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 Collaboratory 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

Local: VMD
Central: NAMD
BioCoRE

coordinates
commands
VMD enables low cost visualization


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

protein

assembly

function

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 training
    - 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)**

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 all 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

Speedup on ASCI RED for ApoA1 (Sligar)

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…


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

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.