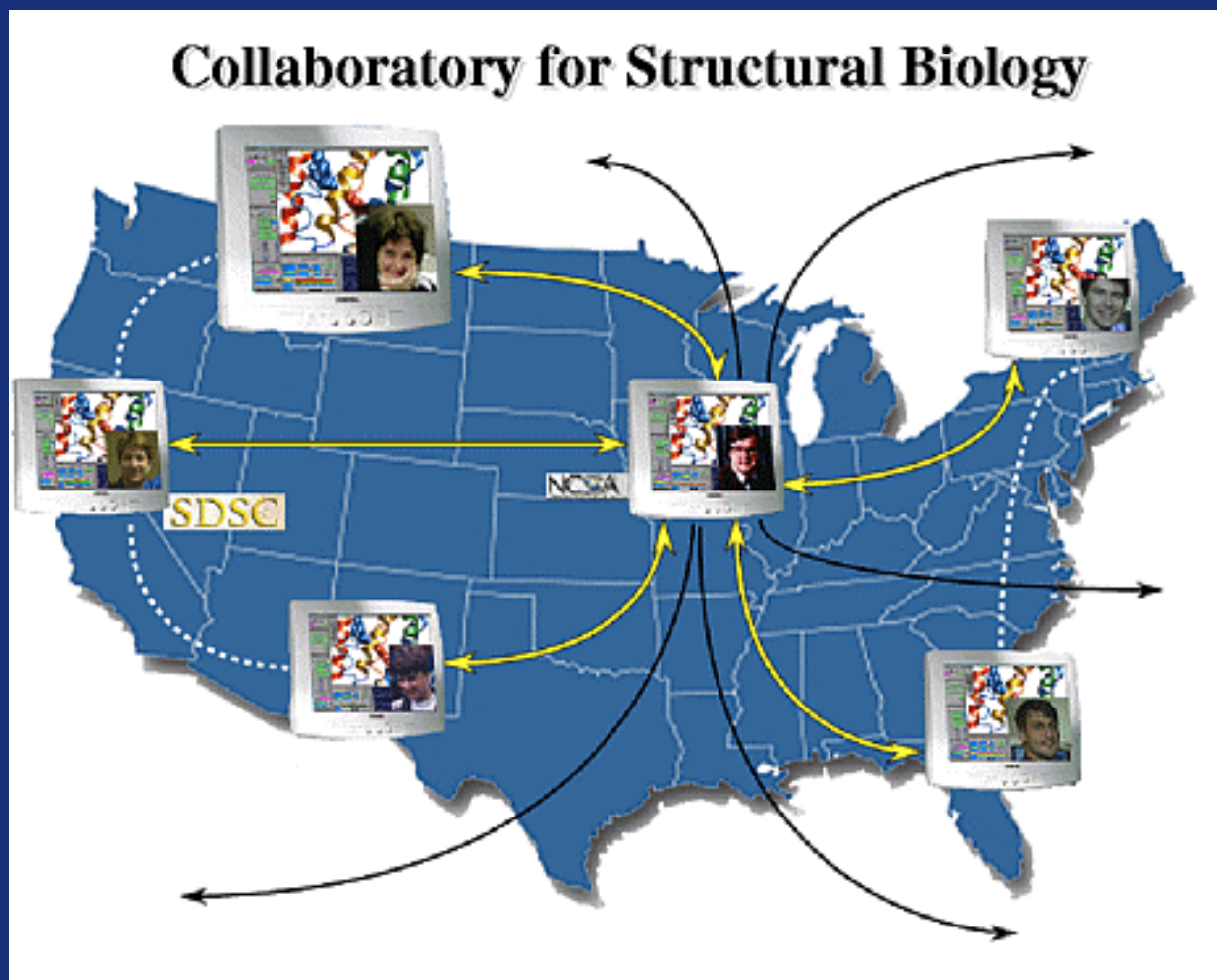


BioCoRE Tools

Developers:
Mike Bach
Robert Brunner
Jay Desouza
Laxmikant V Kale
Sameer Kumar
Kirby Vandivort*
Hui Wang

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 Infrastructure Goals

- ∞ Common access to applications, tools and databases
- ∞ Shared data, computational, and multimedia resources
- ∞ Synchronous or asynchronous interactions
- ∞ Software Engineering

∞ BioCoRE has four main toolboxes:

- Workbench
- Conferences
- Notebook
- Documents

The screenshot shows the BioCoRE Control Center interface. At the top, it says "Current Project: All User Test Project". The main area is divided into several sections: "Workbench" (containing "Monitoring Tool" and "VMD"), "Conference" (containing "Chatting Room"), "Notebook" (containing "Notebook"), "Documents" (containing "Planned For Future"), "Utilities", and "Logout!!". There are also links for "Need Help?" and "Frequently Asked Questions".

BioCoRE Control Center

Workbench
Monitoring Tool
VMD

Conference
Chatting Room

Notebook
Notebook

Documents
Planned For Future

Utilities Logout!!

Need Help? Frequently Asked Questions

Callout Boxes:

- Monitoring Tool:** 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.
- Chatting Room:** 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.
- Notebook:** 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 laboratory, such as chat. And everything is searchable!
- Utilities:** The Utilities section allows you to take care of administrative functions such as changing your password or changing your current project.
- Logout!!:** Always click logout when you want to leave BioCoRE

BioCoRE Servers

∞ Main Server – Can be replicated on remote sites

- Java Servlets
 - Apache Web Server
 - Jserv Servlet Engine
- SQL Database
 - Currently: MySQL (previously used DB2)
- Secure (https/SSL) connections

∞ Centralized Evaluation Server

- Main Servers deposit evaluation data periodically
- Stores registration information, time on task, etc.
- SQL Database
- Secure (https/SSL) connections only

BioCoRE Client

∞ Web Accessibility

- HTML
- Java applets
- Swing

∞ Extends Capabilities of Local Applications

- VMD
- Access to third-party applications planned

∞ Customizability

- Adjustable to user's expertise level
- User-tailored interface

∞ Network Requirements

- Minimal right now (modem OK)
- Will grow as tools are added

Nature of BioCoRE Research Activities

∞ Temporality

- Synchronous
 - Chats
 - Viewing running jobs
 - VMD publishing (soon)
- Asynchronous
 - Notebook stores everything

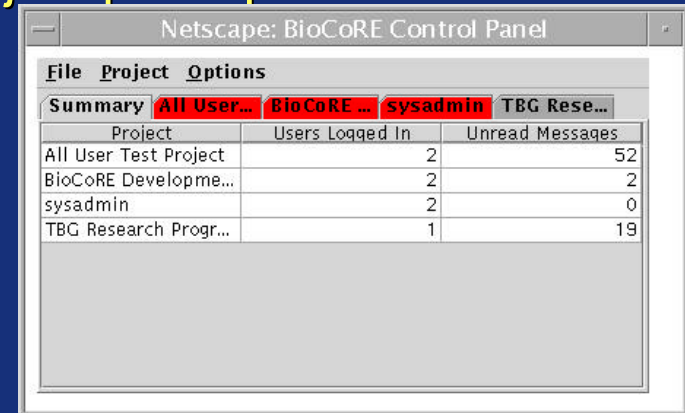
∞ No Central Computing Resource

- Users submit jobs to supercomputers using site-specific procedures
- Users perform analysis of results on own desktop machine

Deployed BioCoRE Tools

Control Panel

- Instant Messaging between logged-on project participants
- Notification of important BioCoRE events
 - Simulations starting/finishing (soon)
 - Users logging in/out
 - New Message Board Entries



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

Workbench Toolbox

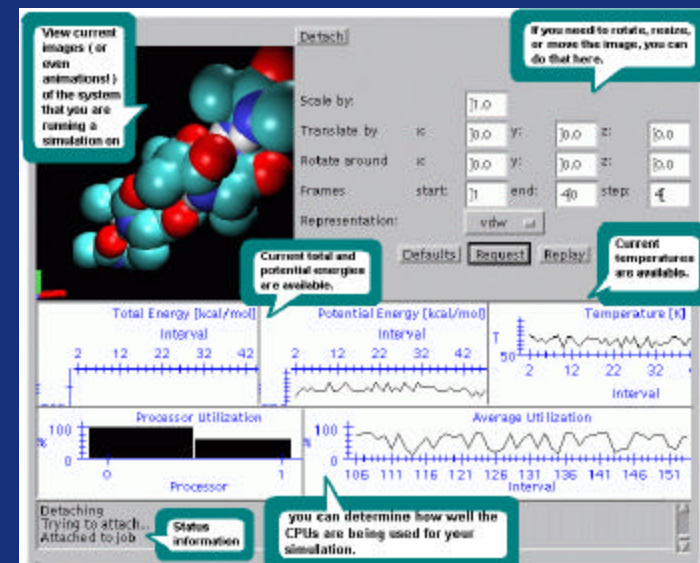
- Web-based job submission and monitoring

Notebook Toolbox

- Message board

Conferences Toolbox

- Subject-specific text conferences



To COTS or not to COTS*

∞ Current BioCoRE tools are not COTS components

- Operating System restrictions. We require more than just Micro\$oft.
- Licensing Concerns. License has to be reasonably flexible.
- Couldn't find high quality pieces for a reasonable price
- Evaluation requirements

∞ BioCoRE provides access to COTS programs

- VMD
- NAMD
- Others soon

∞ COTS components planned for future

- Audio
- Video
- Other suitable components, as they become available

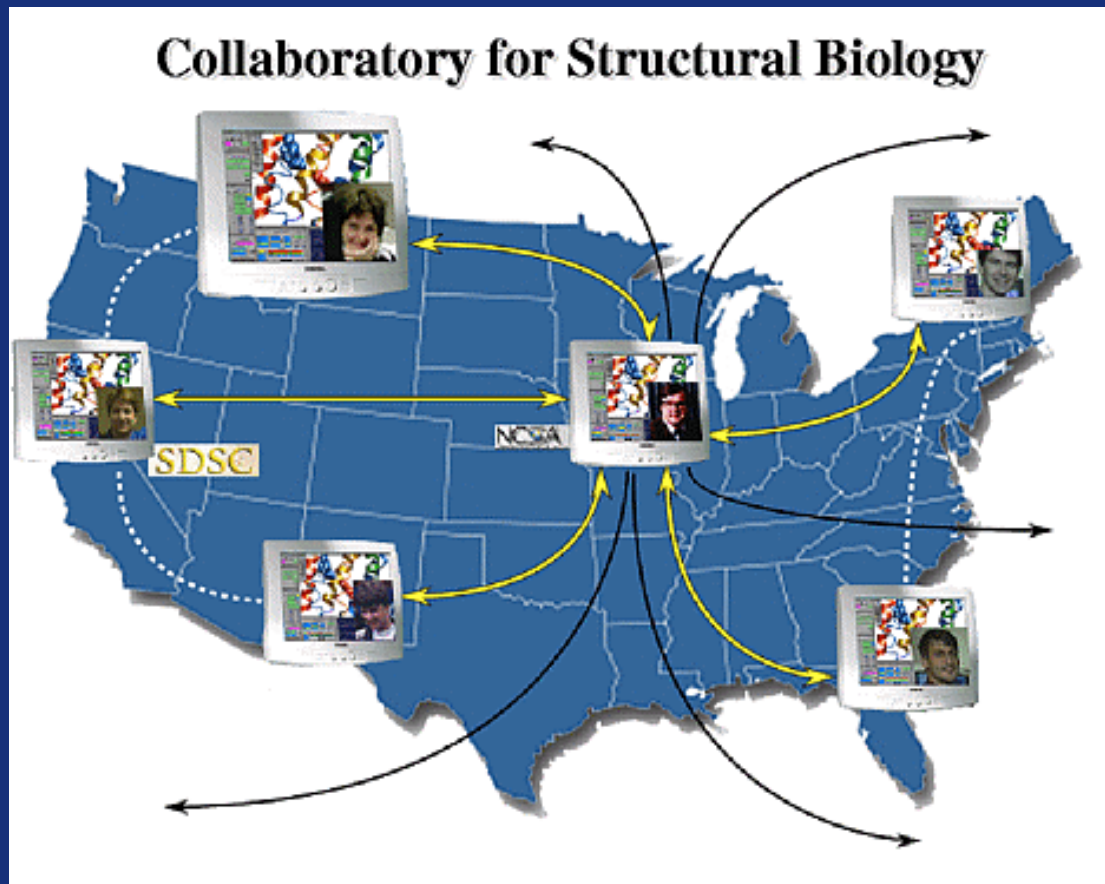
* COTS = Common Off-The-Shelf Components

Outstanding Tasks

- ∞ Convince users that BioCoRE enables better research
- ∞ Give priority to most preferred tools
- ∞ Capitalize on improved browser Java support
- ∞ Interface with more legacy applications

BioCoRE Tools

Questions?



Try us out:

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



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