VMD: Biomolecular Visualization and Analysis

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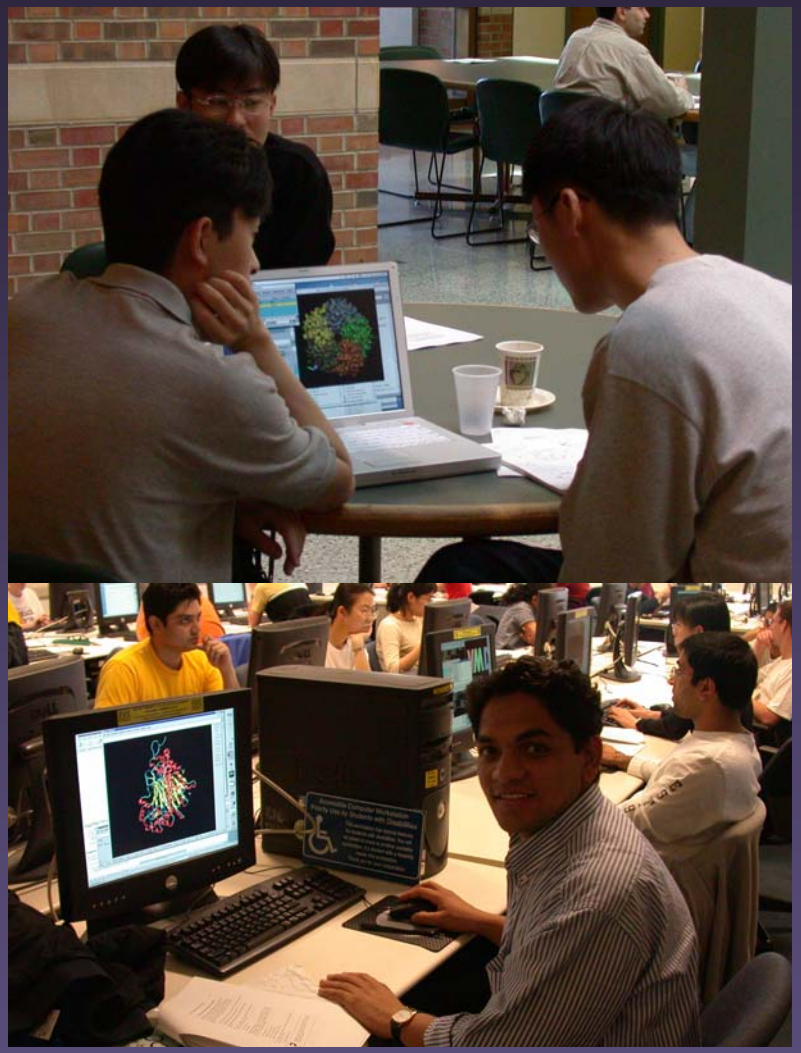
VMD Highlights

- Available on all major platforms.
- Displays large biomolecules and simulation trajectories
- Scene export, ray tracing, solid 3D model printing
- Sequence browsing and structure highlighting
- User-extensible scripting for analysis and customization
- Interactive Molecular Dynamics
- FREE!!! (with source code)



Affordable Visualization with VMD

- Hardware accelerated 3-D graphics not required for simpler molecular representations
- Inexpensive, game-oriented hardware technologies
  - 3-D graphics accelerators
  - Stereo glasses
  - Joysticks and other devices
- Most PCs can be upgraded with 3-D acceleration, stereo glasses, and input devices for about $275

Runs on unaccelerated laptops

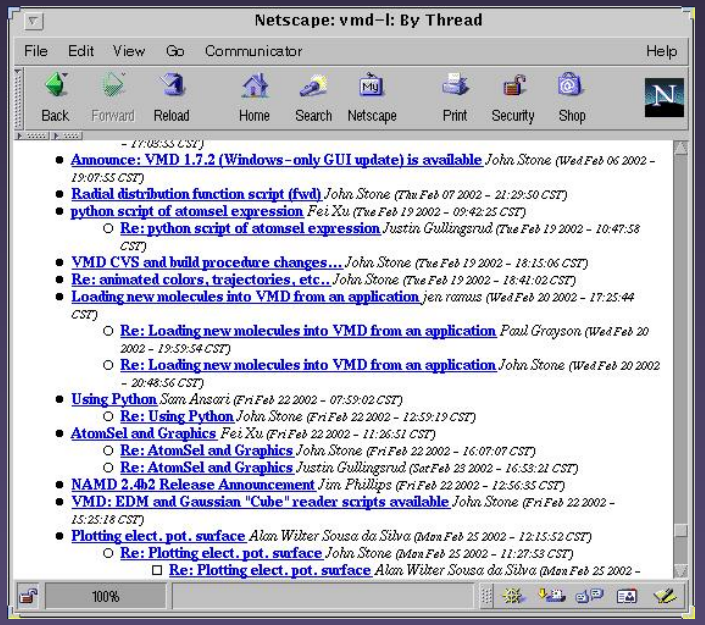
Midrange 3-D accelerator: $100

Stereo glasses $120

Joystick, or a used Spaceball: $50-$100

VMD User Community

- 32,475 registered users (5,857 NIH researchers)
- 7,397 users of multiple versions of VMD
- VMD-L user community mailing list
- E-mail support:
  - 7,000+ emails in 2002
- User-contributed scripts, plugins, tutorials

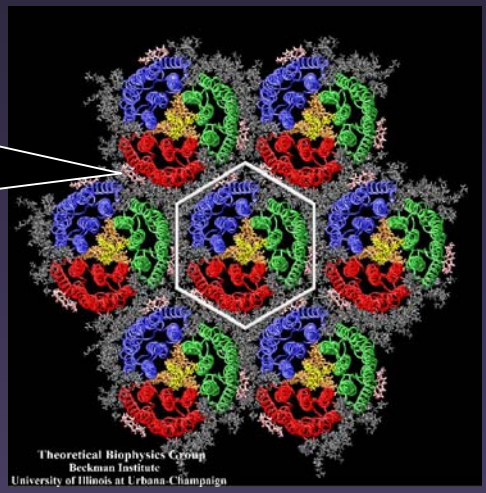


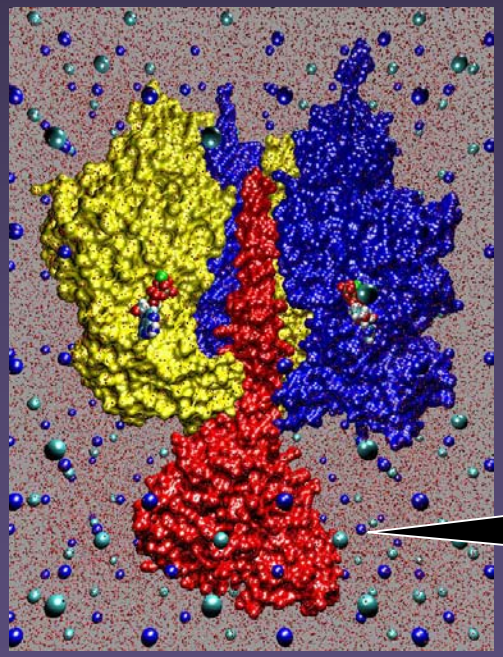
VMD-L mailing list

Large Scale Molecular Visualization

- Large structures: 300,000 atoms and up
- Complex representations
- Long trajectories: thousands of timesteps
- Volumetric data
- Multi-gigabyte data sets break 32-bit barriers
- GlpF: each 5 ns simulation of 100K atoms produces a 12GB trajectory

Purple Membrane 150,000 Atoms

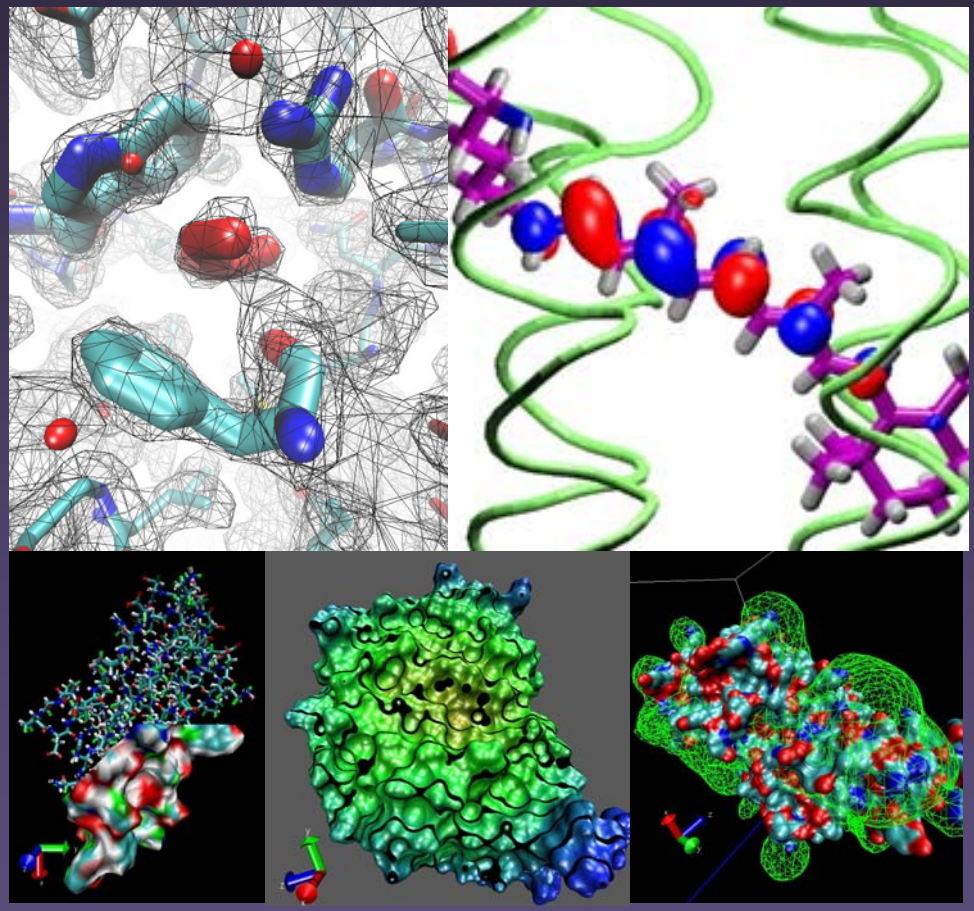




F1 ATPase 327,000 Atoms

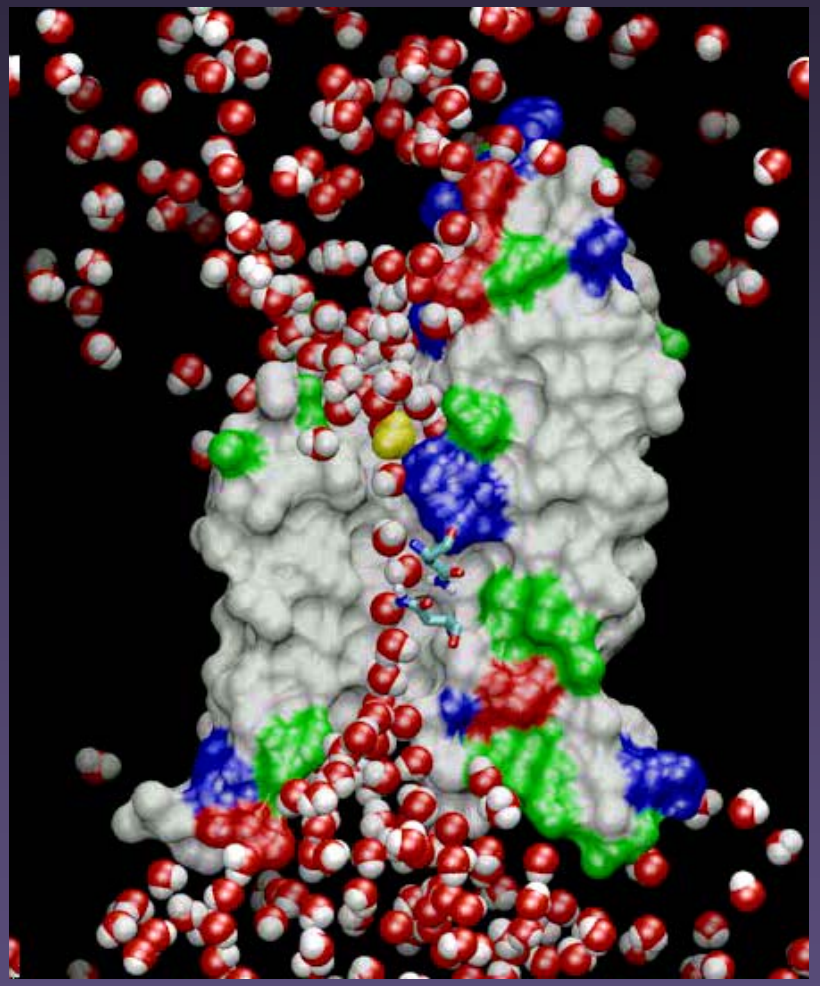
Volumetric Visualization

- Data types:
  - Electron density maps
  - Potential surfaces
  - Electron orbitals
  - User-provided volumetric data
- Rendering features:
  - Isosurface
  - Volume slice
  - Clipping planes
  - 3-D texturing
  - Contour lines



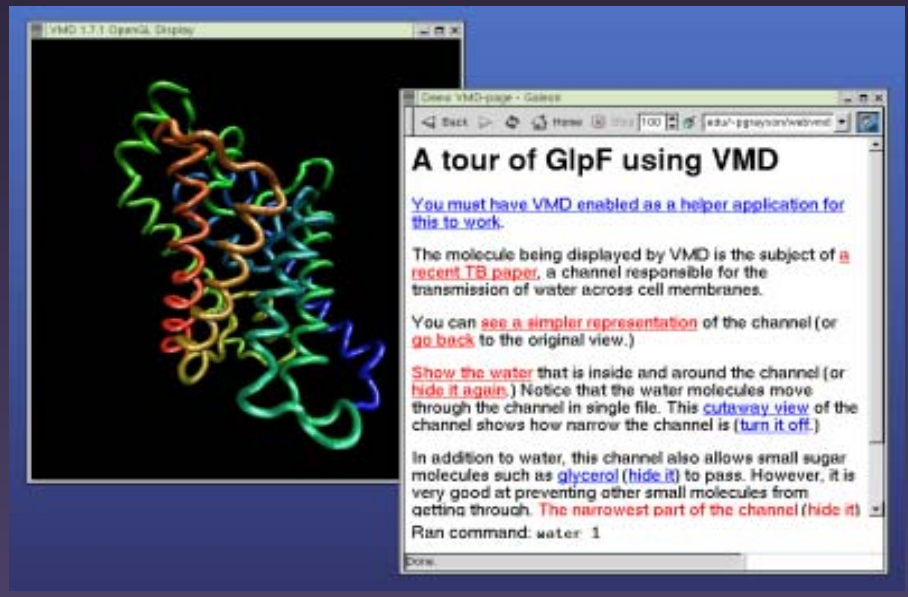
Easy-to-use Movie Making

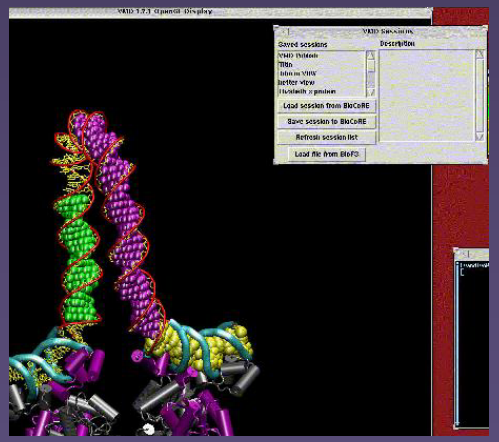
- "Vmdmovie" plugin builds movies in a few minutes
- Uses readily available compression tools
- Several movie types:
  - Rotation
  - Rocking
  - Trajectory animation
  - Trajectory rock
  - Development continues…



Web and Collaboration Features

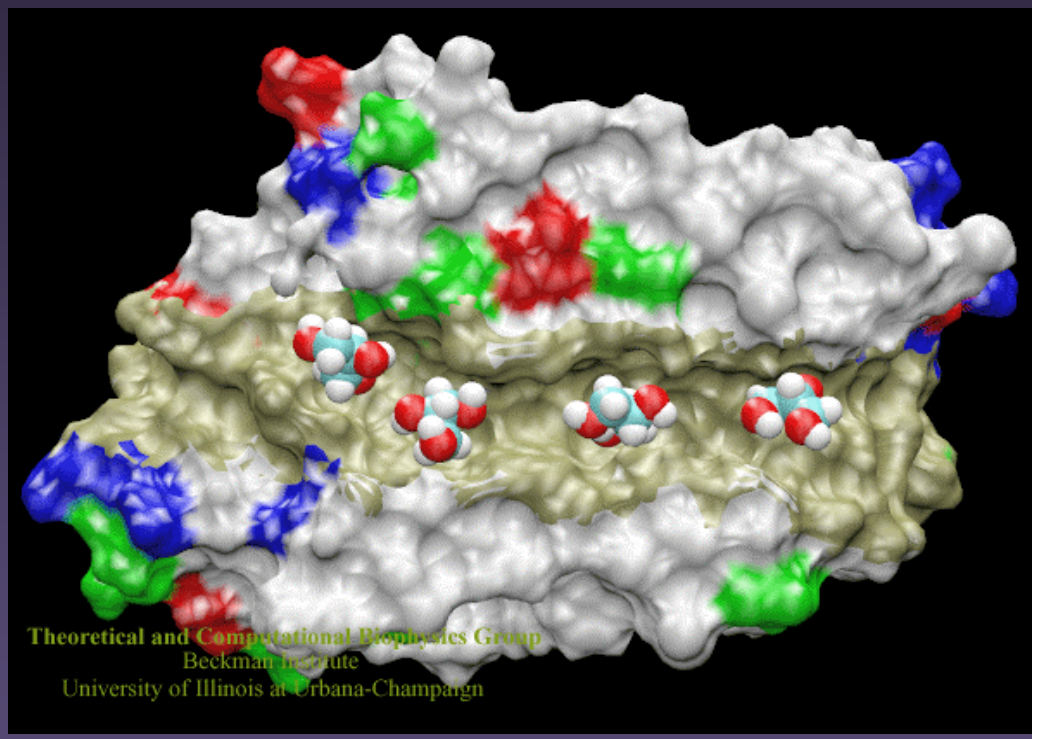
- Web-based VMD scripting
  - Clickable links execute script commands
- BioCoRE
  - Publish VMD sessions to collaboratory
  - Load structures from BioFS





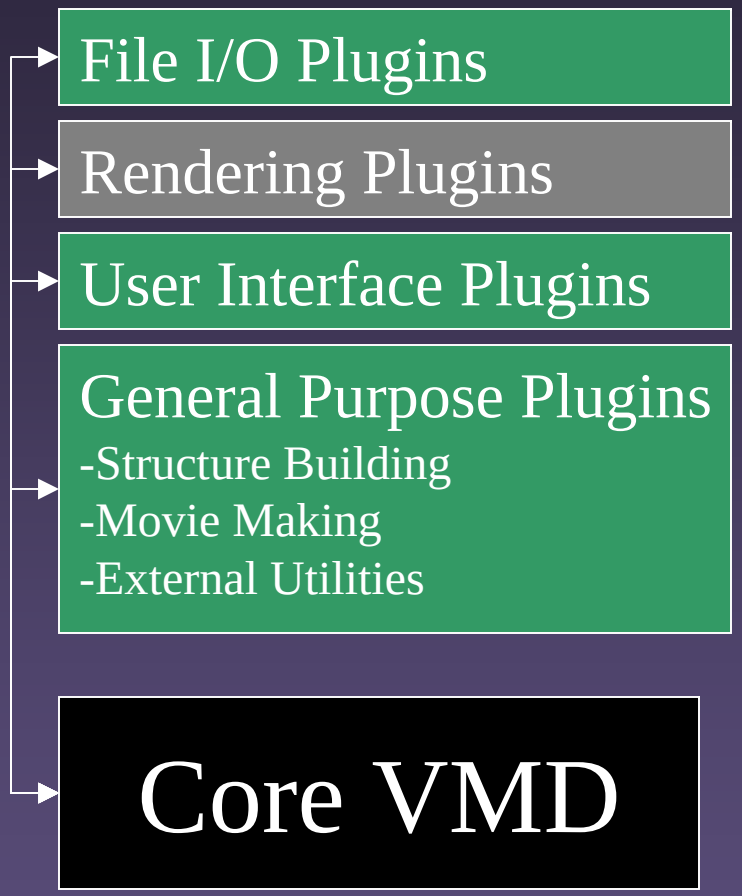
Scripting and Analysis

- Built-in Tcl and Python scripting interfaces
- Interactive command shell
- New commands and routines can be added by users
- Analysis scripts can also be run non-interactively by starting VMD in text-only mode (vmd –dispdev text)



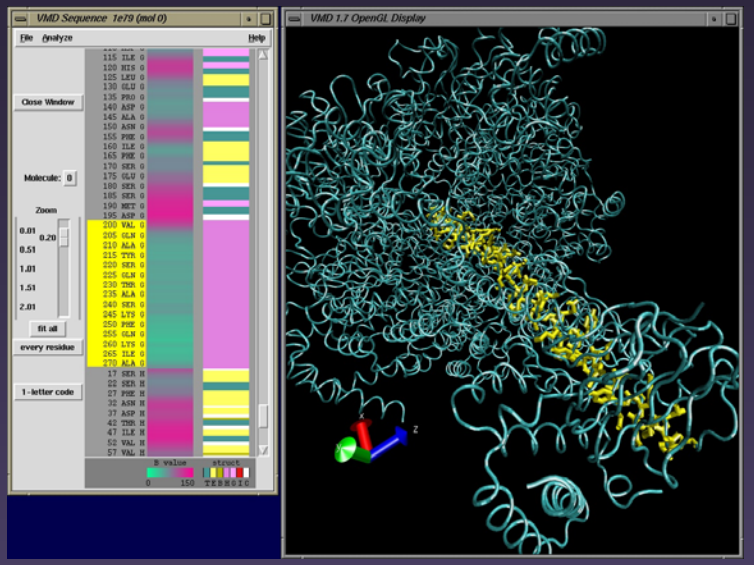
VMD "Plugin" Extensions

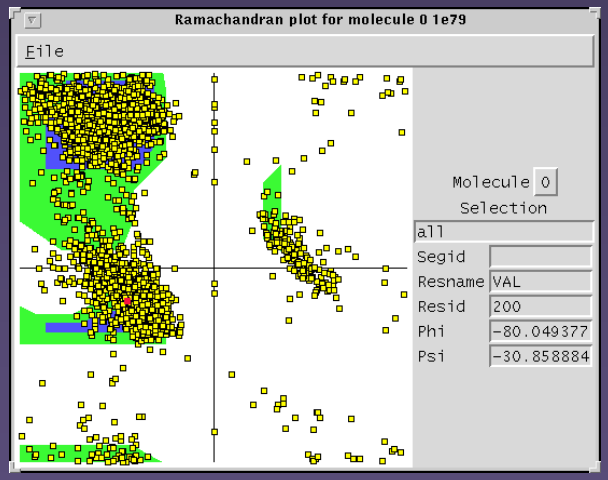
- Similar to web browser plugins
- Written in C, C++, Python, Tcl
- Can extend VMD command language
- Potential for higher performance than pure scripts
- Easier to create and distribute 3rd party VMD extension modules



User Interface Plugins

- AutoIMD
- Sequence Browser
- Ramachandran Plot
- RMS Alignment
- PDB Lookup
- VMD Movie Maker
- More in-progress…
  - Delphi
  - Multiple Sequence Alignment





General Purpose Plugins

- Psfgen: structure building plugin
  - Adds new commands to VMD scripting language
- Plugins can make use of other plugins:
  - Solvate (builds on Psfgen)
  - Membrane (builds on Psfgen)
  - Autoionize (builds on Solvate and Psfgen)

Interactive Molecular Dynamics

National Center for Research Resources

NIH Resource for Macromolecular Modeling and Bioinformatics
http://www.ks.uiuc.edu/

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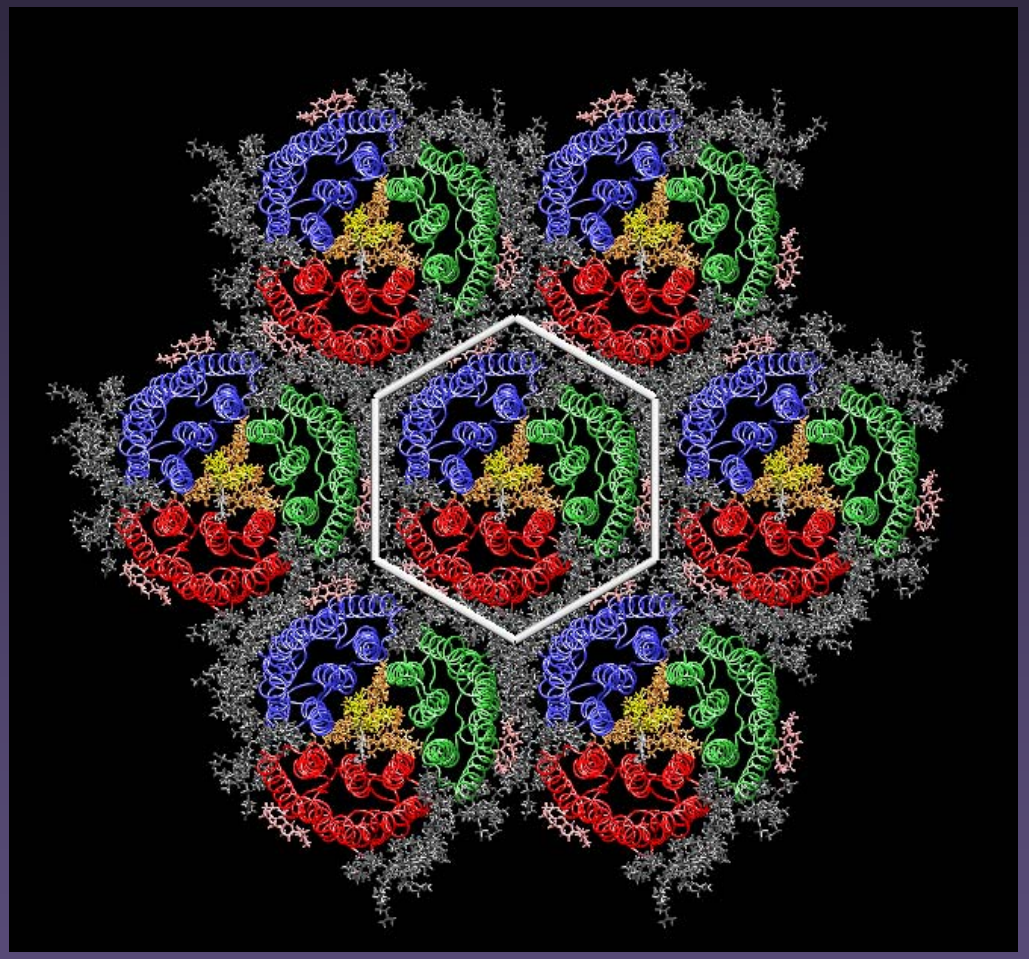
Biomolecular Simulation

- All-atom models of protein, DNA, water.
- 10K-300K interacting particles.
- Time scales of 10-100 ns are accessible, still much shorter than experiment.

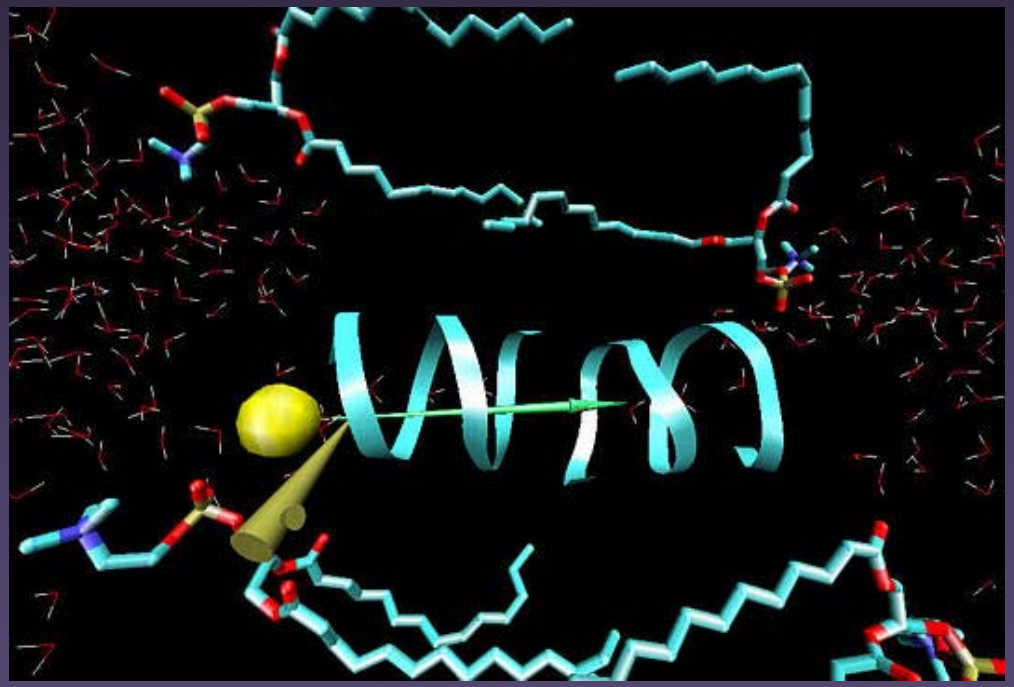


Steered Molecular Dynamics

- Moving restraints pull selected atoms along specified paths.
- Slow processes can be accelerated.
- New flexibility leads to new challenges: how can proteins be manipulated?

A Haptic Interface

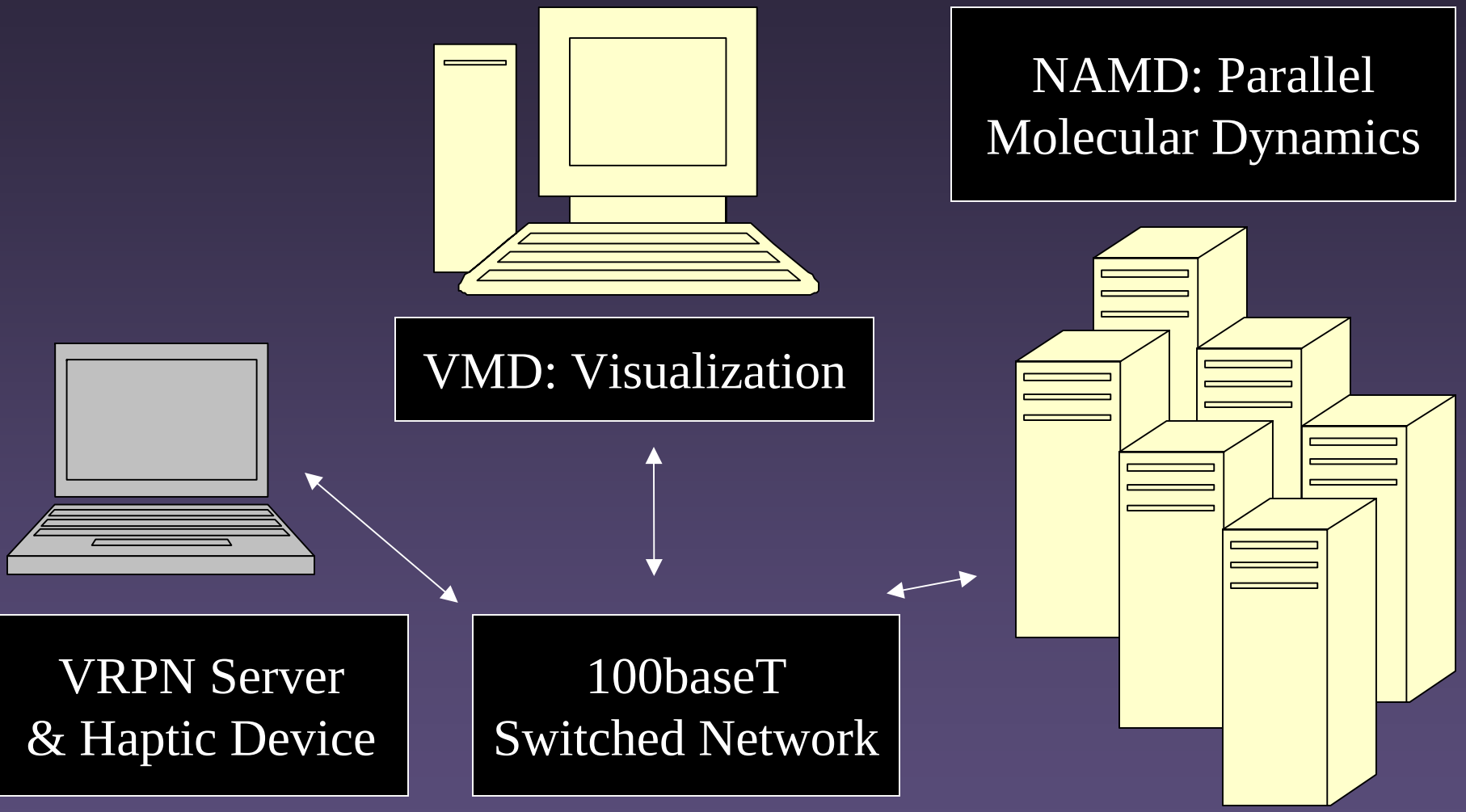
- Haptic devices allow multidimensional manipulation and force feedback.
- Pathways for steered molecular dynamics simulations can be identified interactively.



Interactive Molecular Dynamics

- Replaces pre-determined constraint point and spring with interactive user input and run-time configurable spring parameters;
- Provides user with real-time force feedback through the use of a haptic device;
- Allows user to direct simulation and gain insight by interactive exploration of structure and mechanical properties of molecular system.

IMD Architecture



IMD Simulation Hardware

National Center for Research Resources

NIH Resource for Macromolecular Modeling and Bioinformatics
http://www.ks.uiuc.edu/

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IMD Visualization Hardware

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IMD Force Feedback Model: Parameters

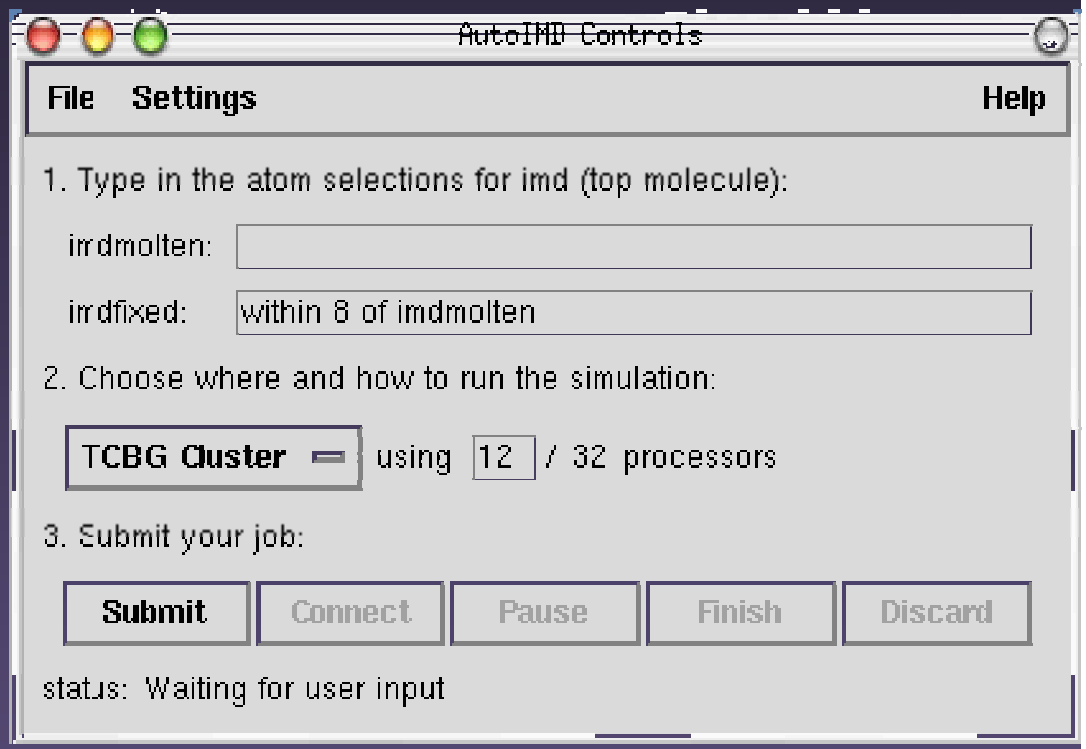
- The response of the IMD system to user input is determined by three parameters:
  - Ratio of wall clock time to simulation time
  - Ratio of user-applied force to simulation force
  - Ratio of atom coordinates to haptic coordinates

IMD Force Feedback Model: Results

- The sensitivity of the haptic interface to atomic interactions goes as the *square* of the speed of the simulation.
- Responsiveness can be improved by increasing the simulation force, but at the cost of sensitivity.
- Stiff restraints give better precision, but result in a noisier haptic interface.

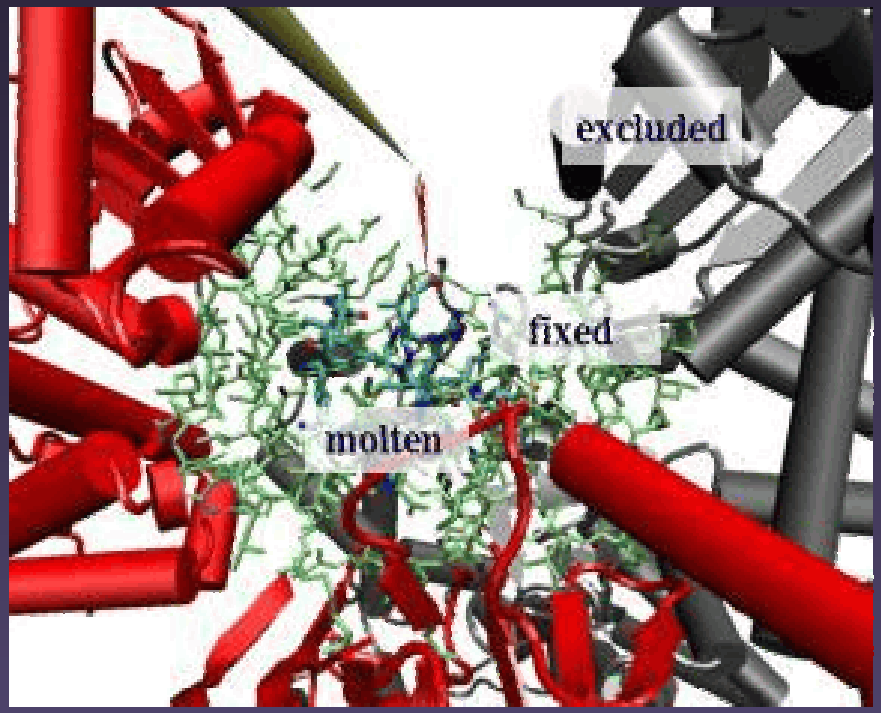
AutoIMD: Easy Simulations

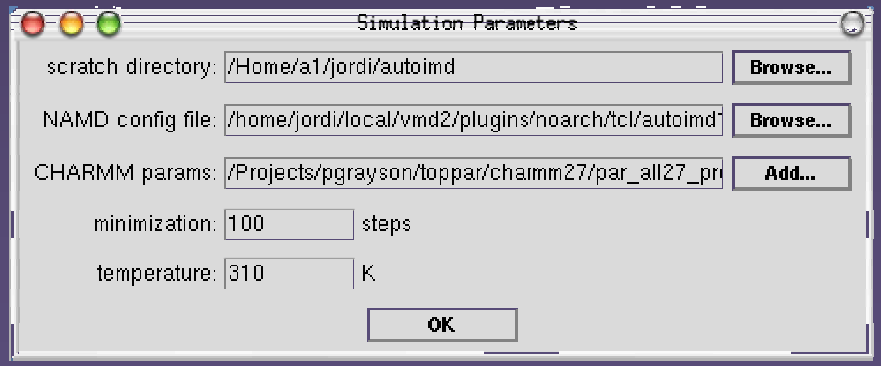
- Simple interface for running IMD simulations
- Run simulations on desktops, laptops, or clusters
- Customizable for local facilities



AutoIMD Uses

- Atom selections choose parts of structure which are simulated
- Works with haptic interface or even with just a mouse
- Aids setup of larger simulations





Thanks!

- Please feel free to ask questions now!
- What would you like to see us implement in future versions of VMD

Molecular Graphics at Siggraph

- Truth before beauty special session
- Electronic theatre: DNA visualization
- Autostereoscopic displays (DTI, VRex)