BioCoRE Tools

Collaboratory for Structural Biology

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

October 27-29, 2000
Pittsburgh, Pennsylvania

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

- **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
Questions?

Try us out:
http://www.ks.uiuc.edu/Research/biocore

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