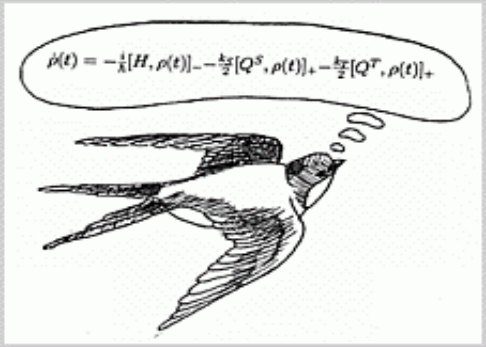
Theoretical Biophysics Group

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



Computational modeling links cryptochrome to magnetoreception in birds and other species

NewStories NEW

Software Releases NEW

New Thesis Projects

NIH Center for Research Resources

Hot Movies

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R Research
At a Glance
Recognition and Assembly
Steered/Interactive MD
Integral Functional Units
Quantum Biology
Various Systems
Sampling and Analysis
Neurobiology

D Development
VMD: Molecular Graphics
NAMD: Molecular Dynamics
BioCoRE: Collaborative Environment
Computing Resources

D Dissemination
Publications
Special Reports
Meetings and Tutorials
Brochures

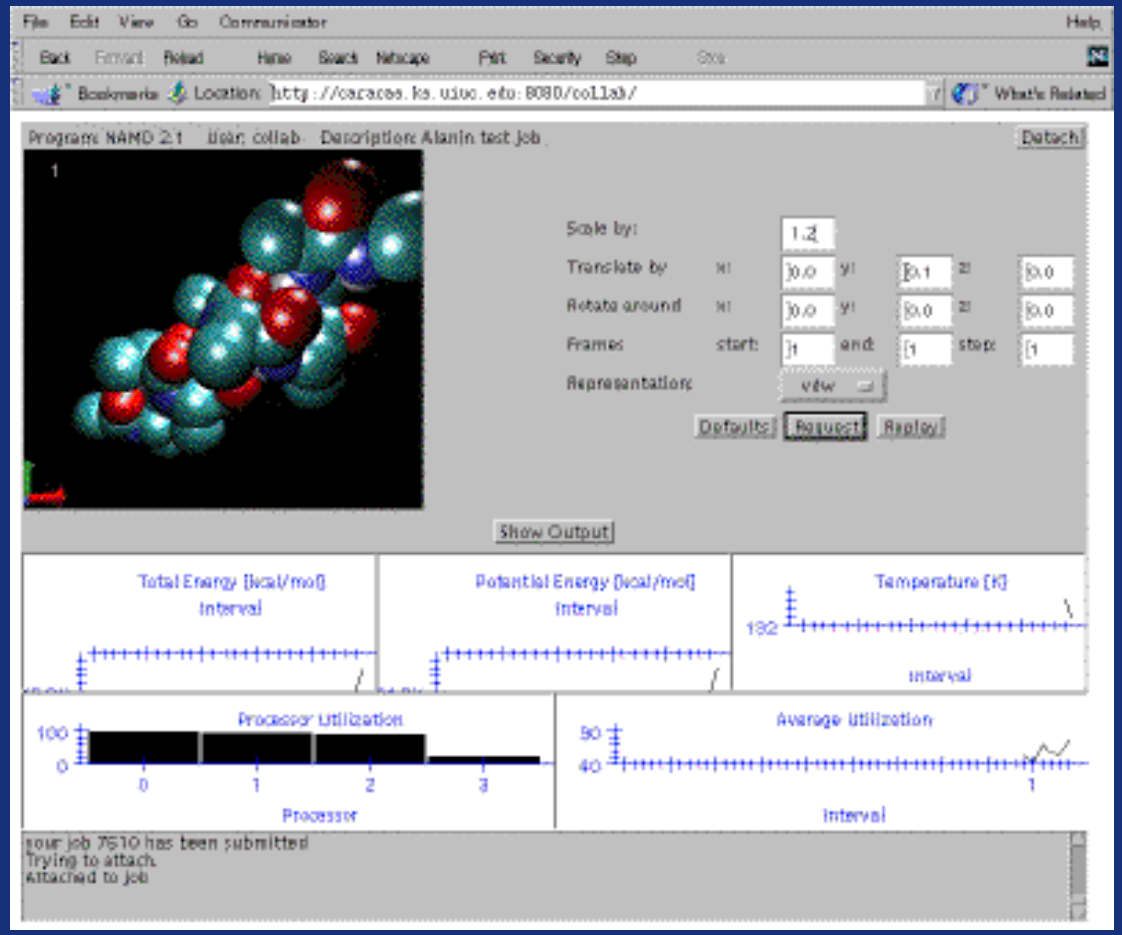
S Services
Seminars
Special Lectures
Classes
Employment
Web Statistics

Overview Research Development Publications Services

Software already available over Resource web site

Deliverables from Collaboratory Project

Access: Use of distant resources (etc, teraflop machines)



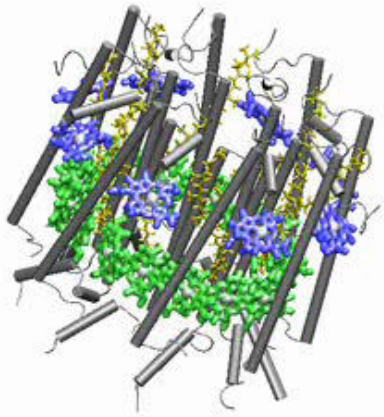
Required:

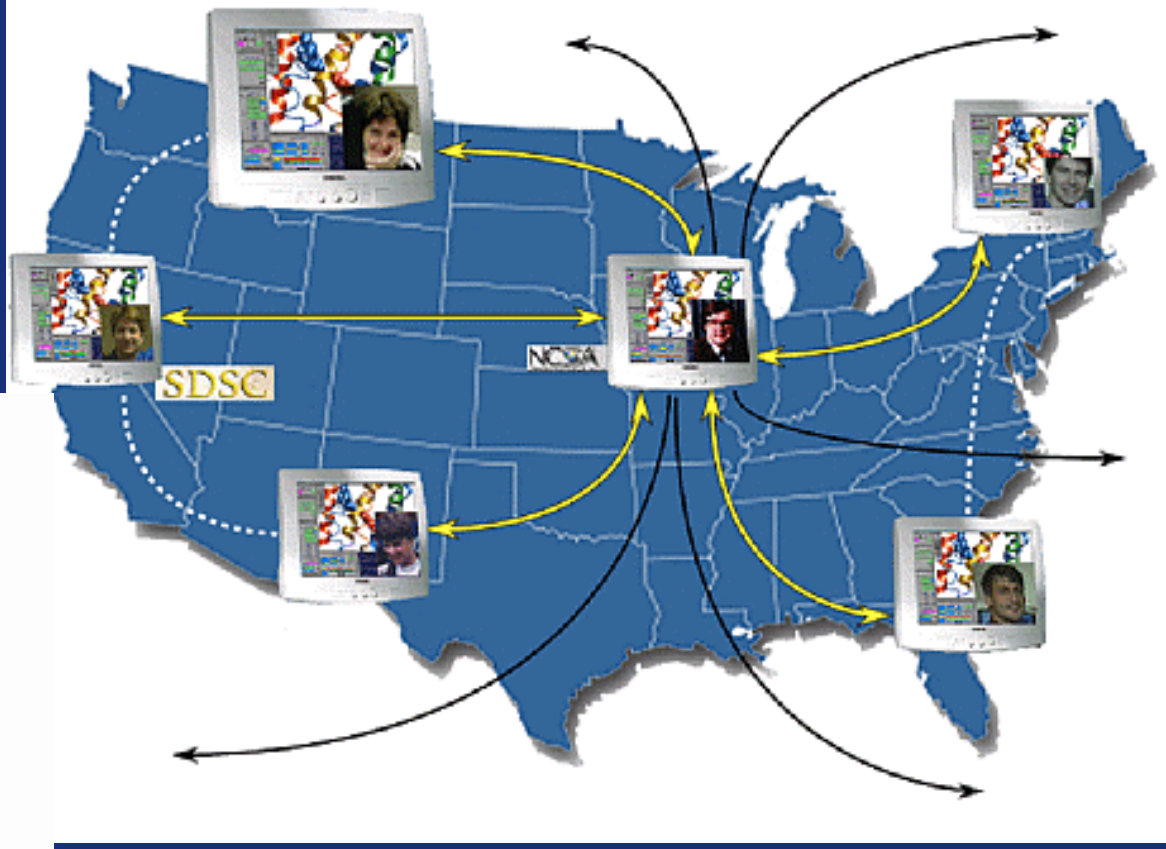
new web software development,
i.e., new expertise, much development effort
(new technology provides better Functionality, but at a price)

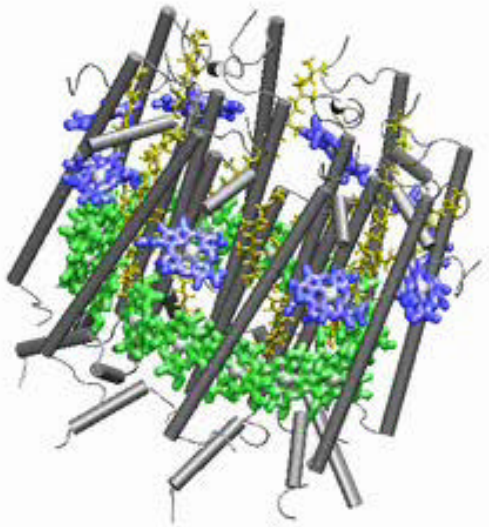
Deliverables from Col-laboratory Project

- **Teleconferencing:**

  Distant sites molecular graphics and modelling sessions

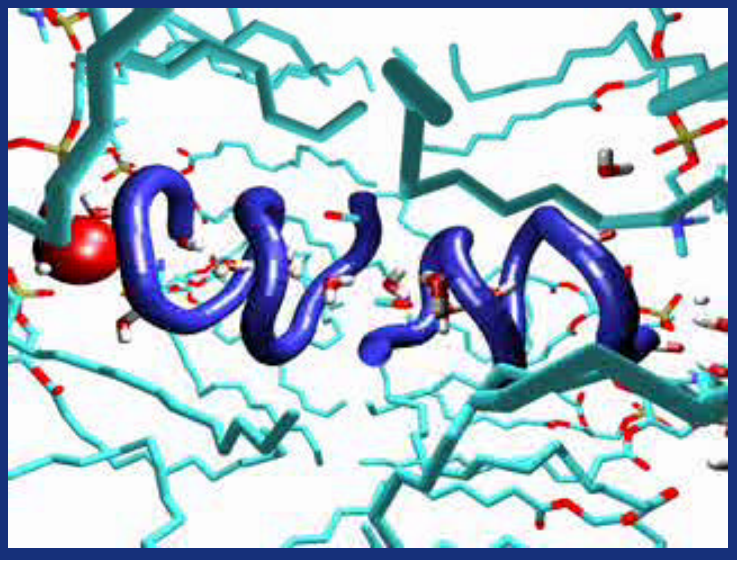


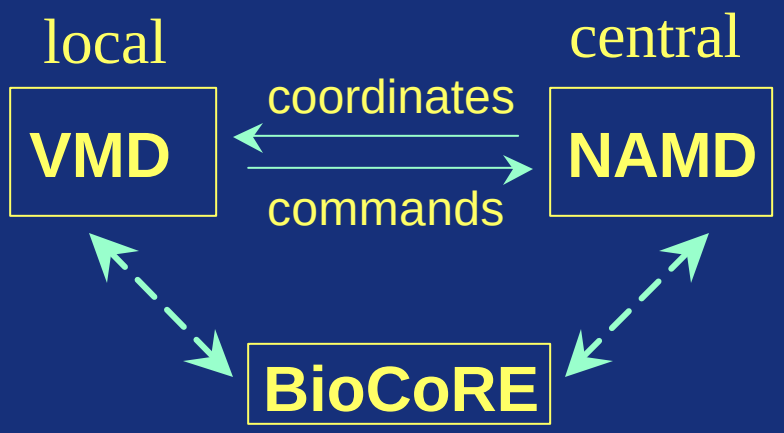




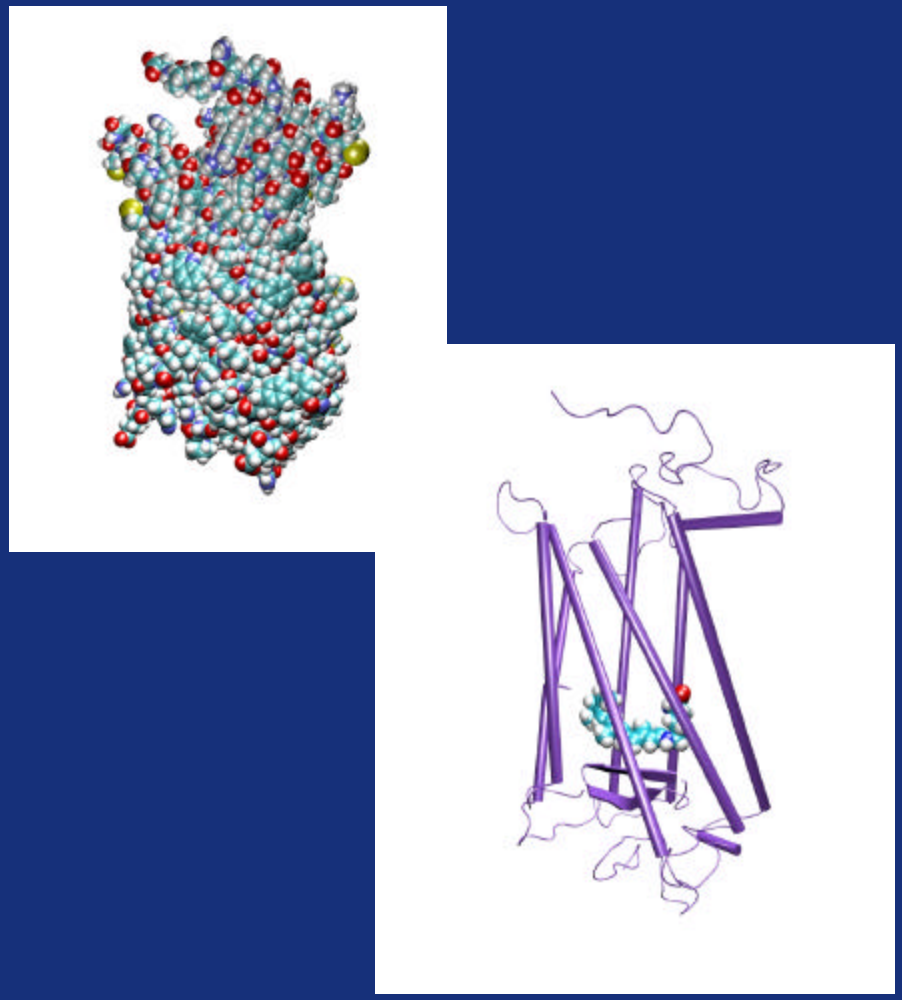
Deliverables from Collaboratory Projects

- **Teleoperation:** interactive MD, a ground breaking new technology of user manipulation of extremely realistic models

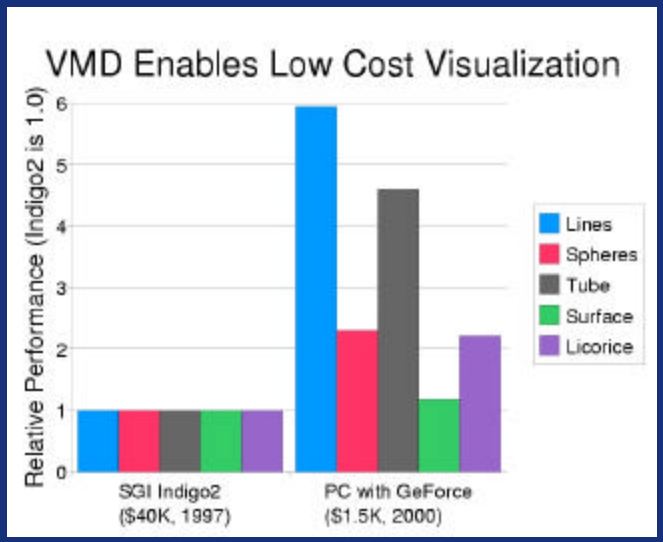




VMD enables low cost visualization



Multiple sessions at distant sites and **Python scripting language** supported in next release (1.6,Jan. 01)

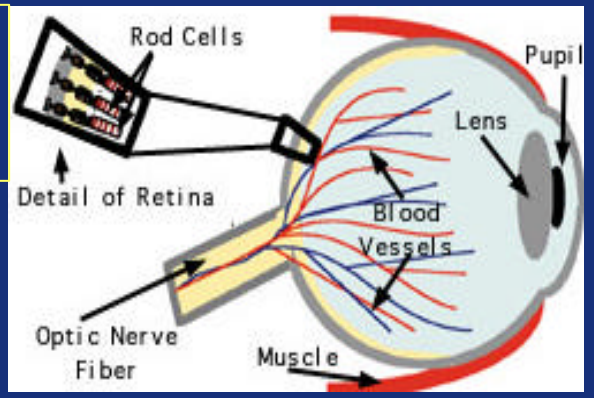


Humphrey et. al., J. Molec. Graphics, **14**:33-38, 1996

Exploring the Process of Vision with BioCoRE

K. Schulten (UIUC, IL)

Modeling and Molecular Dynamics



S. Suhai (Heidelberg, Germany)

Quantum Chemistry

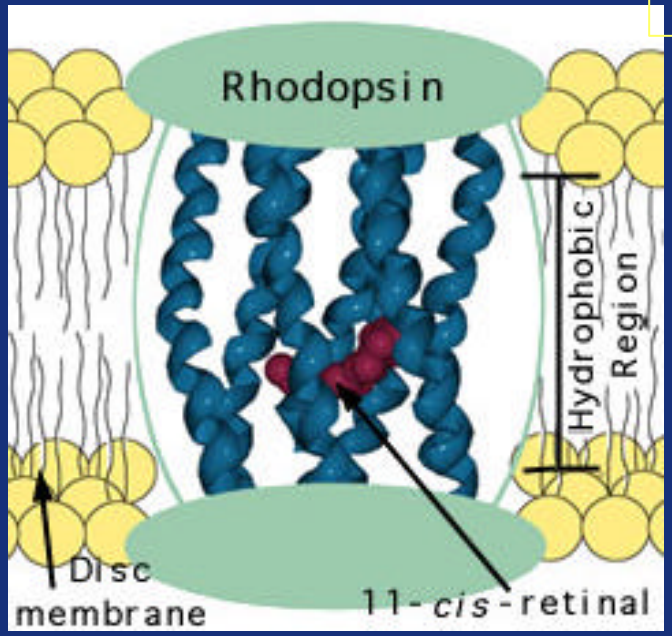
M. Olivucci (Siena, Italy)

Modeling of Excited State

BioCoRE

H. Kandori (Kyoto, Japan)

Hydration and Spectroscopy



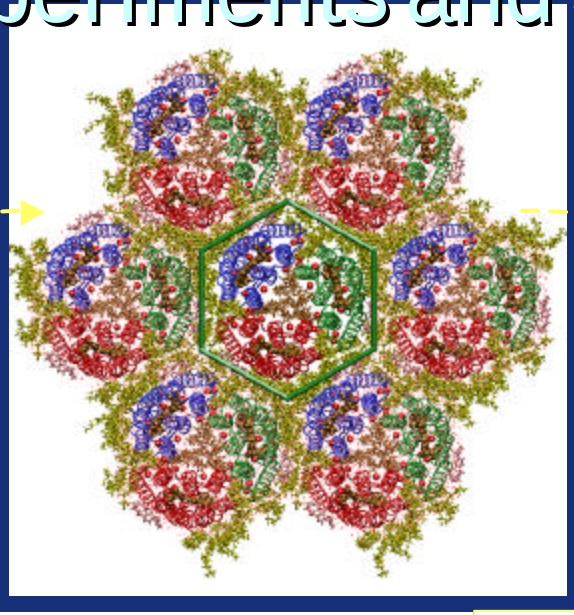
M. Sheves (Rehovot, Israel)

Spectroscopy and Chemistry

H. Weinstein (Mount Sinai, NY)

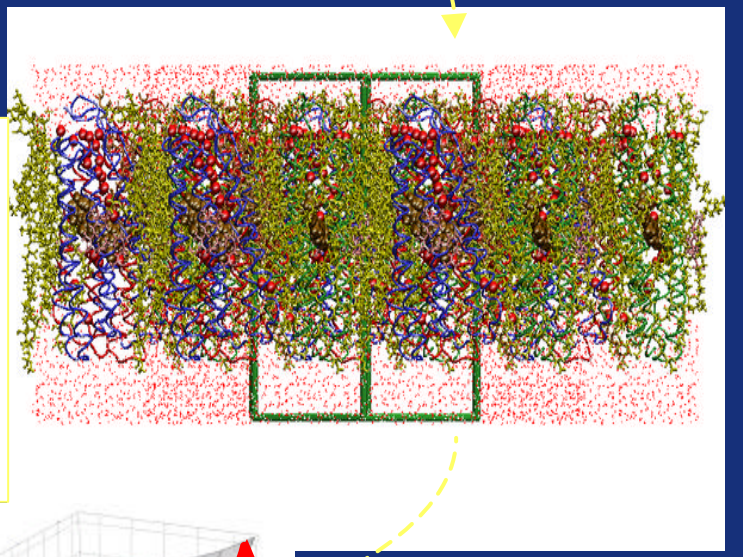
Biology and Modeling

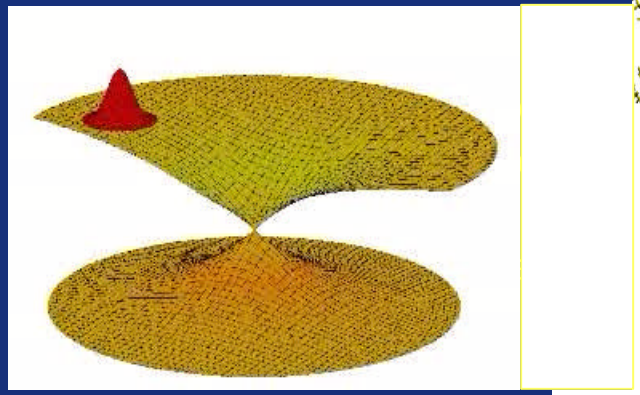
Combining Experiments and Simulation

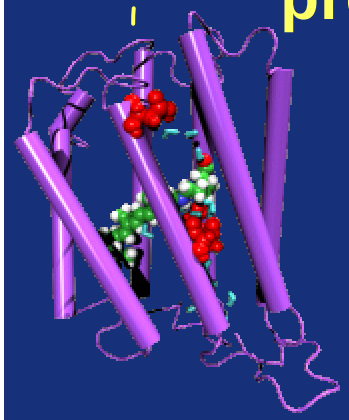


assembly

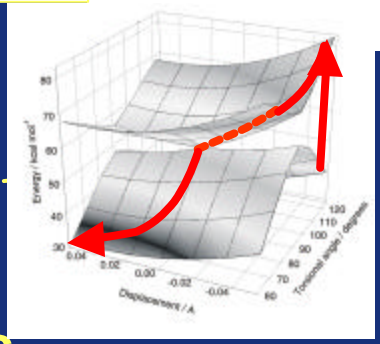
function

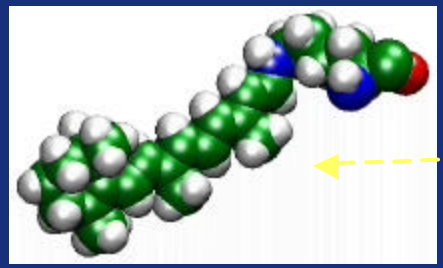






protein





molecular electronics

Shortcomings in Scientific Productivity of Collaboration due to Geographic Separation

- Limited Access to Computational Resources
  - Main machines available at few US sites
  - Limited expertise, e.g., in Unix file systems
  - Sharing of job monitoring impossible
  - Desired: easy, web-based joint access to runs and resources
- In-depth discussions of structures and dynamics rarely possible
  - Participating researchers met and discussed never as a group
  - Work requires joint viewing of structures to interpret data
  - Desired: joint graphics sessions, regular (daily) meetings
- Joint Depository of publications, technical documents, data lacking
  - Desired: shared data for multiple formats
- Proposal and report writing cumbersome
  - Desired: joint document preparation system

Timeline, for BioCoRE into research environment

- Initial use for training (2000)
  - As a communication tool, BioCoRE is very suitable for traning
    - BioCoRE-based MD Course at EMBL, Japan Grad. University, UIUC
- Use for joint projects at UIUC site (2000/ 2001)
  - Reporting
  - Initiating projects
  - Graphics sessions shared between distant local sites
- Linking Weinstein and Schulten laboratories (2001)
  - Grad student from NYC initiated work in Urbana, and continues contacts through BioCoRE; use of Workbench for submission, etc
  - Implementing joint graphics sessions, and then other capabilities
- Linking Olivucci, Kandori, Schulten labs (2001)
- Linking nanobiology collaborators in Seattle (2000-2001)

Scientists‘ Interactions with the Tool Development and Support Teams

- UIUC users and developers share lab space with daily contacts
  - Ideal situation, common mission, frank and frequent discussions
- BioCoRE use and development discussed at weekly group meeting
  - Initially very tough debates; scepticism on the side of users
- First break through
  - BioCoRE recognized as enabling technology for distant learning
    - PI and users had to develop MD course taught in Germany and Japan
- Users began to adopt BioCoRE and suggest features
  - User suggestion mainly easy to implement, but extremely valuable
    - Affects priorities (joint graphics sessions)
    - Adapts features (e.g., file access privileges, add AND delete features)
    - Suggest new uses (training; use in small groups)

Biomedical Researchers' Interactions with the Evaluators

- Evaluator tested prototypes with users
- Evaluator’s questionnaire reinforced that BioCoRE is considered by many users a good teaching tool
- Evaluator provides feedback on
  - design,
  - user concerns,
  - preferences,
  - priorities

Positive Effects Already Experienced

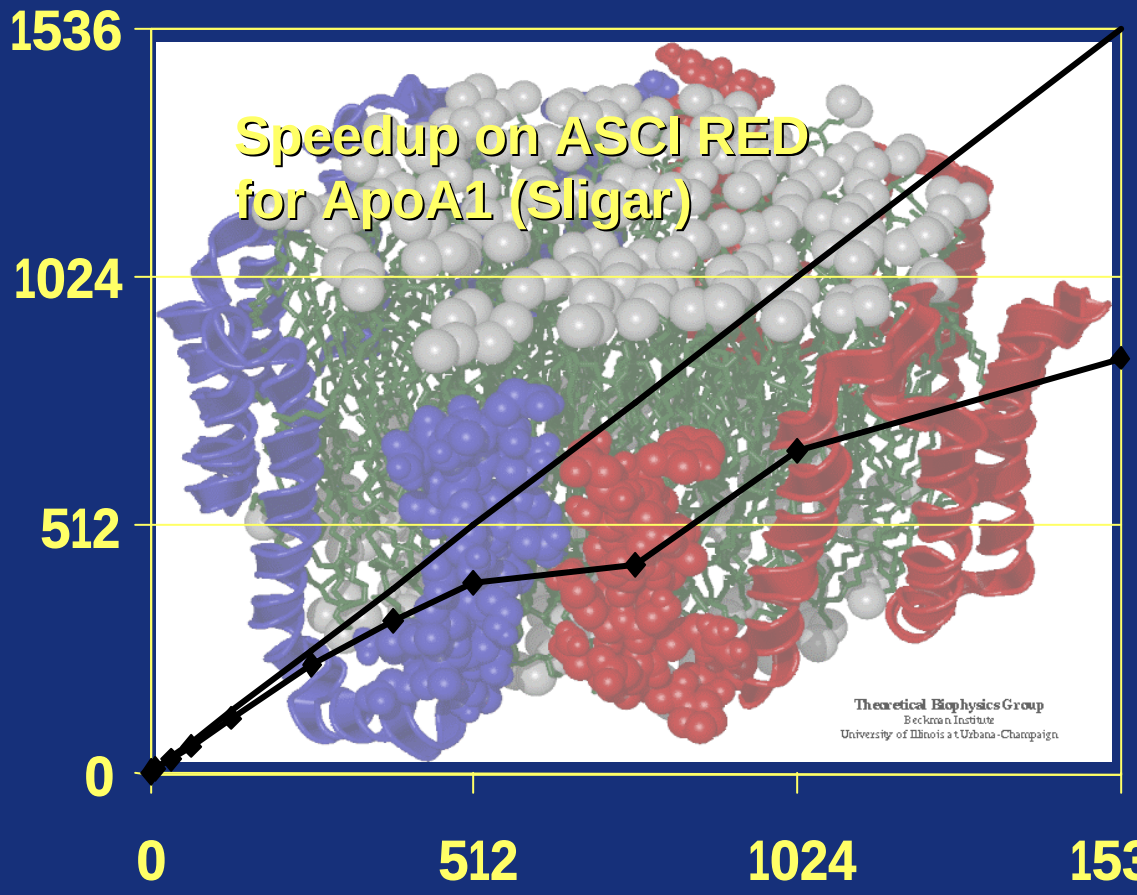
- Use central resources and staff
  - Web-based program submission eliminates need for implementing programs at local sites (save resources, staff time; reduces error)
- Joint graphics sessions of extreme value
  - Improves dramatically the research process
  - Eliminates need to travel, more so for large teams
- Keeping up with research progress in a team
  - Having access to up-to-the-minute entries of collaborators
  - Having access to al past entries with an opportunity to address past problems or check on
  - All team members are informed on progress
  - Real time chat using the Control Panel
  - Great joint lab notebook and project management tool
  - Direct communication, faster than e-mail due to alerts
- Greatly improved depository of heterogeneous information
- Good security
- Good portability through use for web browsers

User Concerns (mainly temporary)

- Need to provide central portal (other sites available soon);
- Another software to learn;
- Project management too hierarchical (solution exists!);
- Missing functions make it presently hard to integrate into one's work;
- Archiving taken too far; elimination (filing away) of material necessary; also user should have personal scratch space.

End

NAMD: Scalable Molecular Dynamics



For SP3, Origin, T3E, clusters…
PSC teraflop, IBM Blue Gene.

Scalable to 1000's of CPUs.

Data file compatible with CHARMM and X-PLOR.

Fast full electrostatics and constant pressure ensembles.

Flexible Tcl scripting language.

Ready for
10^6 atoms
and beyond…

Design of NAMD: Kalé *et al.,* J. Comp. Phys., **151**, 283 (1999)

Freely available with C++ source code from http://www.ks.uiuc.edu/Research/namd/

VMD: Molecular Visualization (1.5, release Jan. 00)

Interactive Molecular Dynamics

Flexible Tcl scripting language

Stereoscopic 3D display

Runs on Windows and Unix

No limits on size of molecules

Animates dynamics trajectories

Exports scenes to ray tracers for publication quality rendering.

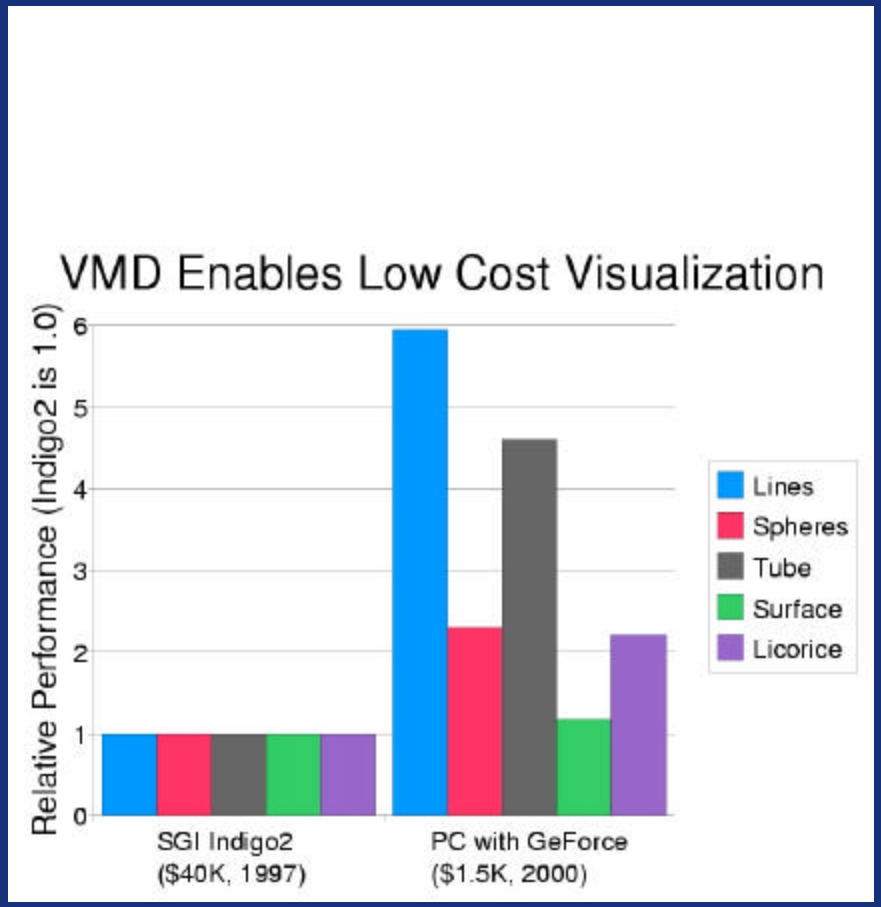
Multiple sessions at distant sites and **Python scripting language** supported in next release (1.6,Jan. 01)

Humphrey et. al., J. Molec. Graphics, **14**:33-38, 1996

Freely available, with source code from http://www.ks.uiuc.edu/Research/vmd/

VMD enables low cost visualization

VMD now runs on PCs with low cost OpenGL “game boards”, video boards that are designed for use with games like Quake. Game boards cost less than $300, but can provide good 3D rendering performance with VMD. (example “NVidia GeForce 256 board”)



Through its sophisticated rendering algorithms VMD is able to achieve molecular visualization performance several times better than what was possible with a high-end SGI Indigo2 Maximum-Impact, costing $40,000 just 3 years ago, using a cheap $300 GeForce 256 graphics board in a commodity PC today.

VMD
Visual Molecular Dynamics