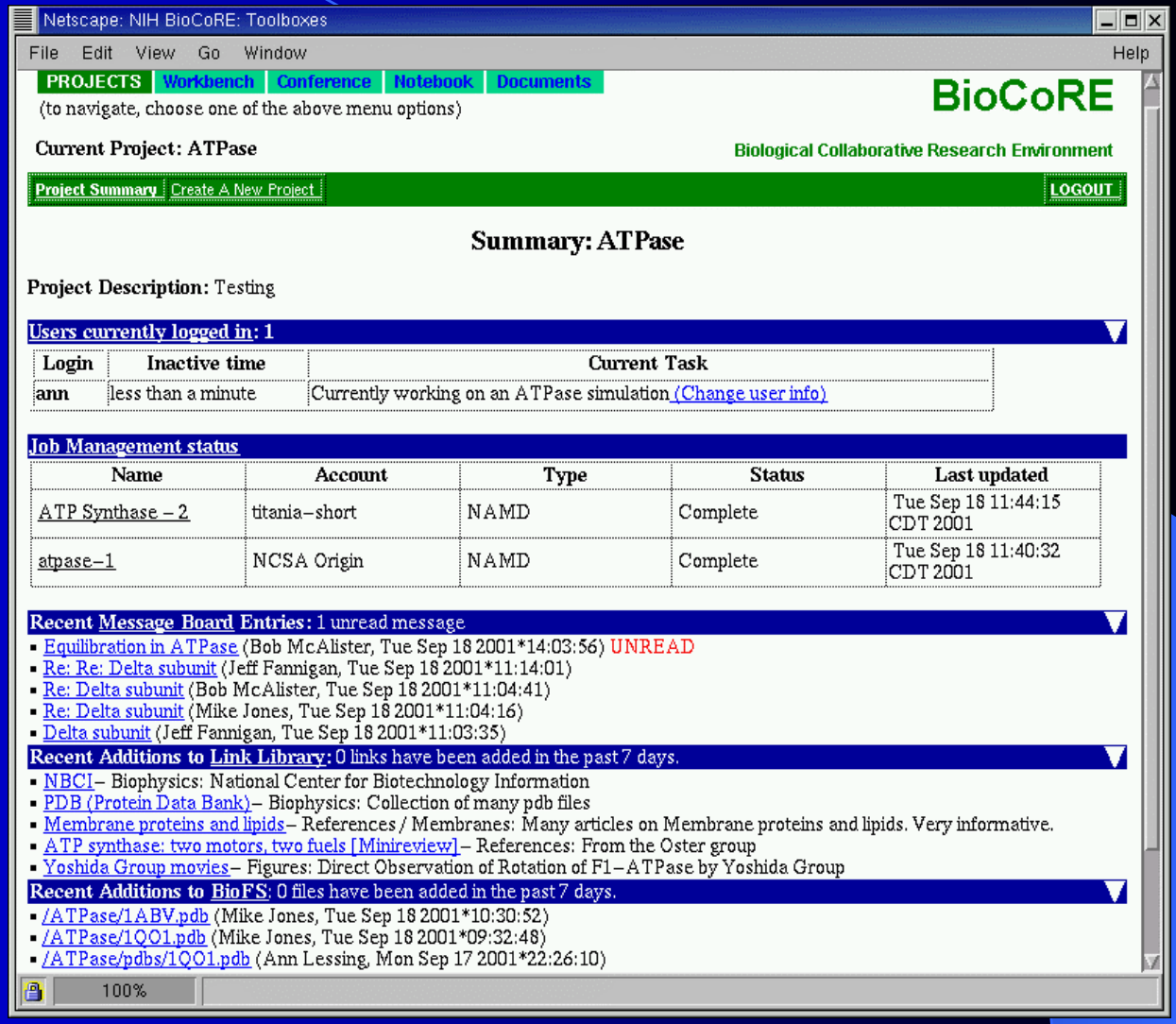
BioCoRE Projects

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



BioCoRE Tool Areas

- Workbench
- Conferences
- Notebook
- Documents



Workbench Tools

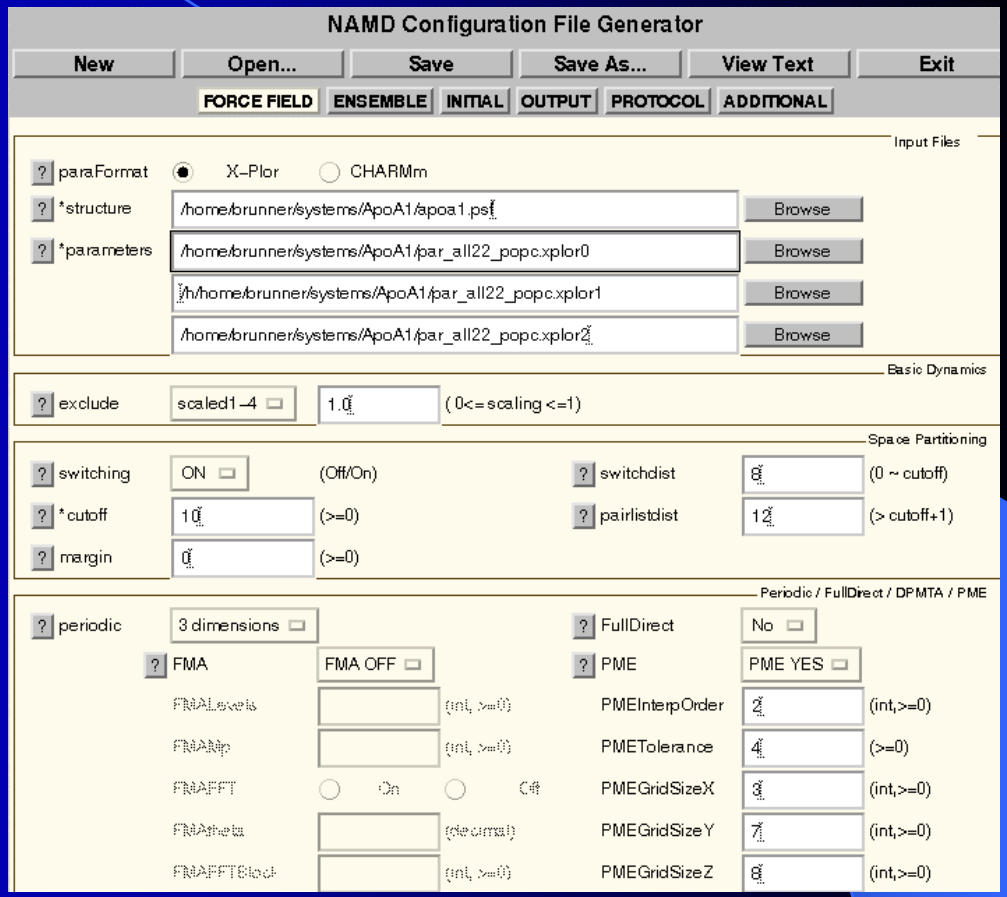
- Simulation Configuration File Generator
- Supercomputer Job Management
- VMD* Save/Load state
- JMV** – Java Molecular Viewer – Java3D applet

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

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

Configuration File Generator

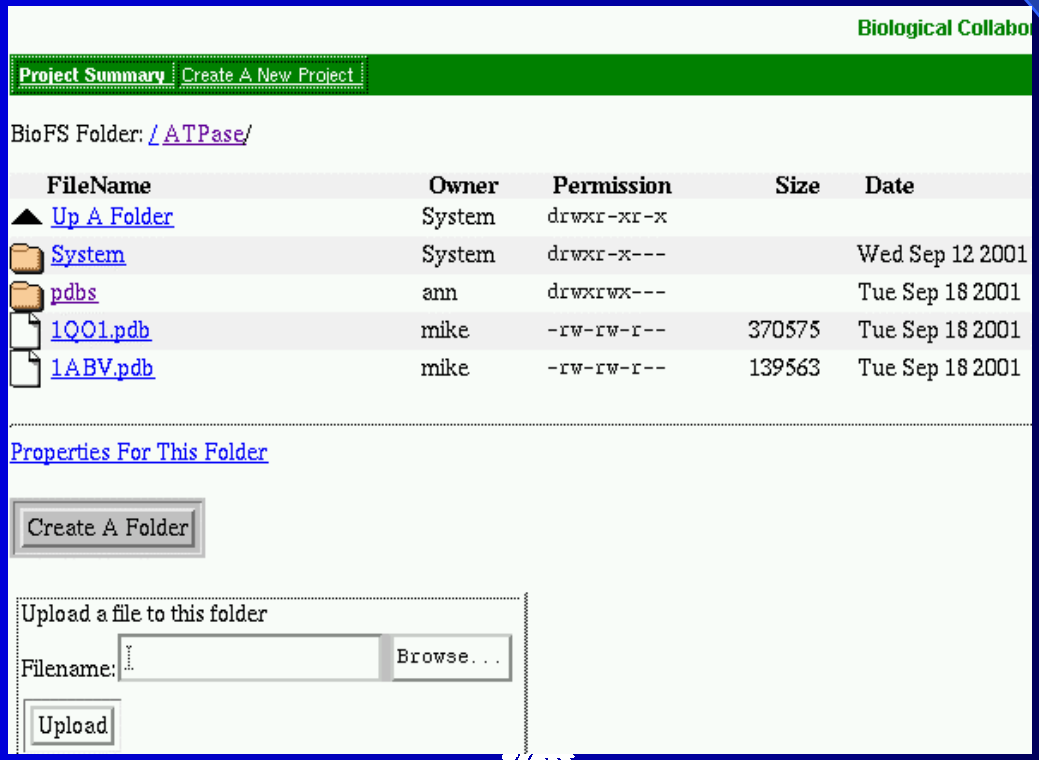
- Simplifies creation of NAMD* input files
- Checks for common input errors
- Java applet



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

BioFS File System

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

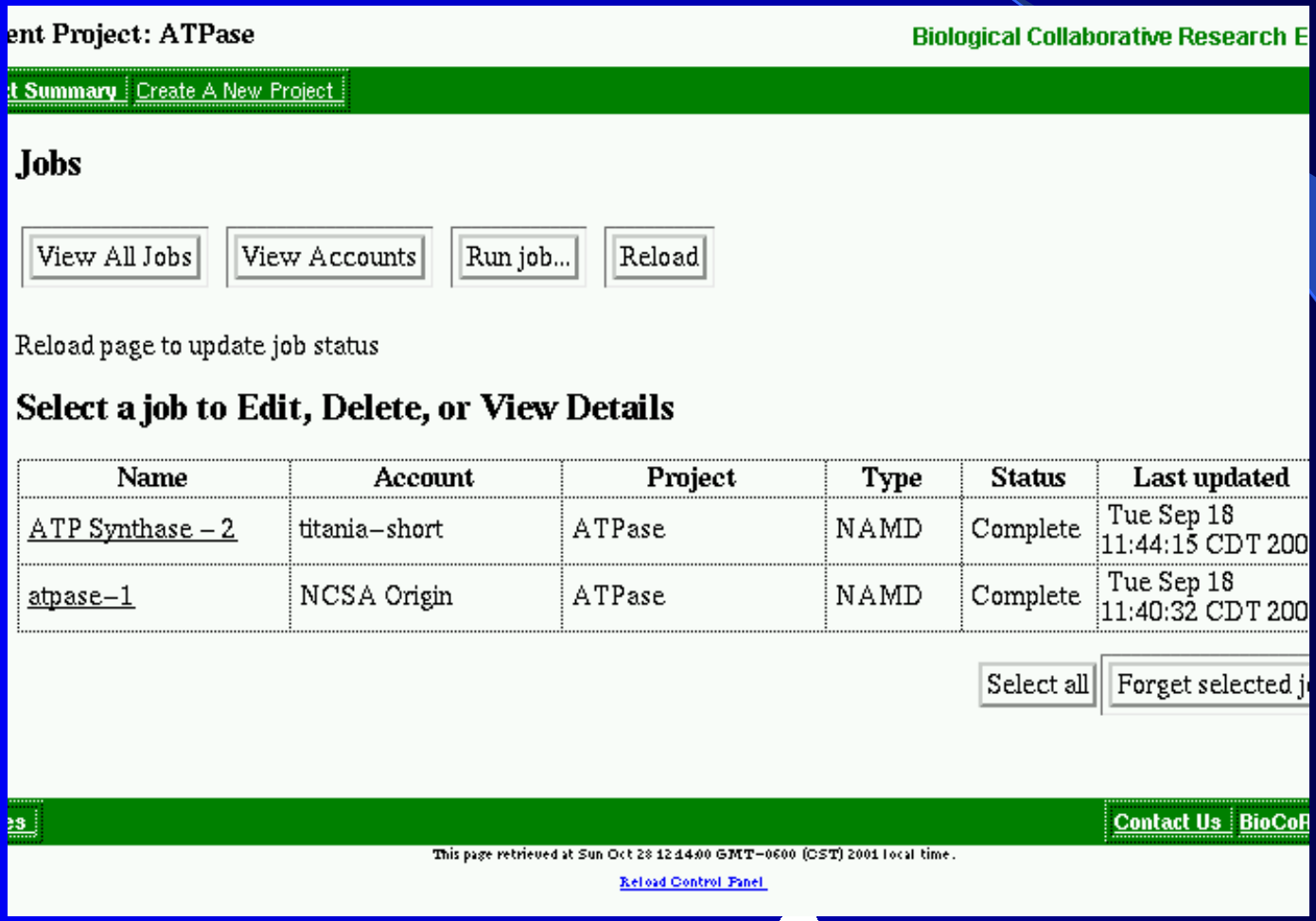


Supercomputer Job Management

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

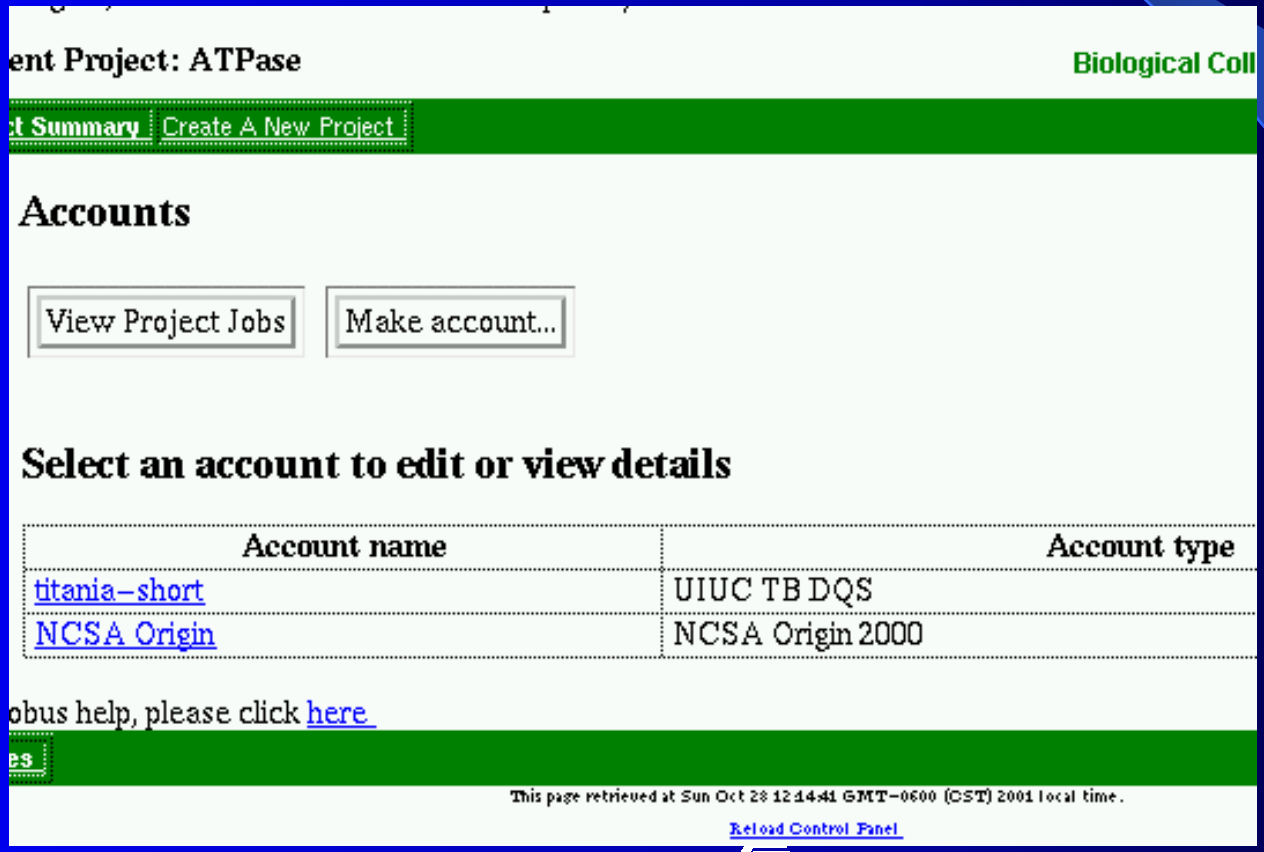
Supercomputer Job Management

- Single-screen summary of jobs



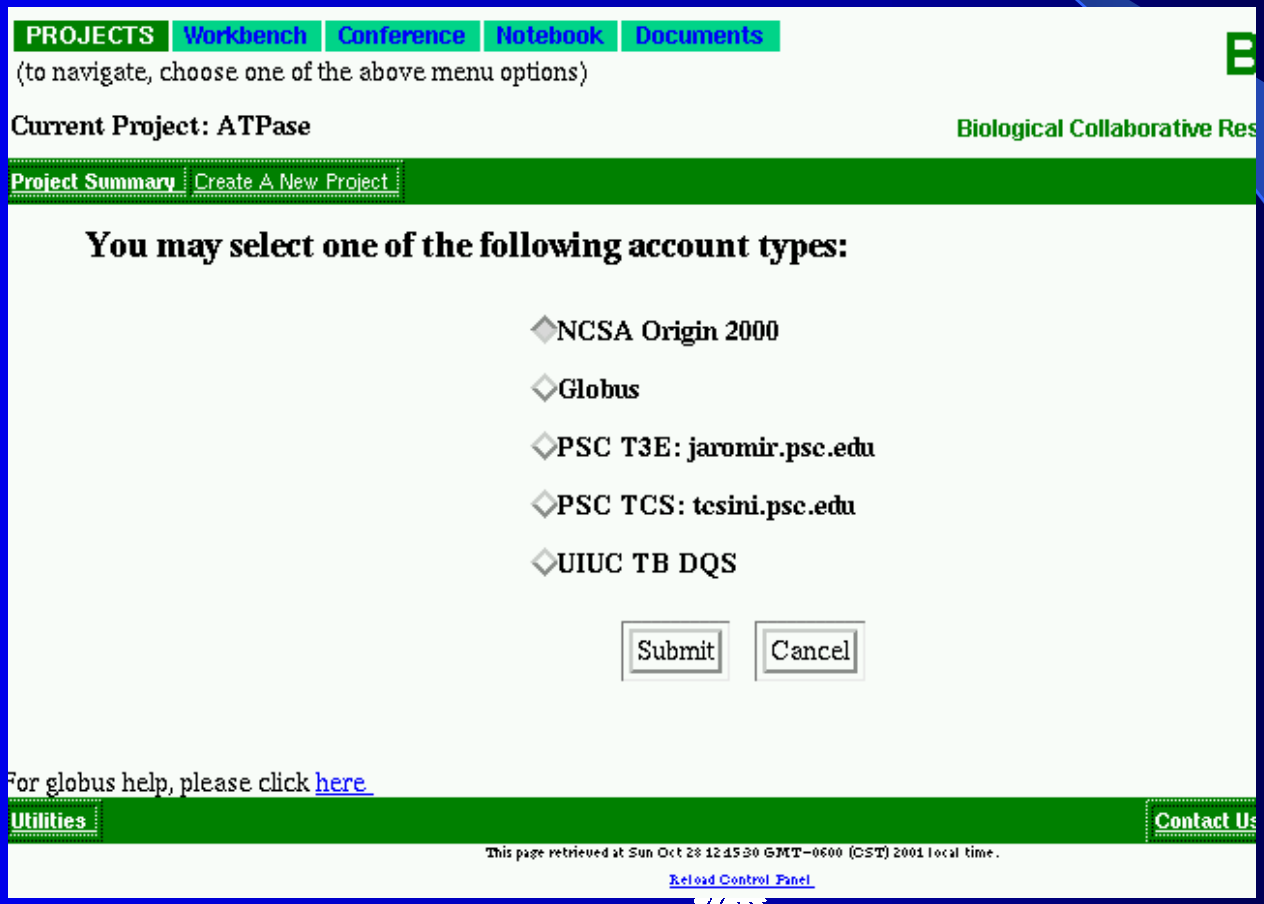
Registering Supercomputer Accounts with BioCoRE

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



BioCoRE Account Registration

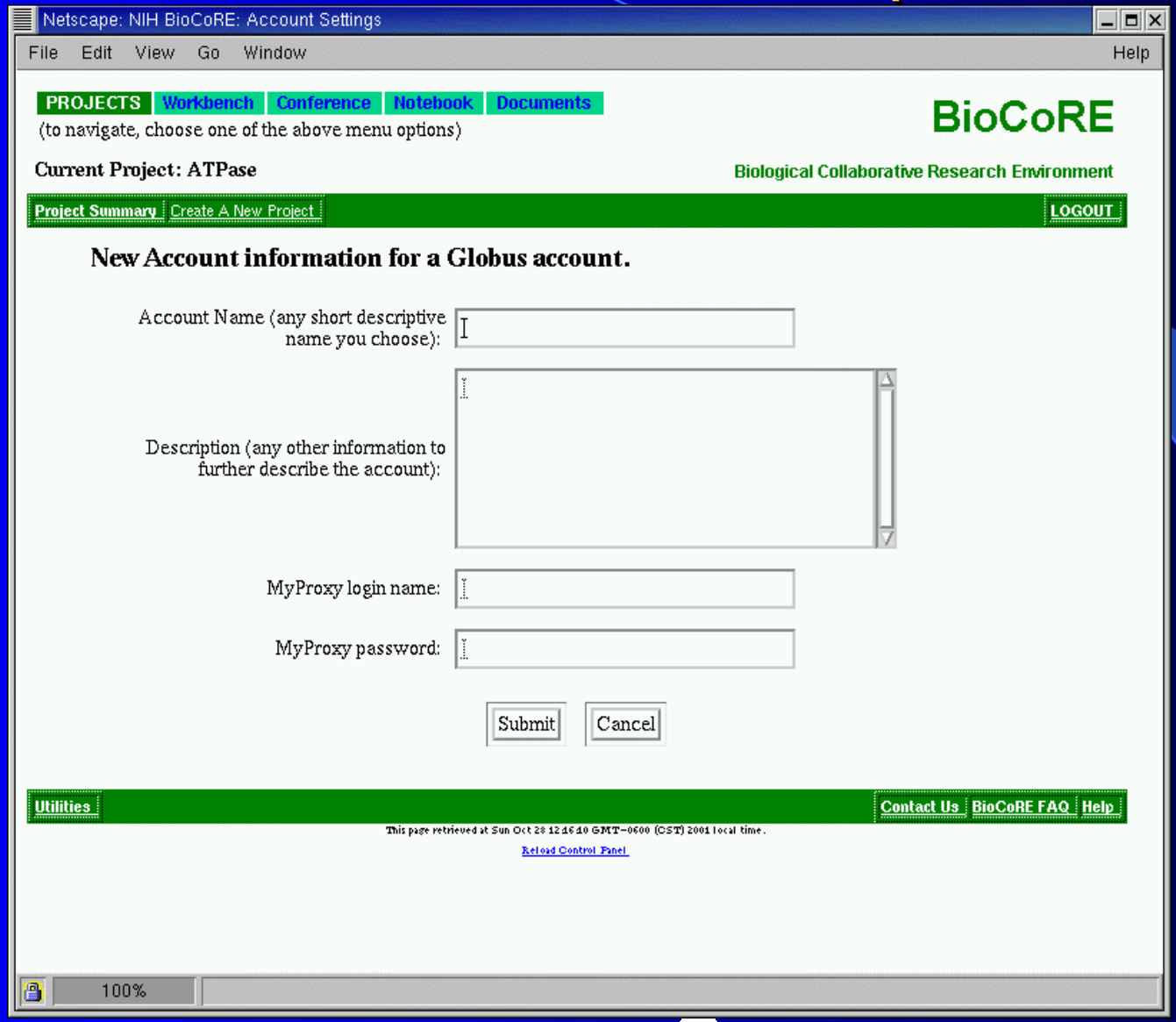
- User selects supercomputer
- SC account accessed via Globus or SSH



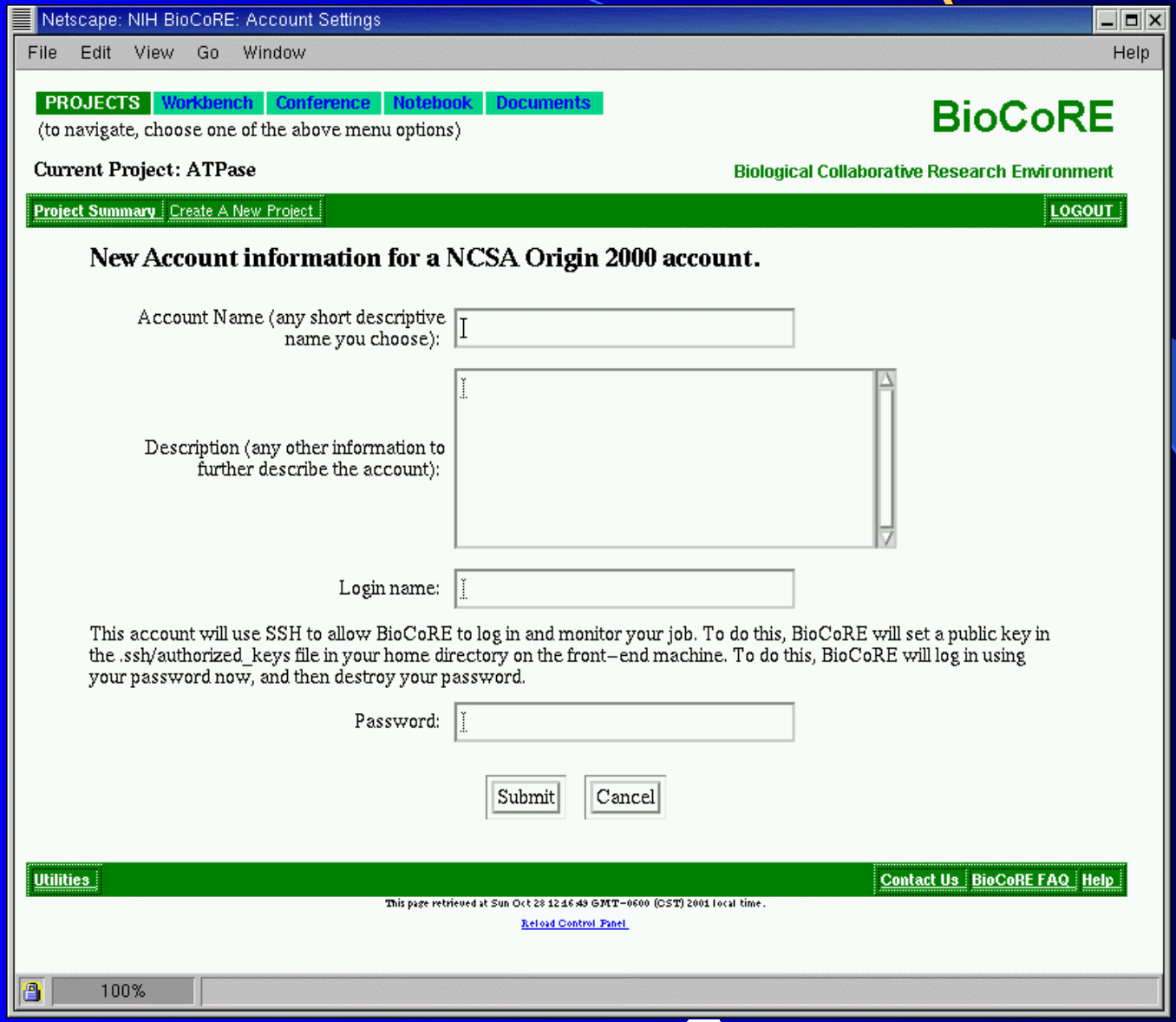
Globus Support

- 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)

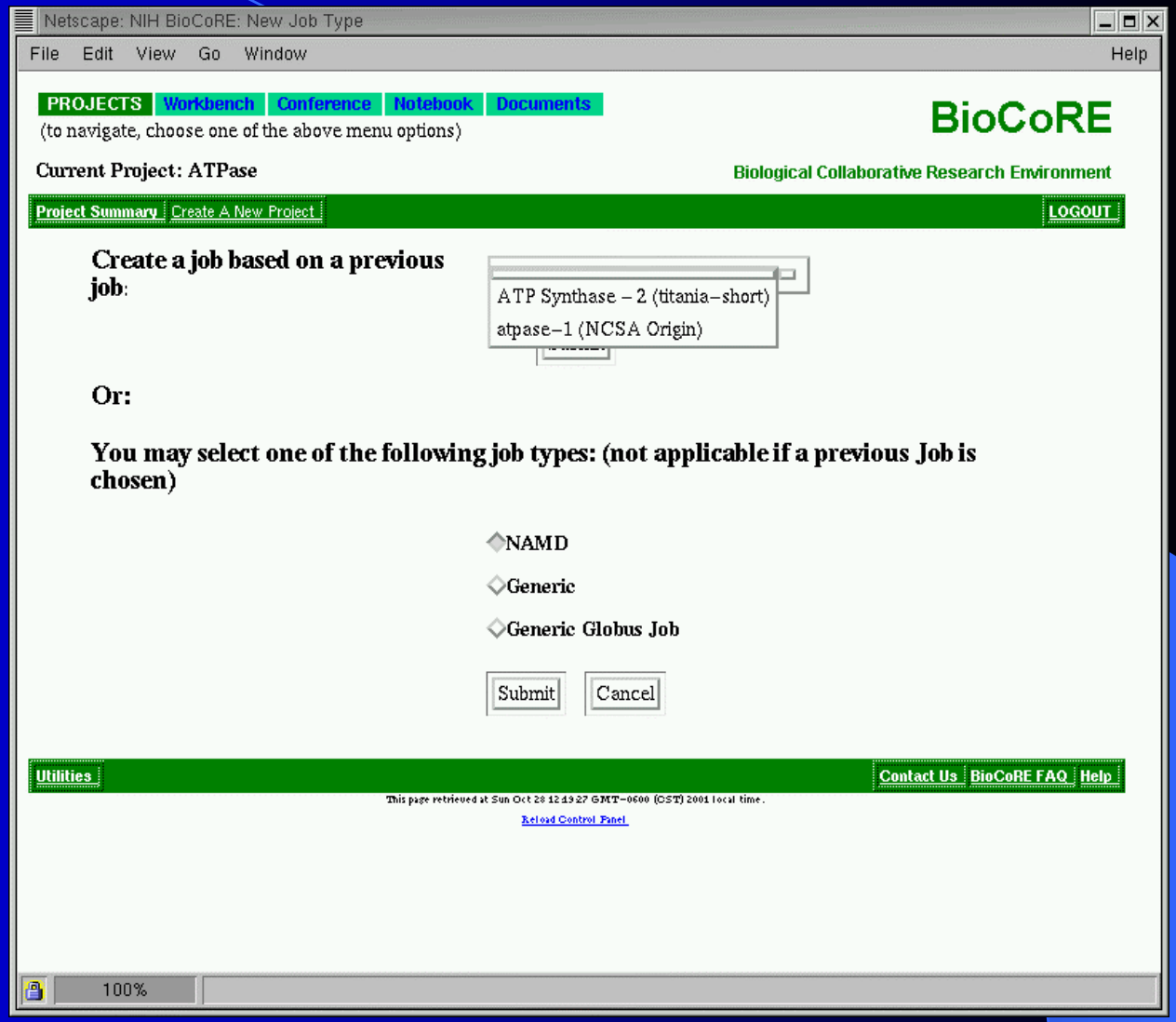


Account Details (SSH)



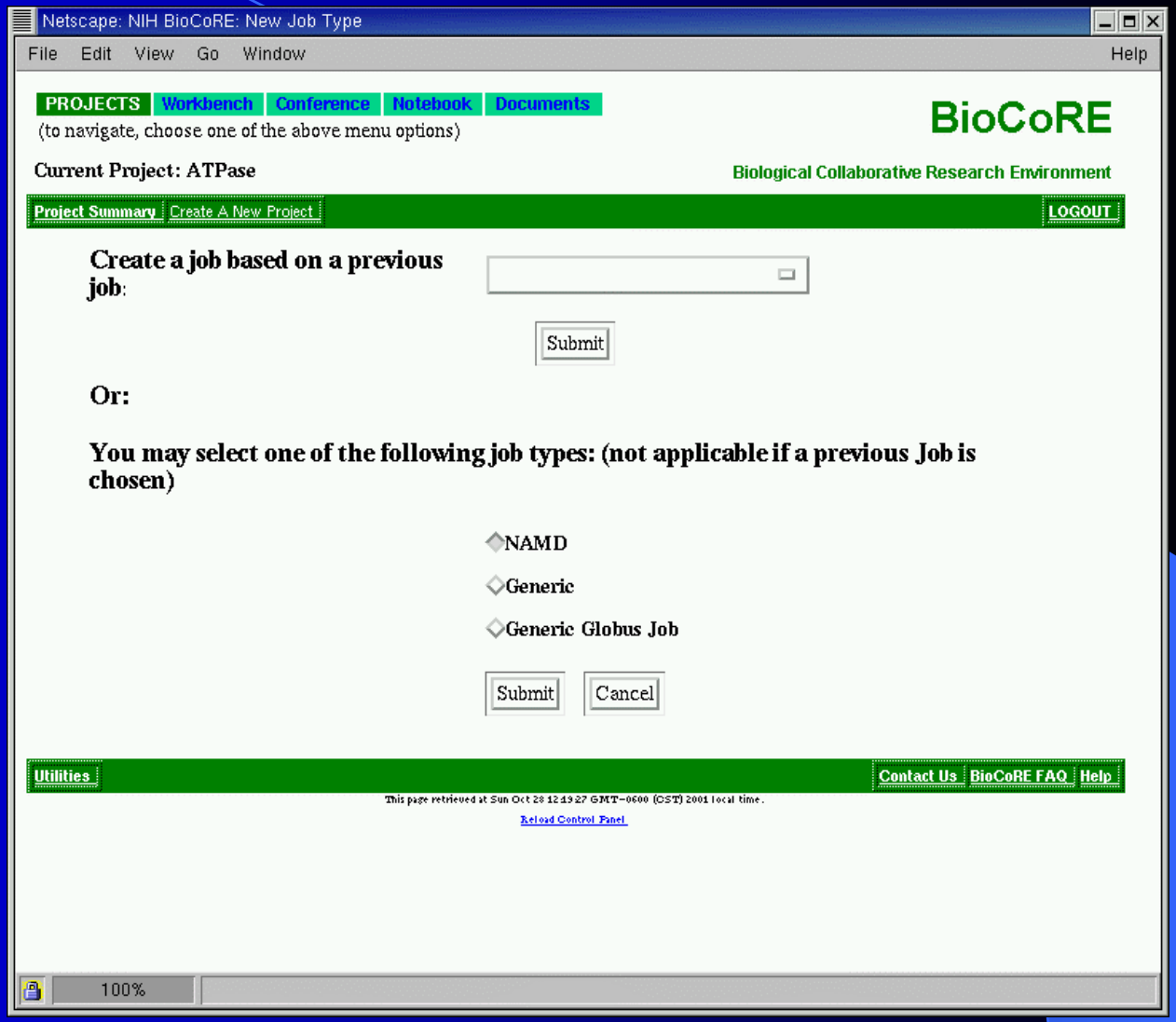
Job Submission via BioCoRE

- Submit a new job based on previous job parameters



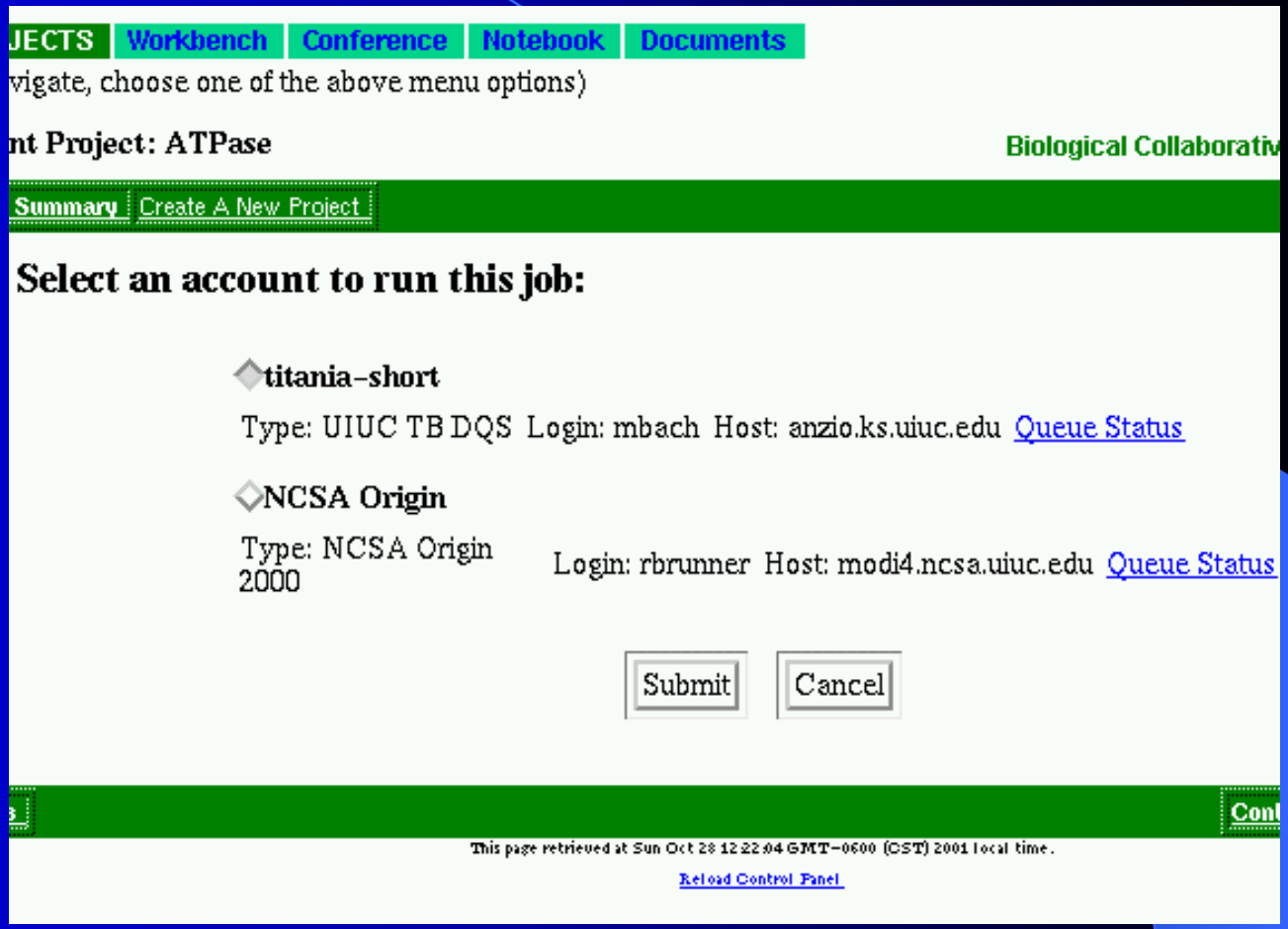
Job Submission via BioCoRE

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



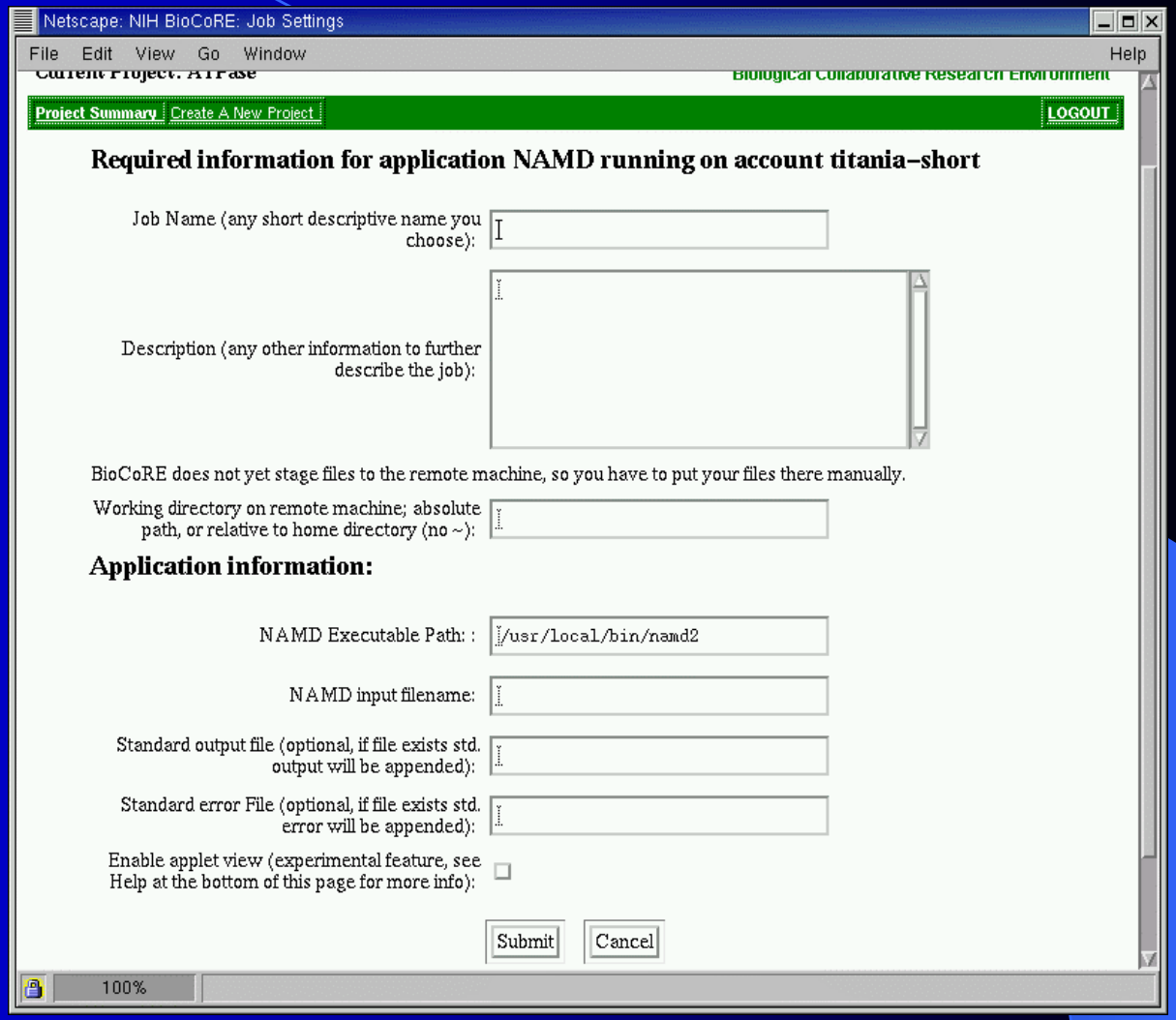
Job Submission via BioCoRE

- Select account
- Check queue status



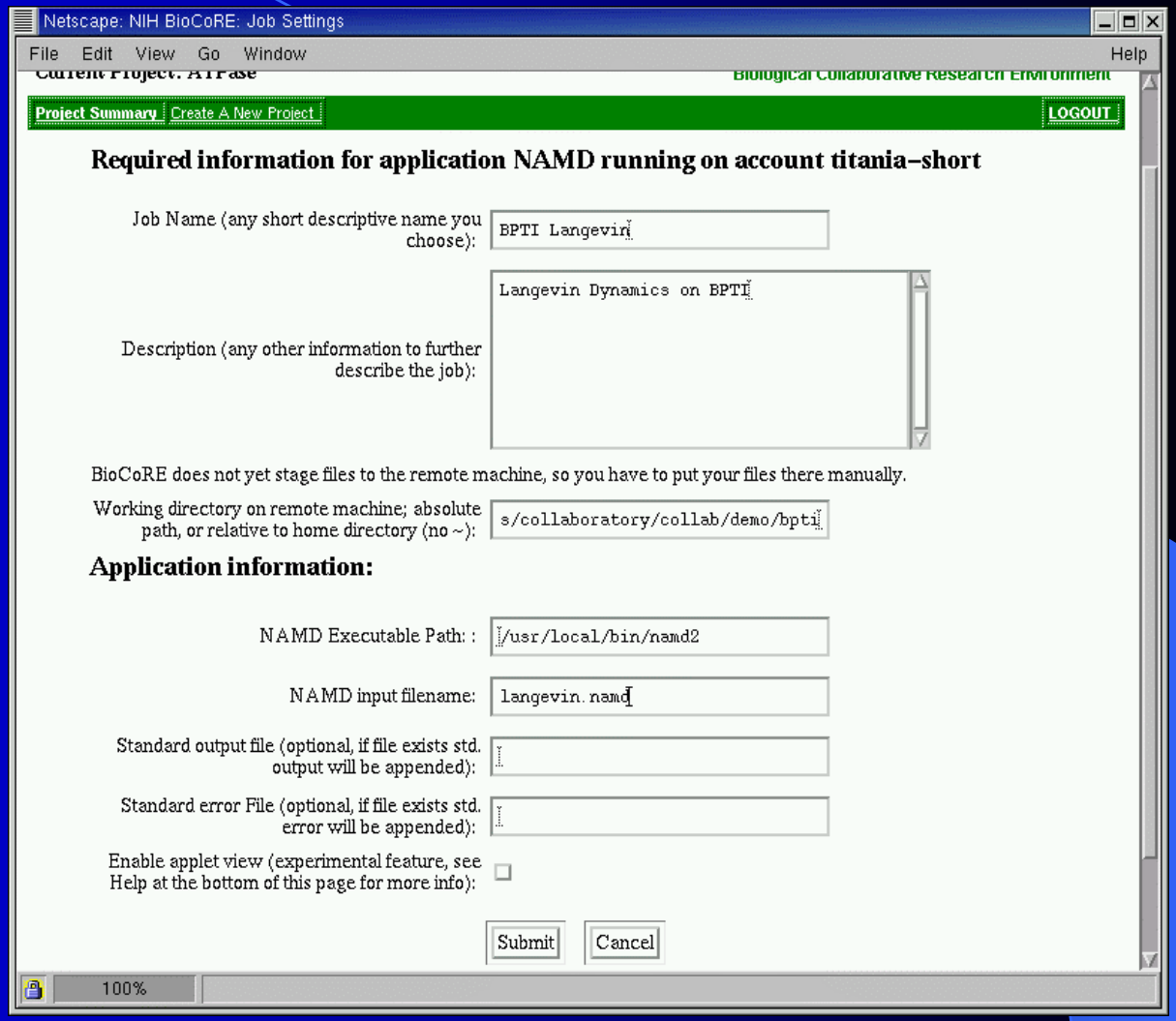
Job Submission via BioCoRE

- Set the job parameters



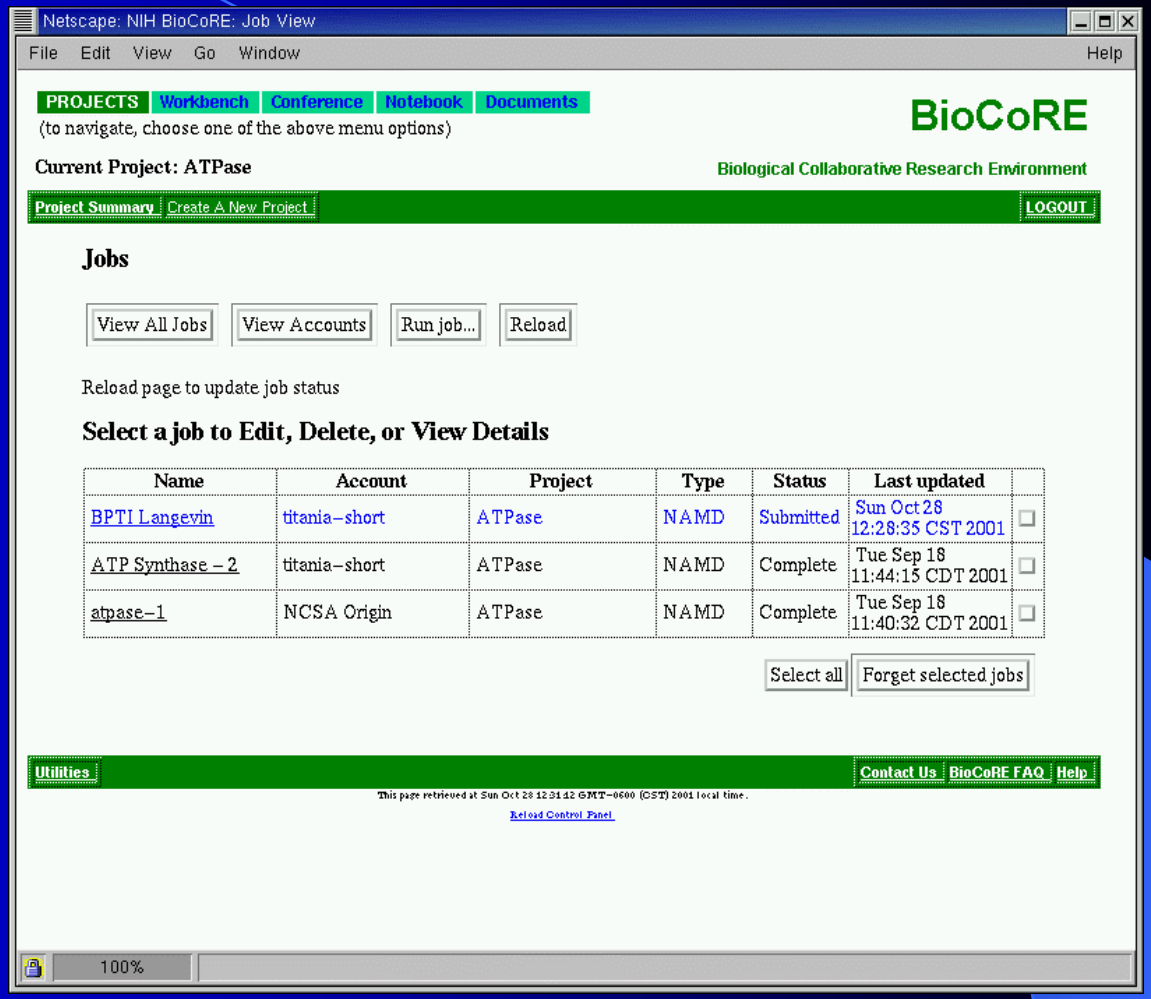
Job Submission via BioCoRE

- Set the job parameters
- Submit job



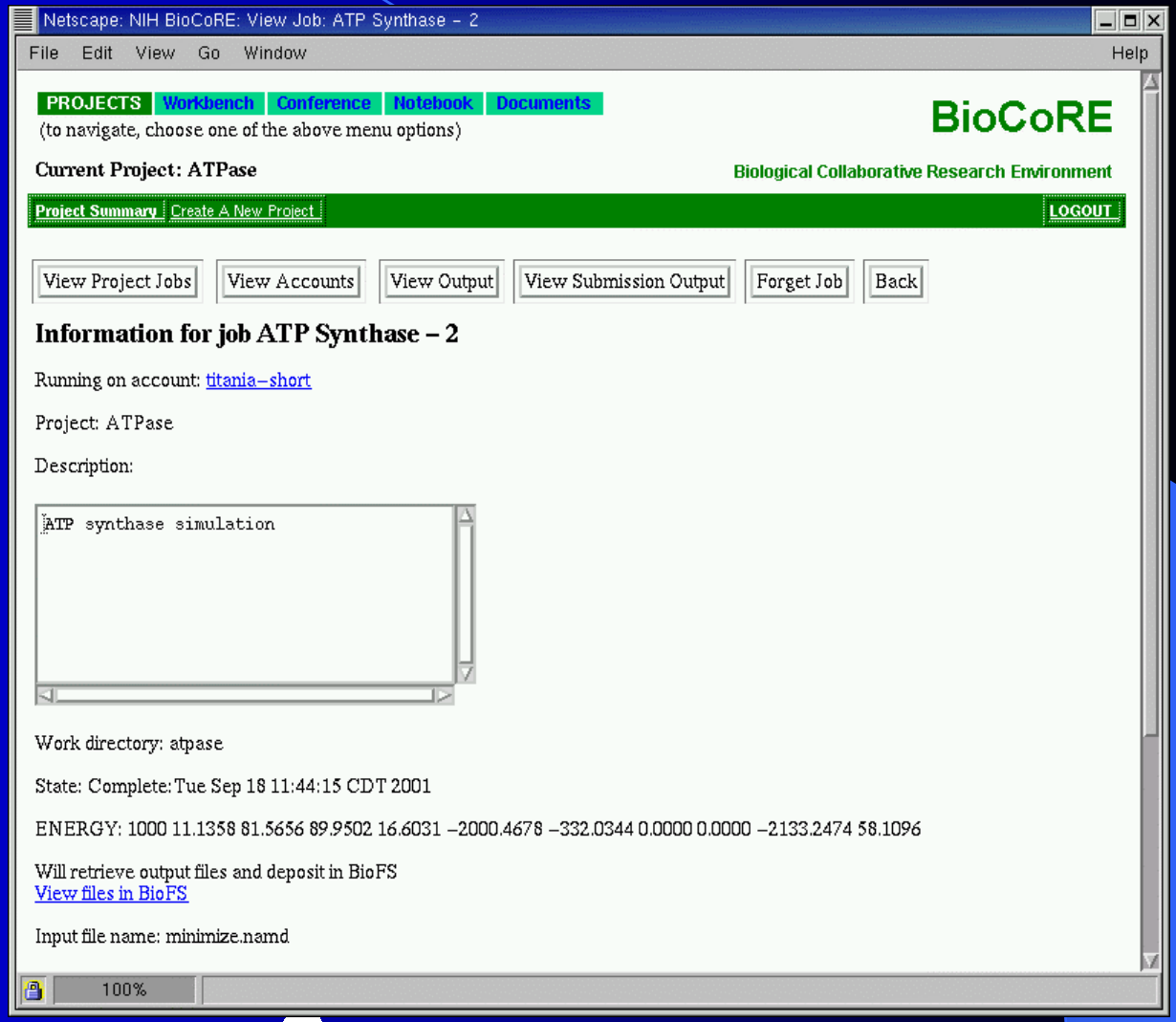
Monitor Running Jobs

- The new job has been submitted



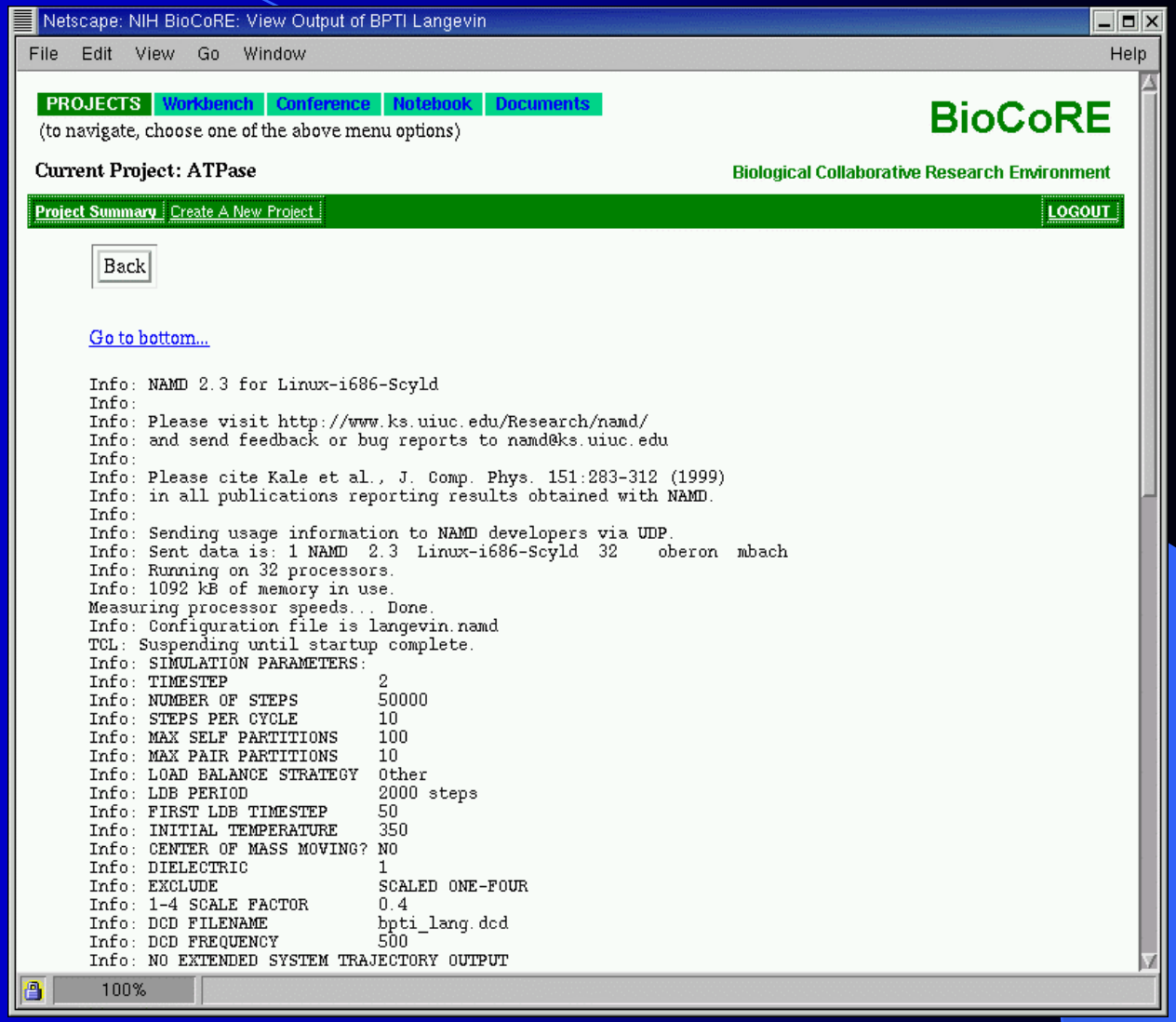
BioCoRE Job Details

- Details of running jobs can be displayed



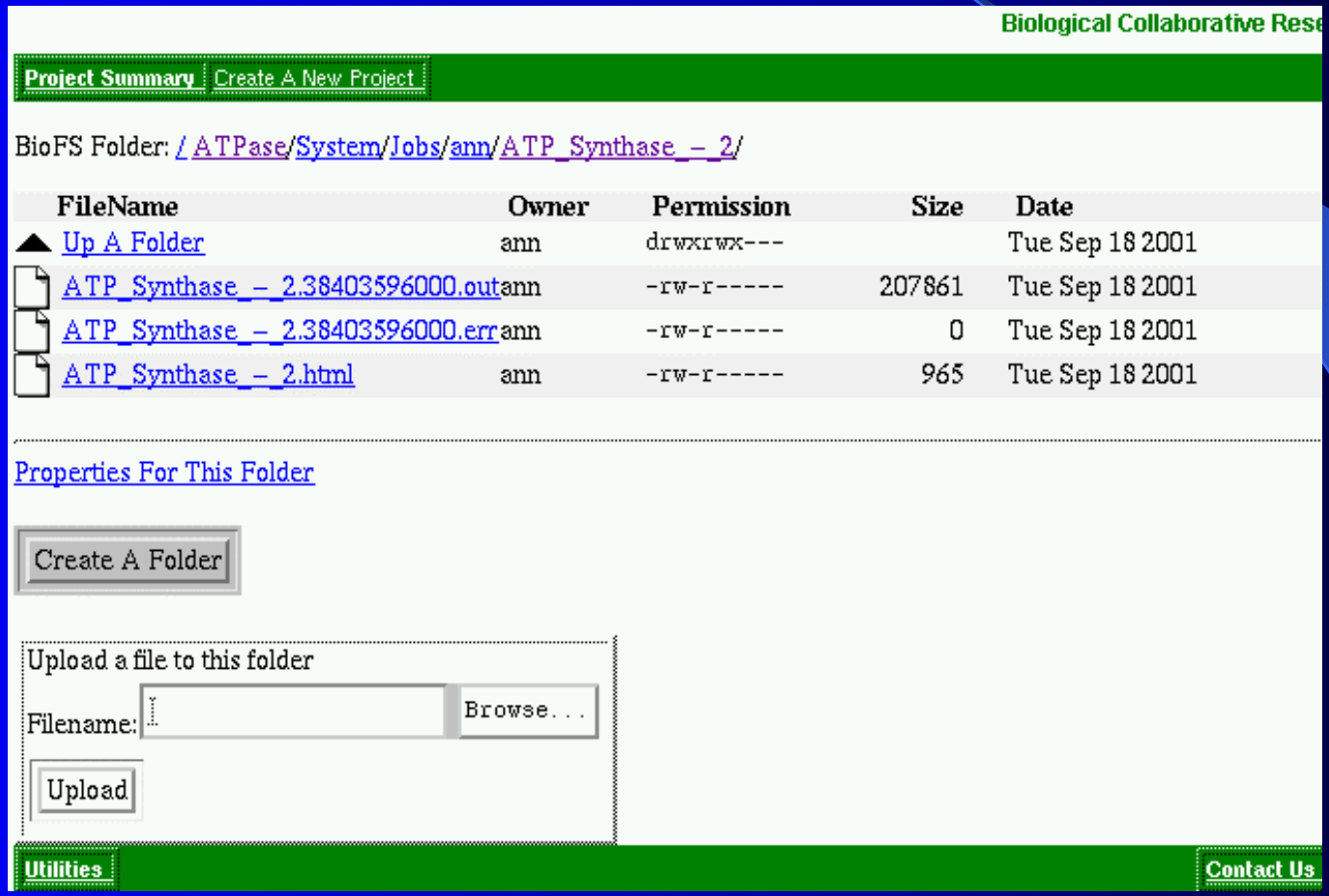
BioCoRE Job Details

- Standard output of the job



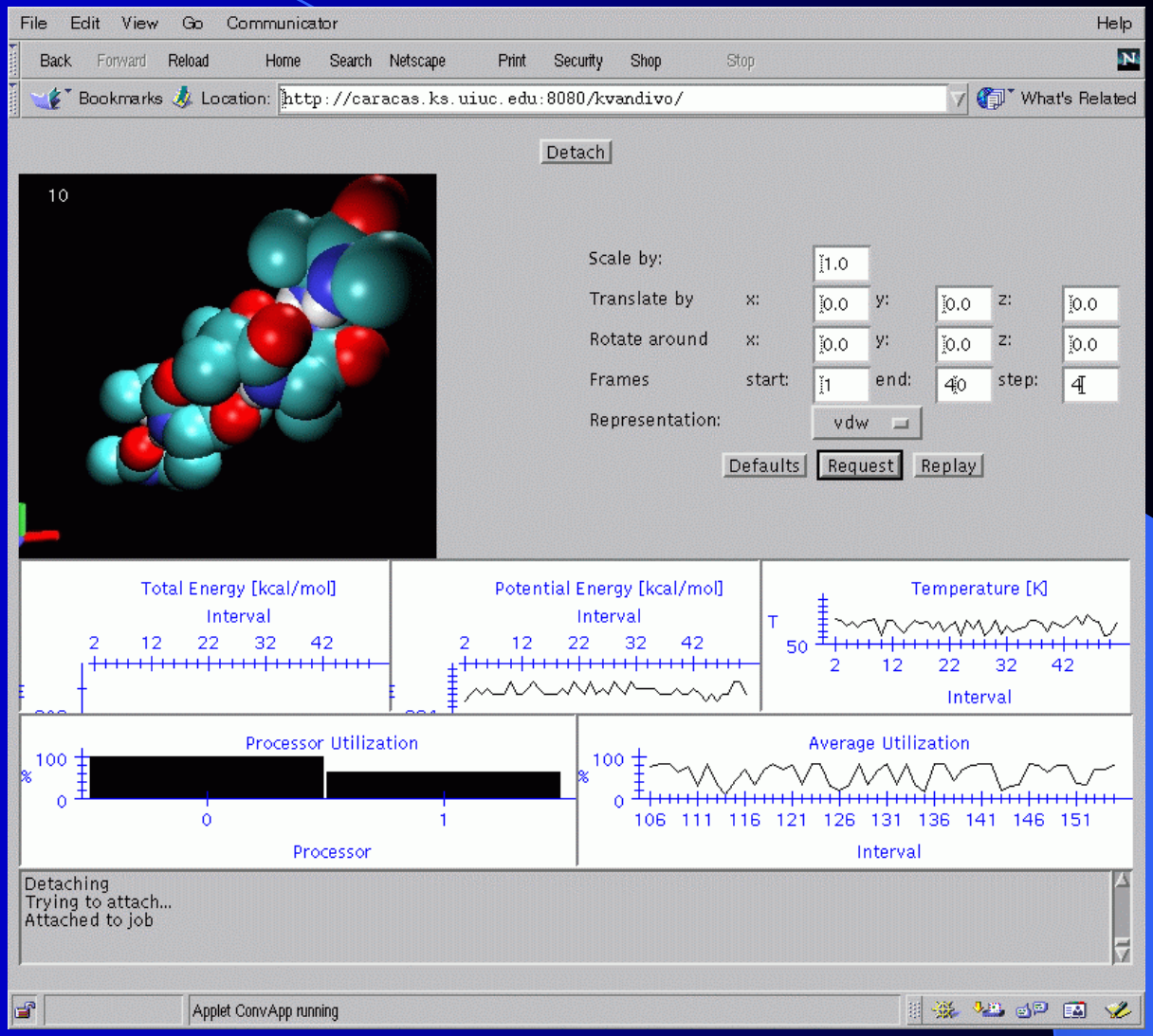
Job Details Saved To BioFS

- Accessible to all project members

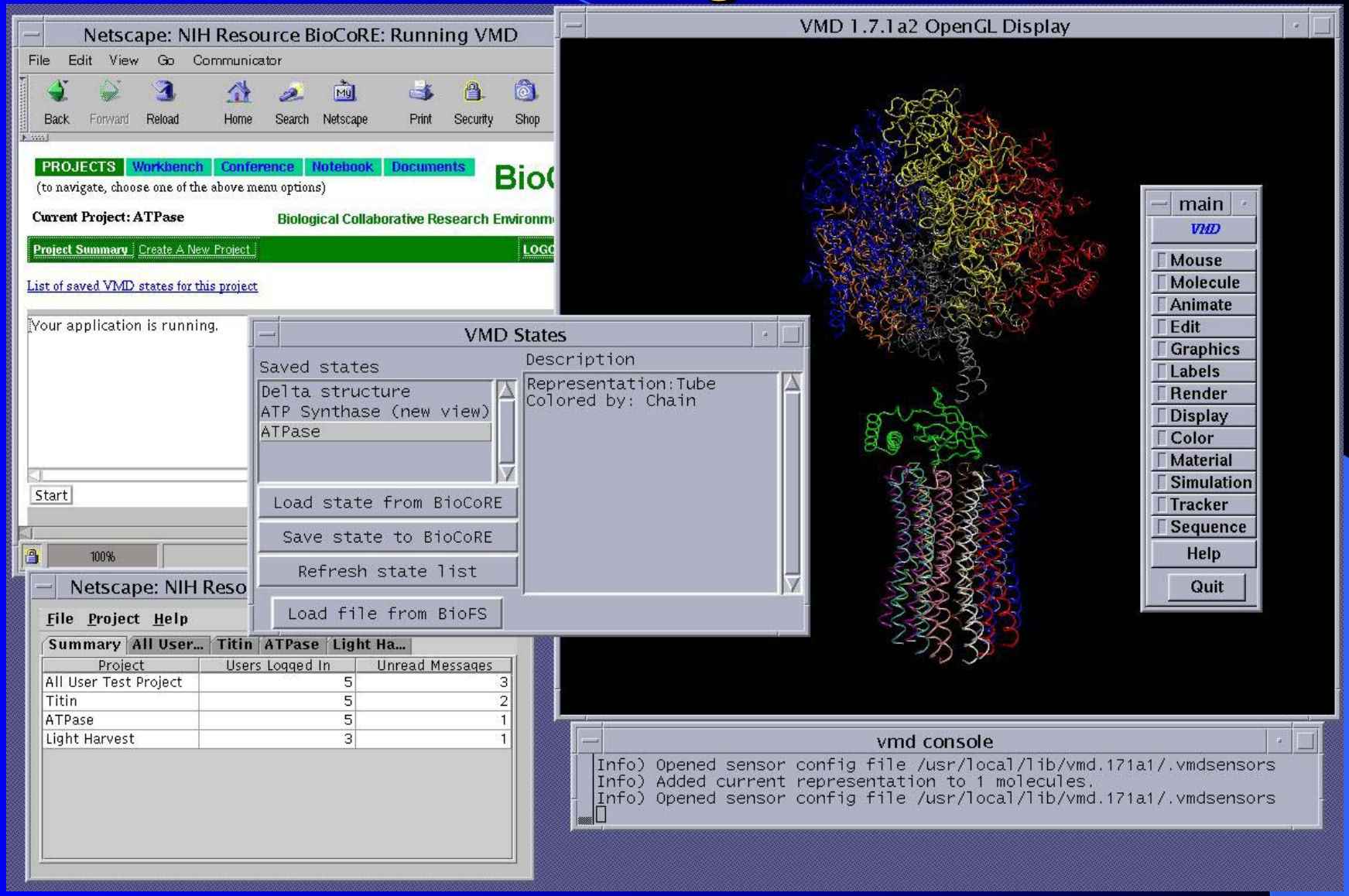


BioCoRE Job Details

- Graphical capabilities when running NAMD

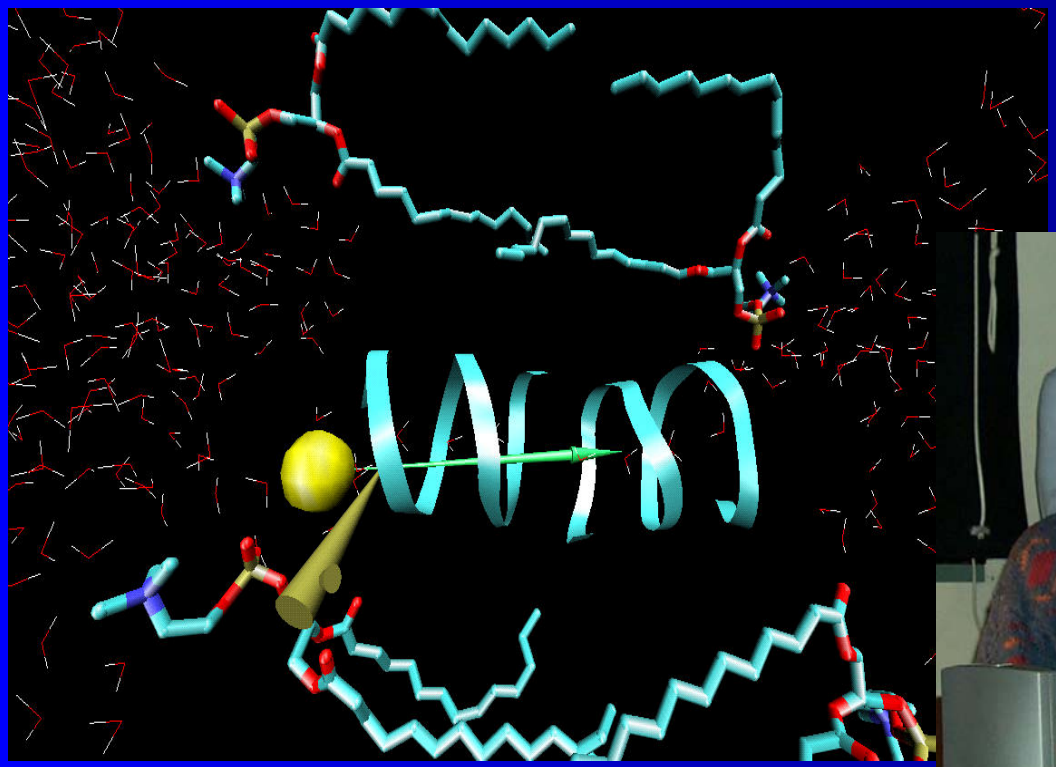


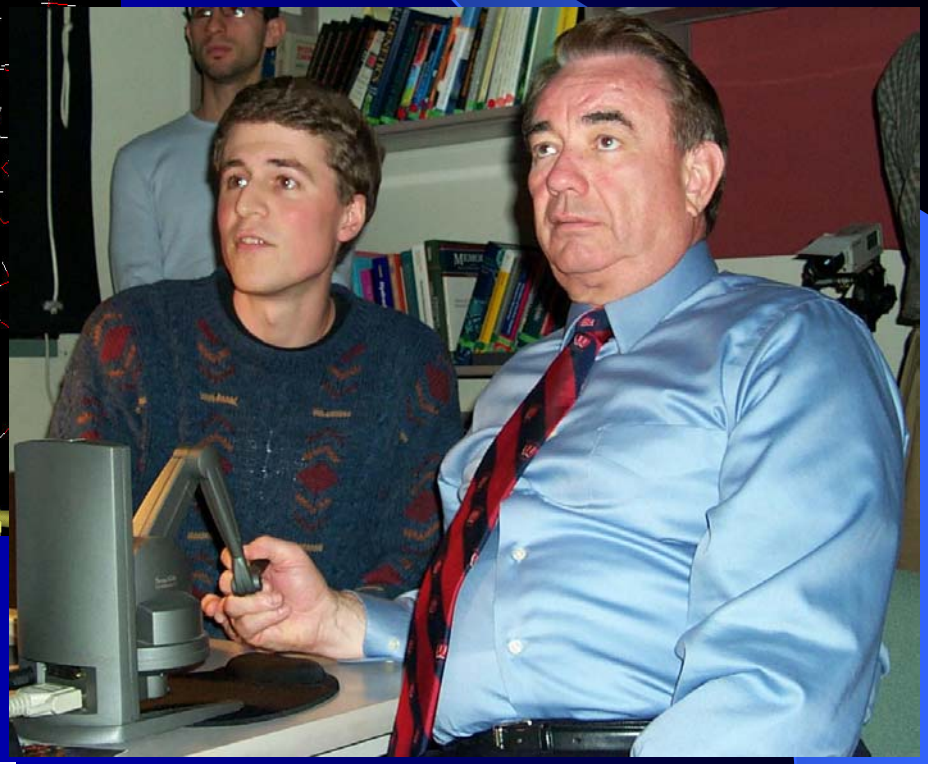
Launching VMD



Interactive MD

- Real-time interaction between VMD/NAMD



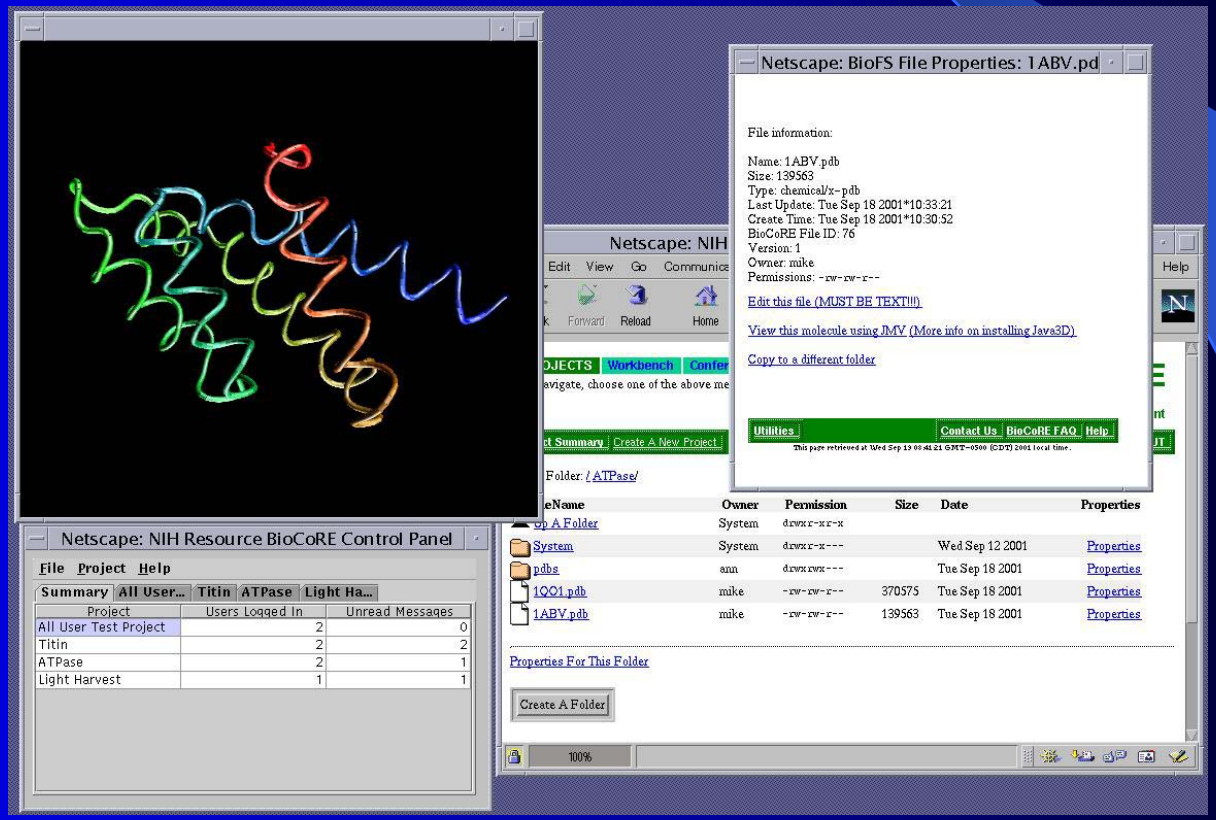


http://www.ks.uiuc.edu/Research/biocore/

Theoretical Biophysics Group,
Beckman Institute, University of Illinois at Urbana/Champaign

JMV Support Within BioCoRE

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

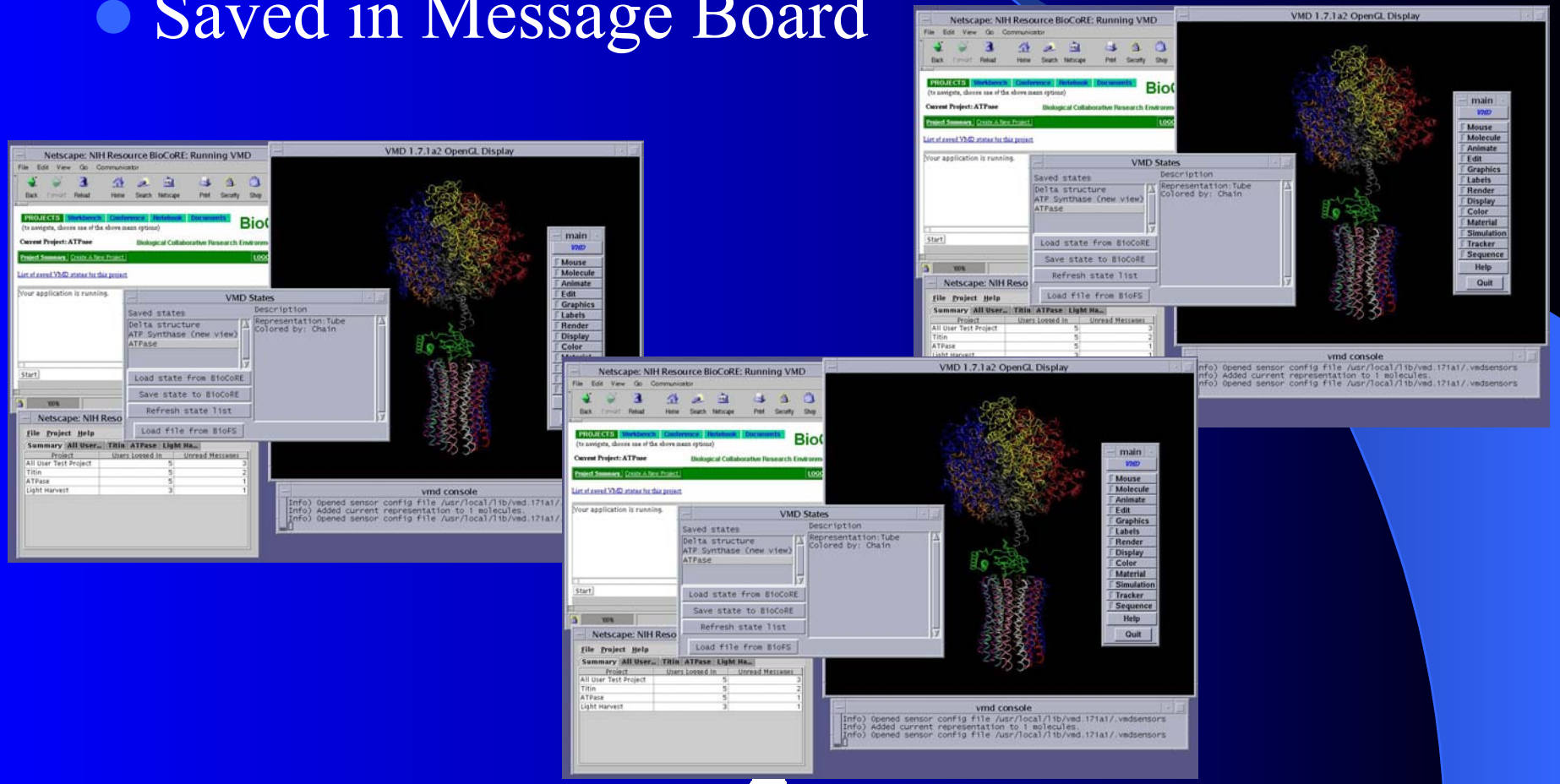


Collaboration Tools

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

Collaborative VMD

- Load/save visualization states
- Saved in Message Board



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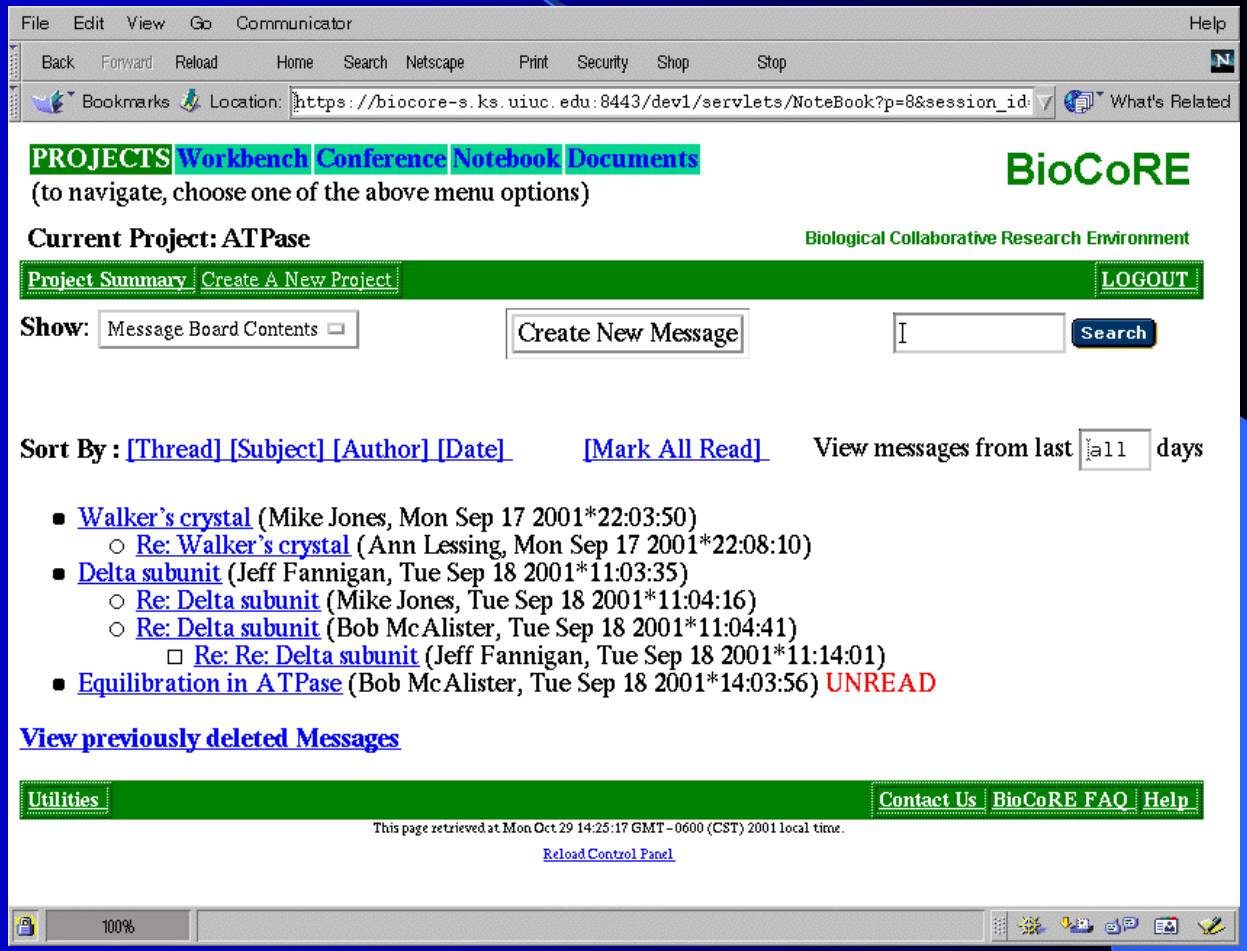
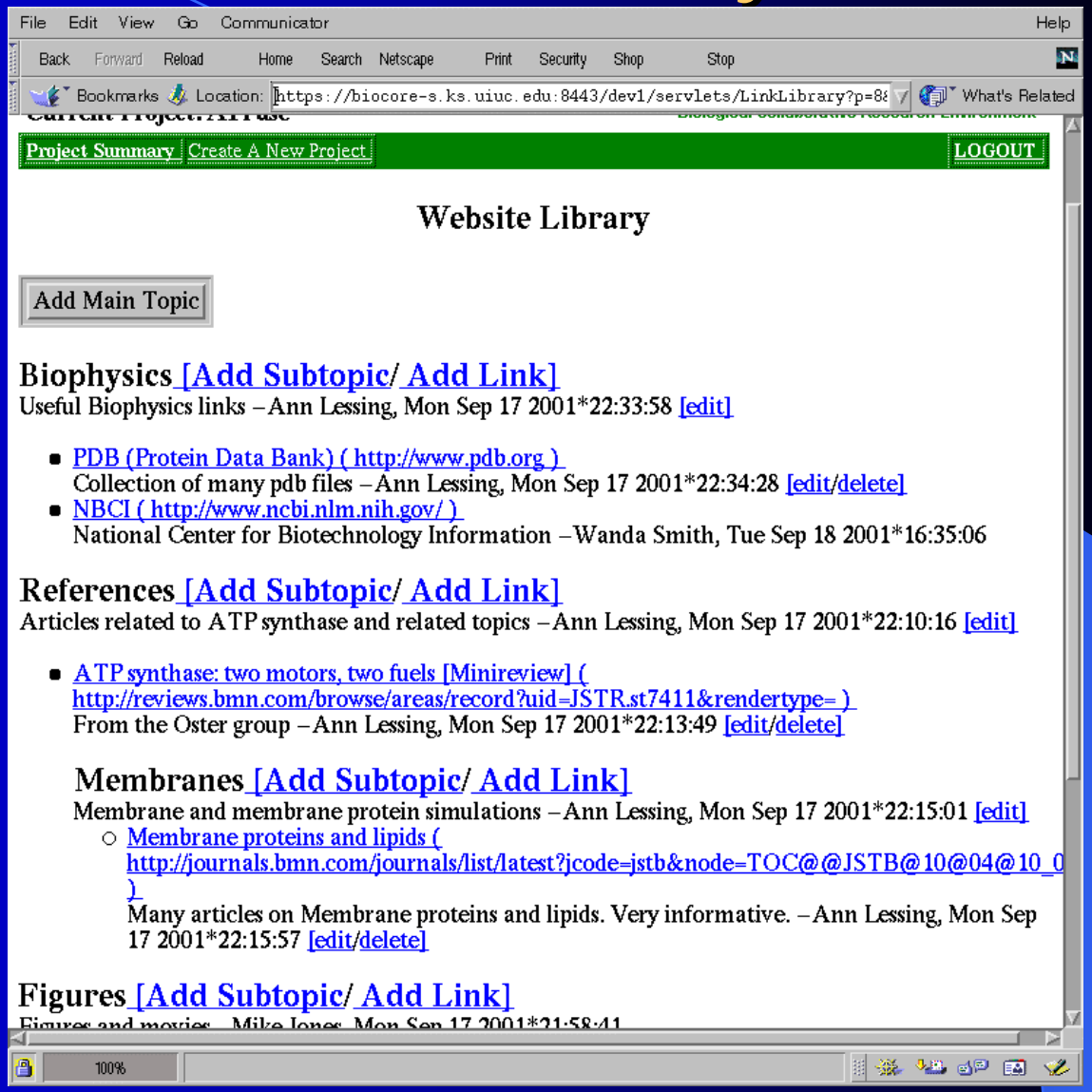
BioCoRE Message Board

- Asynchronous
- Threaded
- Sortable
- Searchable



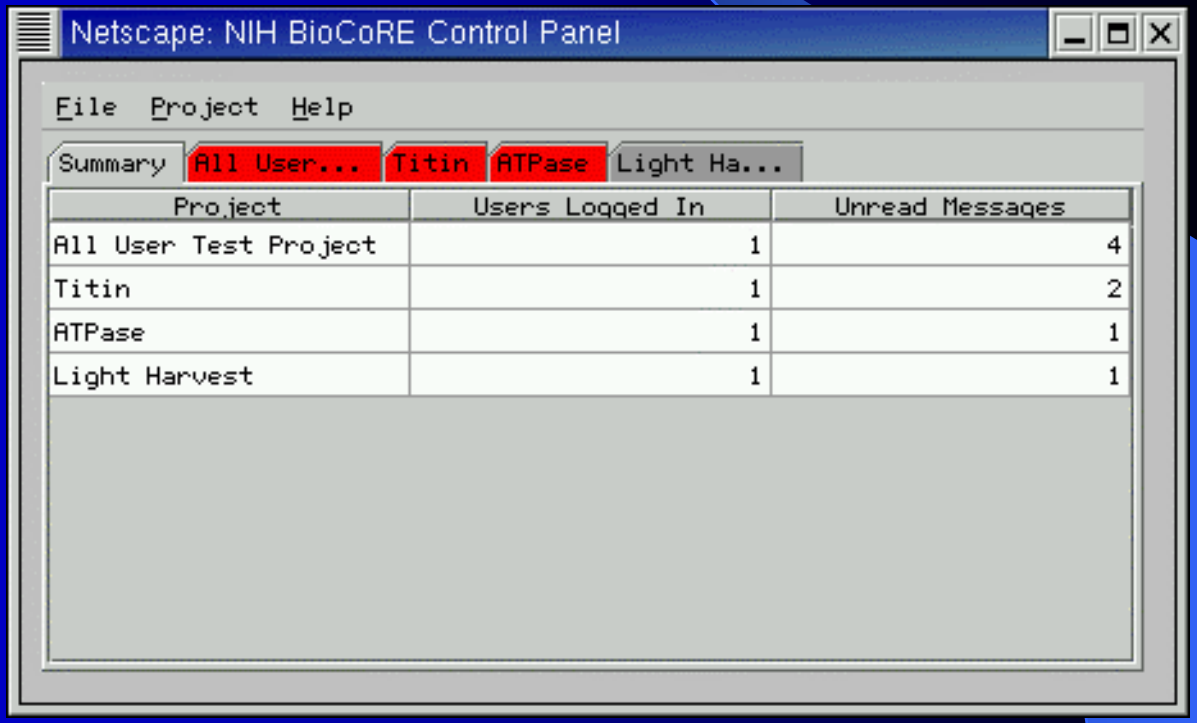
Website Link Library

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



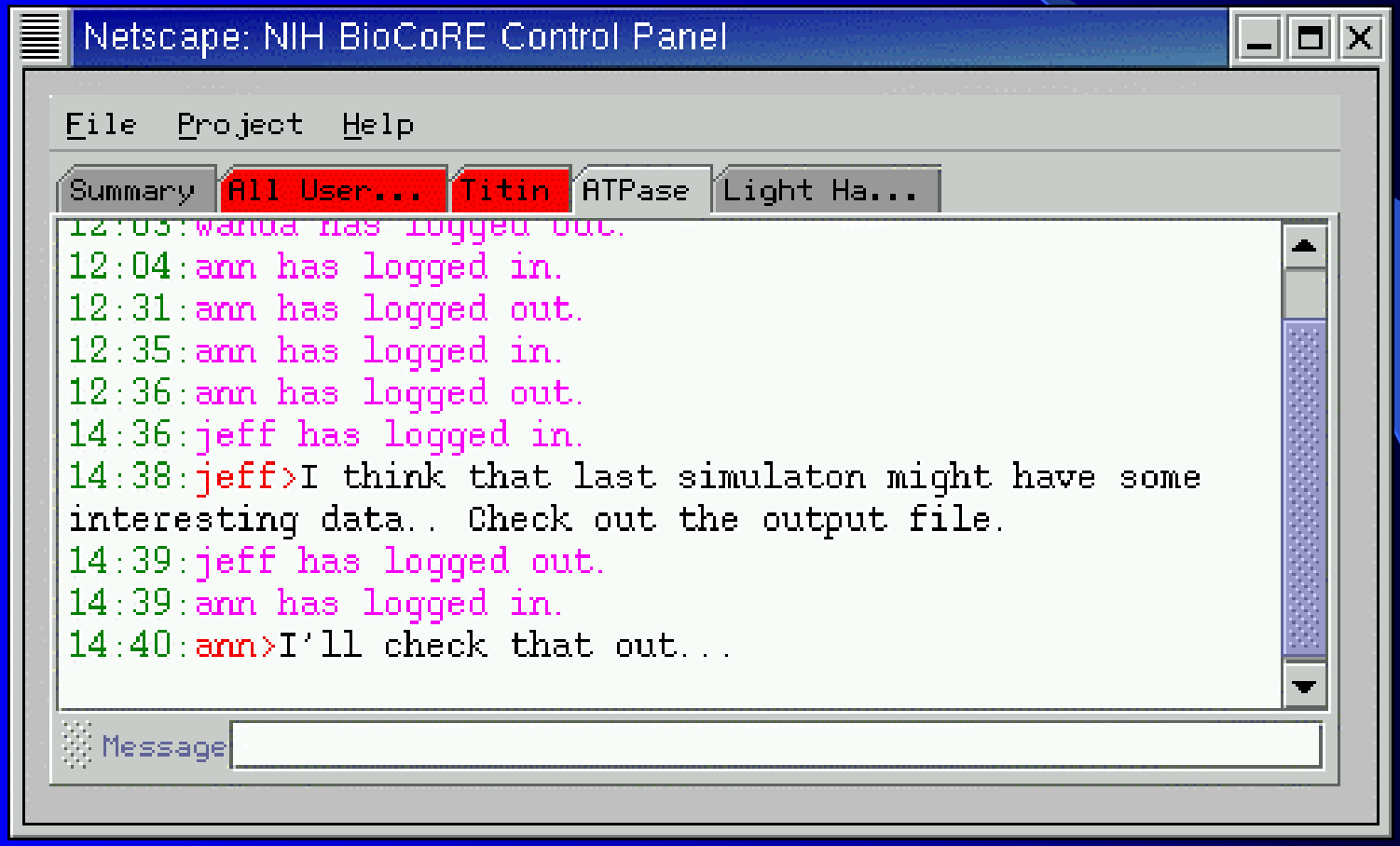
BioCoRE Control Panel

- "Always-on"
- Automatic event notification
- Java Swing



Control Panel Chat

- Saved to Message Board



Publication Tools

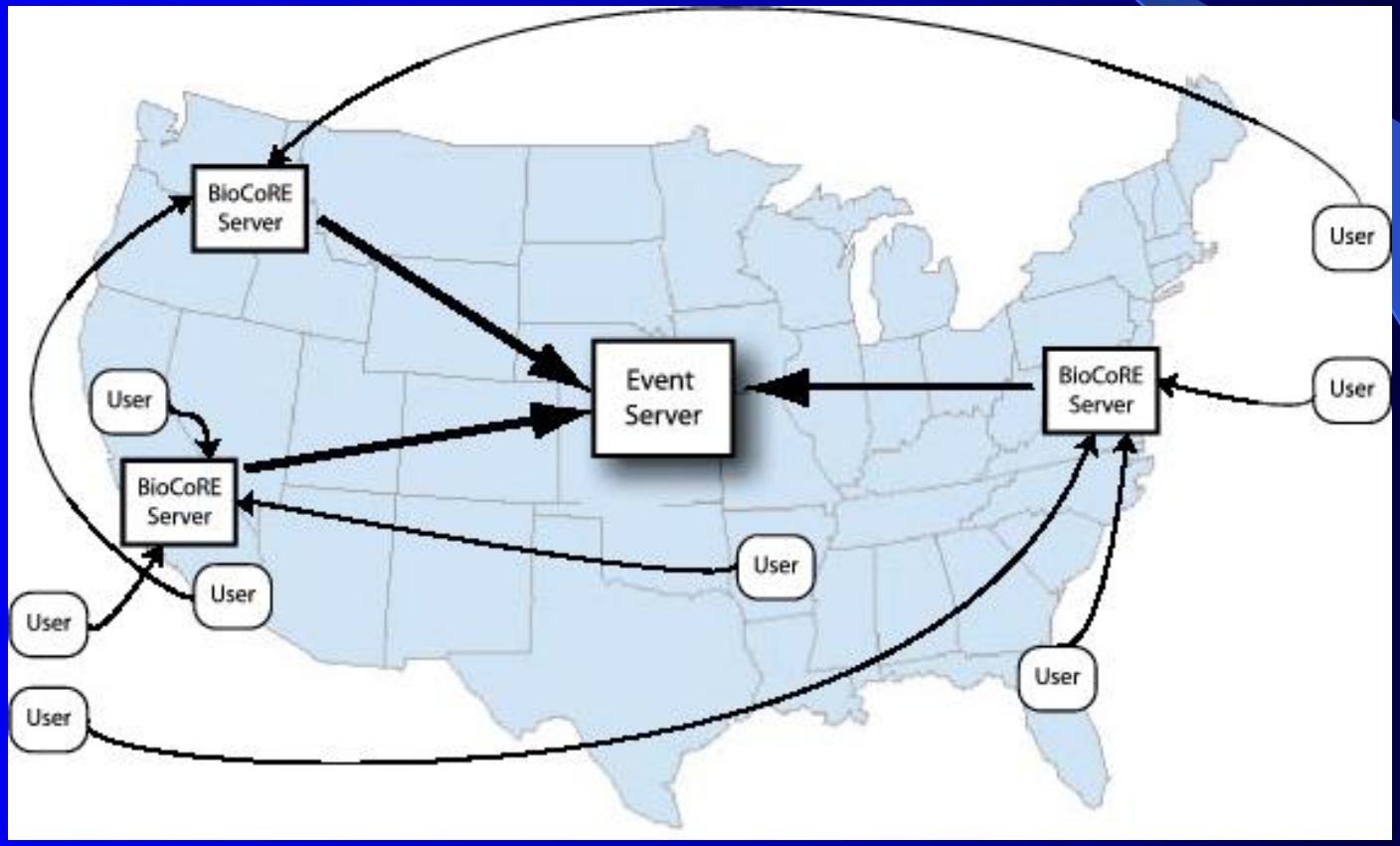
- BioFS support for seamless file transport across platforms
- File conversions planned (Word→TeX, TeX →Word, etc.)
- WebDAV for easy access

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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