

VMD: Visual Molecular Dynamics

Computational Microscope / Tool to Think

amino acid tyrosine

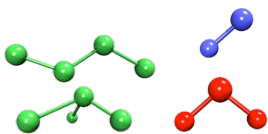
enzymatic control
BPTI
VMD tutorial

trafficking
Ubiquitin
case study

<http://www.ks.uiuc.edu/Training/CaseStudies/>
<http://www.ks.uiuc.edu/Training/Tutorials/>

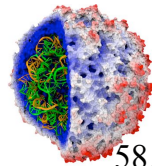
Our Microscope is Made of...

Chemistry



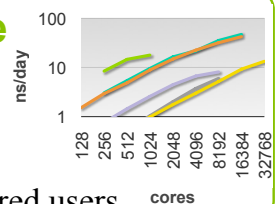
$$U(\vec{R}) = \underbrace{\sum_{\text{bonds}} k_i^{\text{bond}} (r_i - r_0)^2}_{U_{\text{bond}}} + \underbrace{\sum_{\text{angles}} k_i^{\text{angle}} (\theta_i - \theta_0)^2}_{U_{\text{angle}}} + \underbrace{\sum_{\text{dihedrals}} k_i^{\text{dih}} [1 + \cos(n_i \phi_i + \delta_i)]}_{U_{\text{dihedral}}} + \underbrace{\sum_i \sum_{j \neq i} 4 \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]}_{U_{\text{nonbond}}} + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}$$

NAMD Software



Virus

58,000 registered users



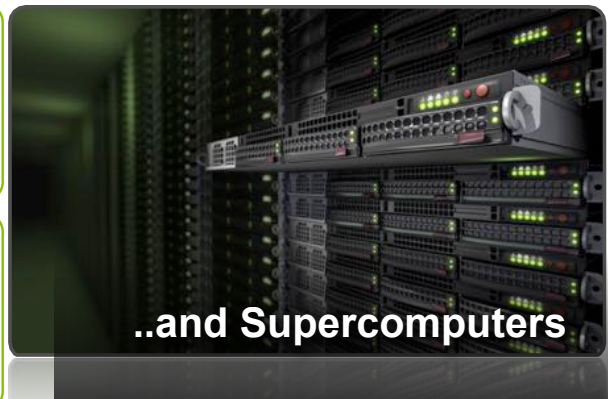
Physics

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i = -\vec{\nabla} U(\vec{R})$$

Math

$$\vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \frac{\Delta t^2}{m_i} \vec{F}_i(t)$$

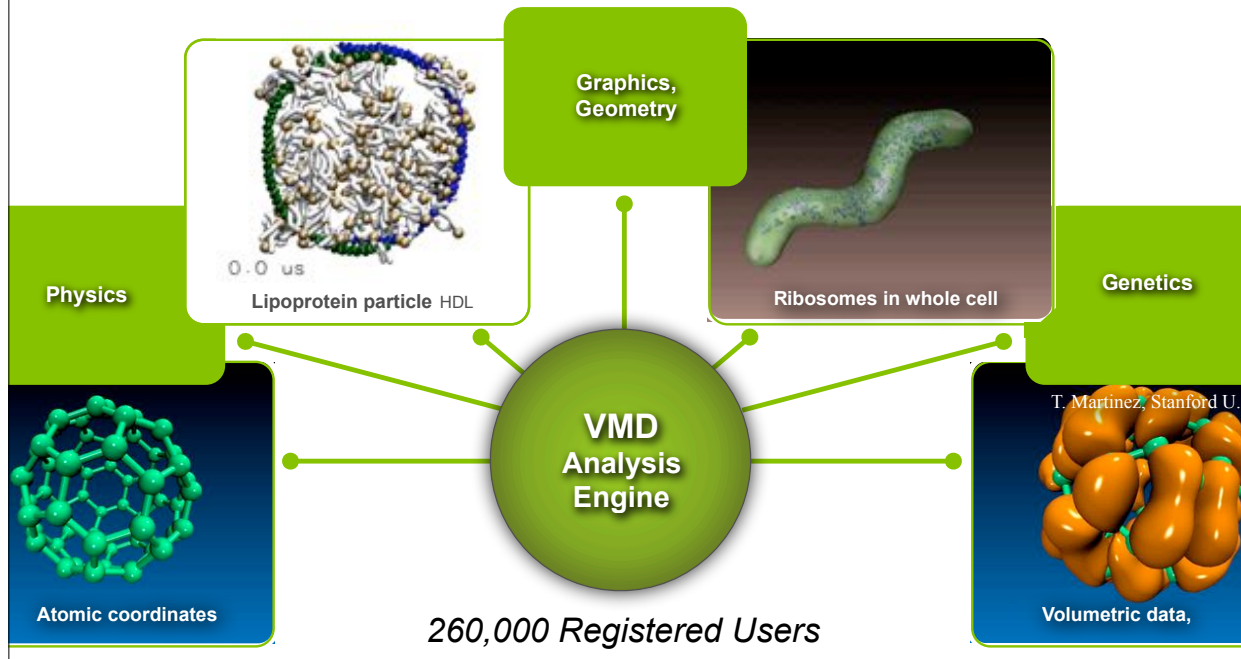
(repeat **one billion times** = microsecond)



..and Supercomputers

Our Microscope is Made of...

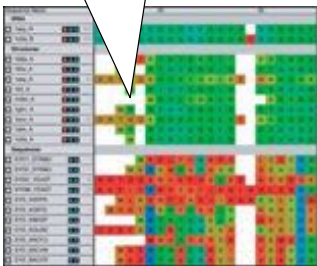
and of...



VMD – A Tool to Think

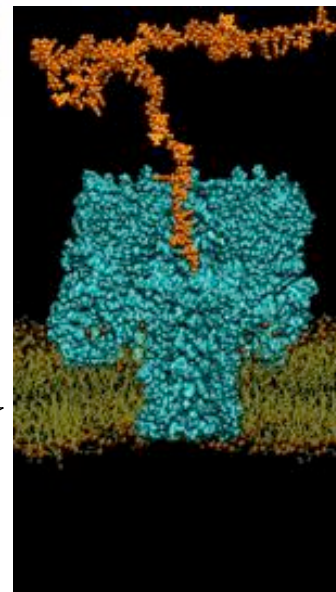
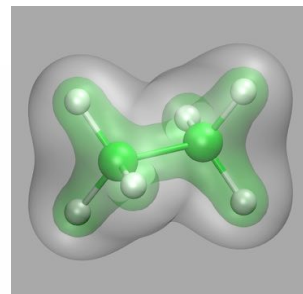
Volumetric Data:
Density maps,
Electron orbitals,
Electrostatic potential,
Time-averaged occupancy, ...

Sequence Data:
Multiple Alignments,
Phylogenetic Trees

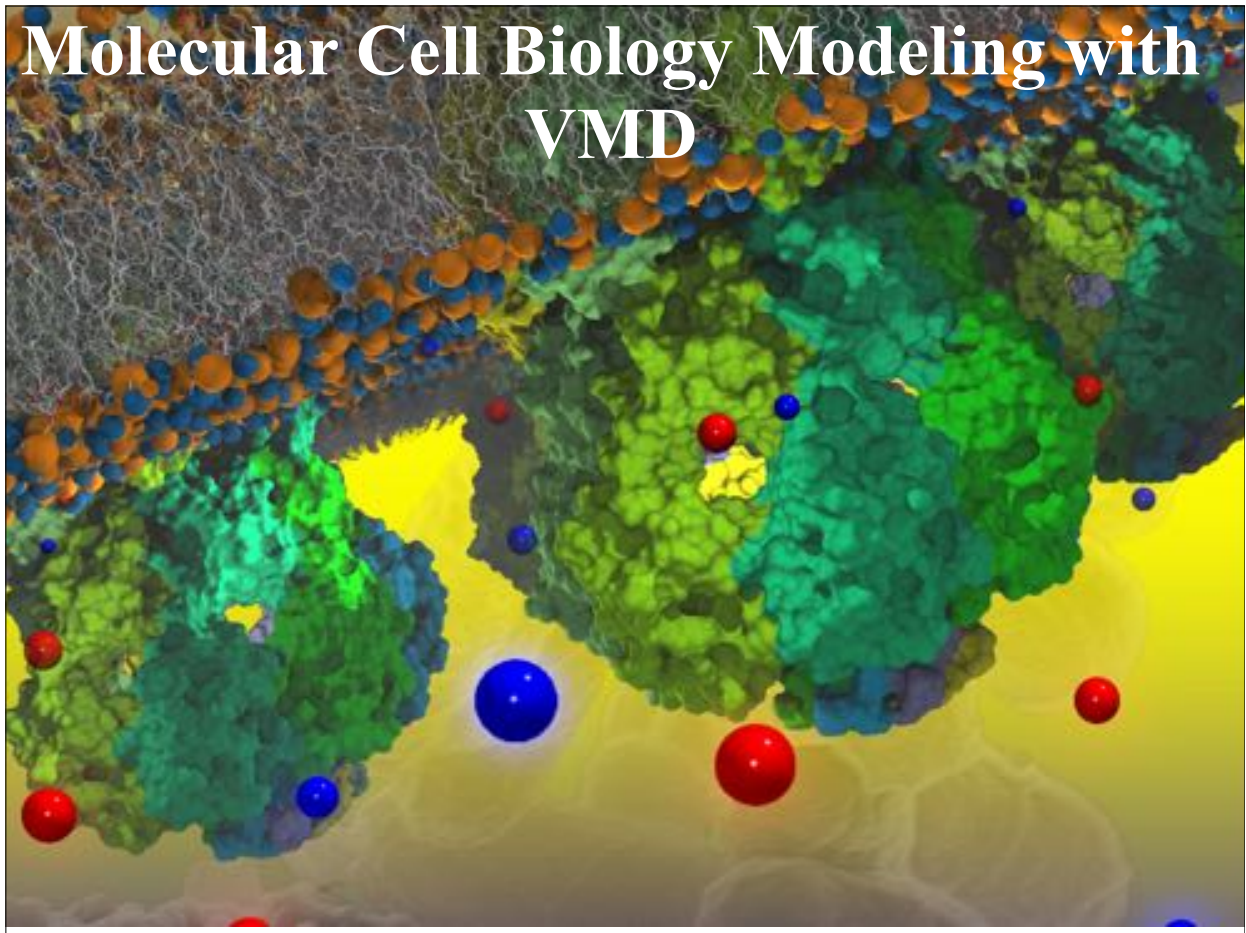


VMD

Atomic Data:
Coordinates,
Trajectories,
Energies,
Forces, ...



Molecular Cell Biology Modeling with VMD



Molecular Graphics with VMD

TkConsole

Main Menu

Output console

Representations Menu

Graphics Window

typical VMD session

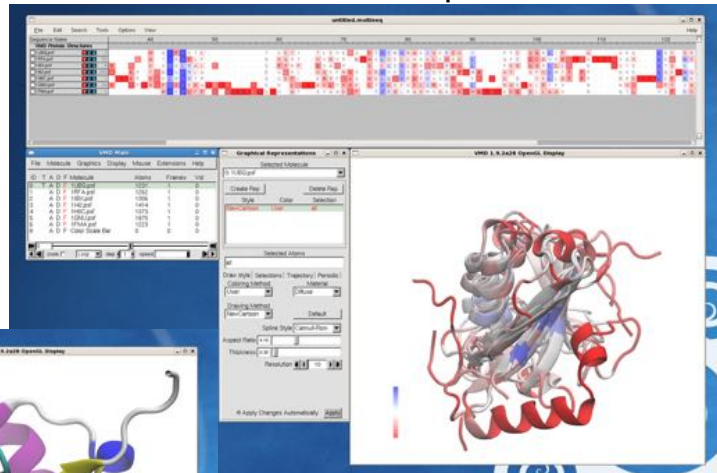
Bioinformatics

MultiSeq

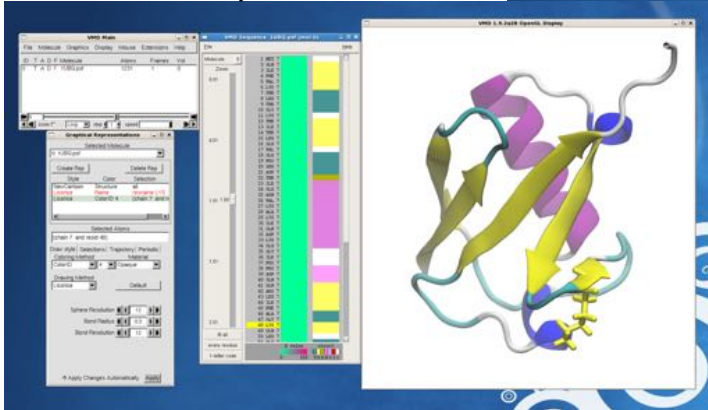
Link sequence to structure

Multiple sequence/
structure alignments

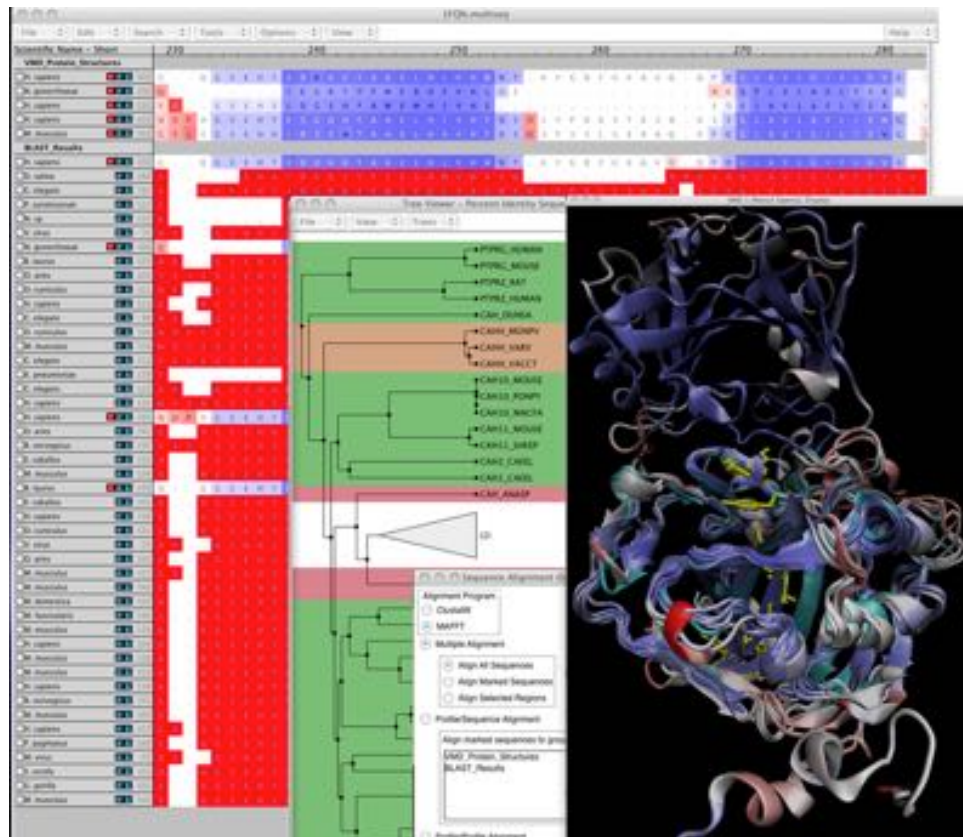
Phylogenetic trees



Sequence Viewer



Structure, Sequence and Phylogenetic Analysis with VMD

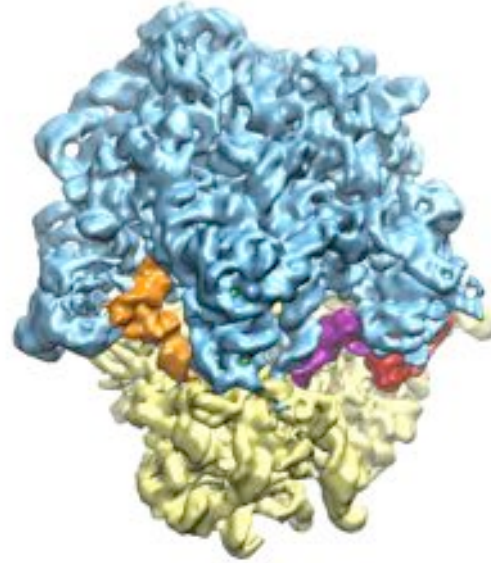


VMD Handles Volumetric Data

Cryo-EM map of the *E. coli* ribosome at 6.7-Å resolution

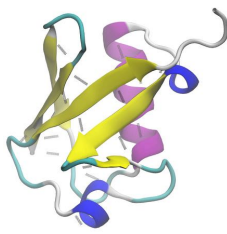


electron density
from QM/MM
calculation
Martinez, Stanford

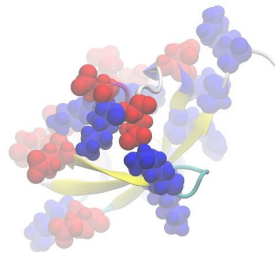


cryo-EM density

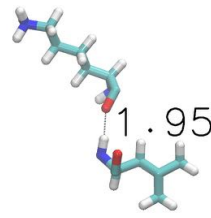
VMD Determines Physical Properties



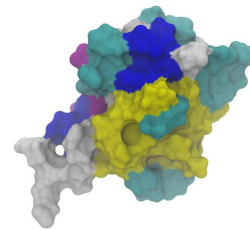
hydrogen bonds



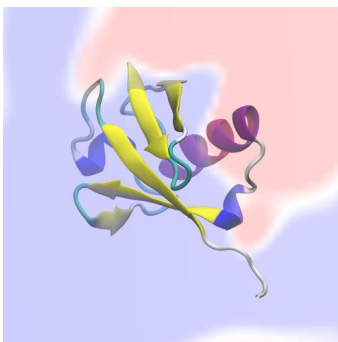
salt bridges



distances



SASA



electrostatics

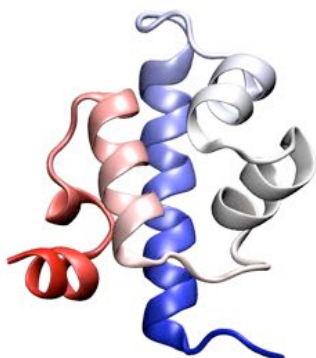
- SASA
- secondary structure
- interaction surfaces
- hydrogen bonds
- salt bridges
- electrostatics
- distances
- angles
- dihedrals
- RMSD
- RMSF
- interaction energies
- forces
- free energy profiles
- normal modes

Trajectory Graphics/Analysis with VMD

**VMD Plugin:
Timeline**

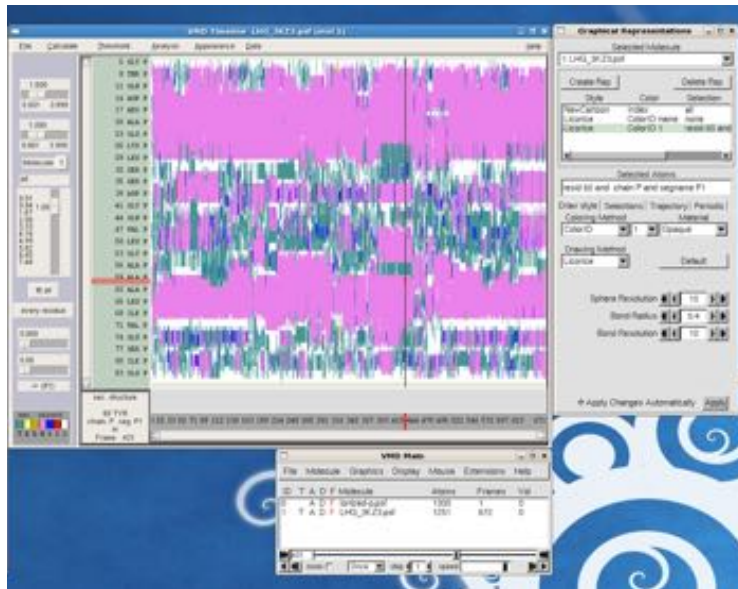
plugin to analyze MD trajectories for events
plot properties, e.g. RMSD, secondary
structure, hydrogen bonds, for each residue
across a trajectory

Example: protein folding



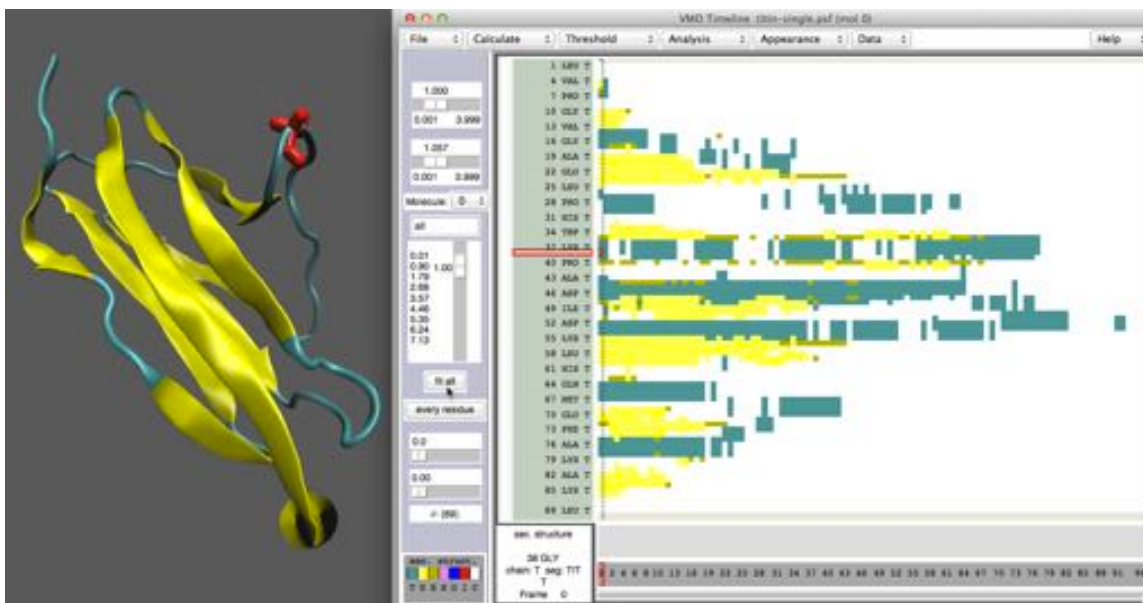
lambda repressor (2012)
80 amino acids, 100 μ s

Journal of Physical Chemistry Letters, 3:1117-1123,
2012. *Proceedings of the National Academy of
Sciences, USA*, In press, 2013.



VMD Session 2:
trajectory of villin head piece

Timeline: a graphing and analysis tool to identify events in an MD trajectory

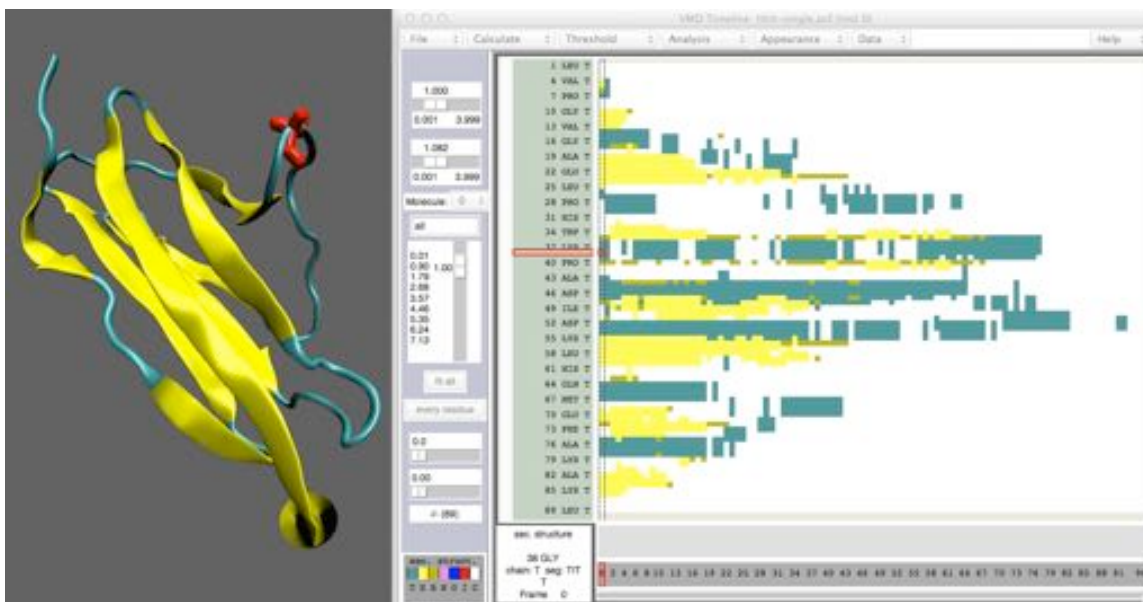


■ Beta turn ■ Extended beta ■ Isolated bridge □ None (coil)

1/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory

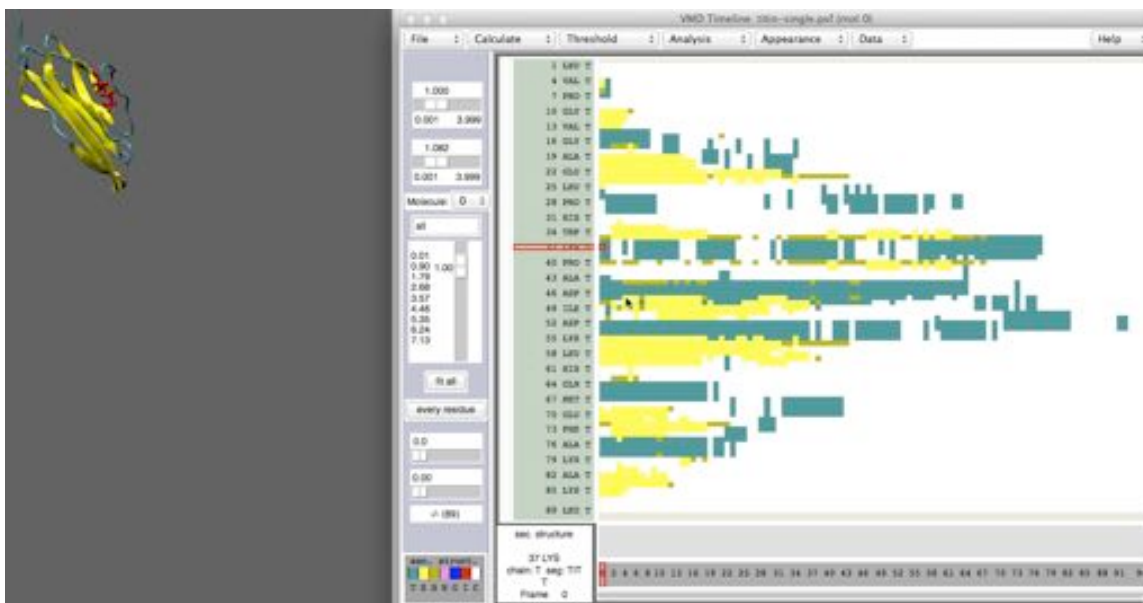


■ Beta turn ■ Extended beta ■ Isolated bridge □ None (coil)

2/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory

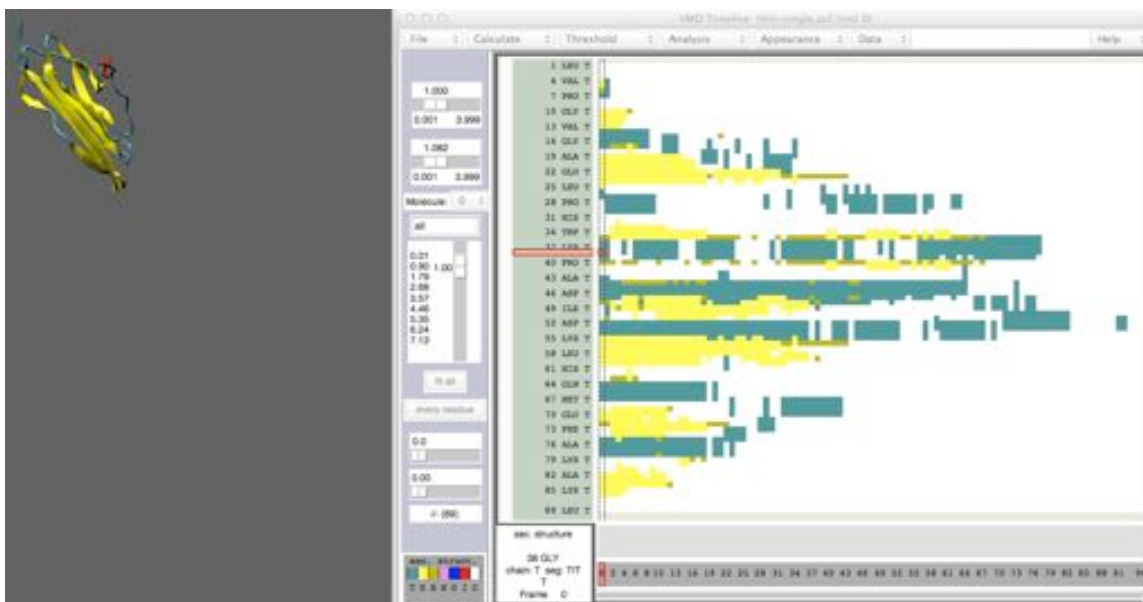


■ Beta turn ■ Extended beta ■ Isolated bridge □ None (coil)

3/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory

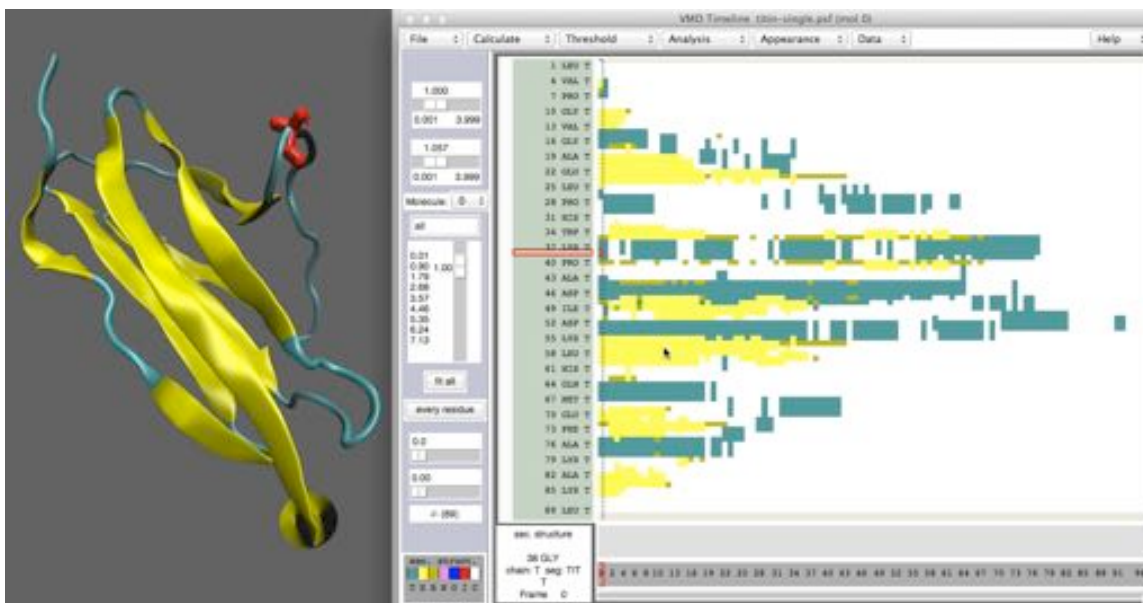


■ Beta turn ■ Extended beta ■ Isolated bridge □ None (coil)

4/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory

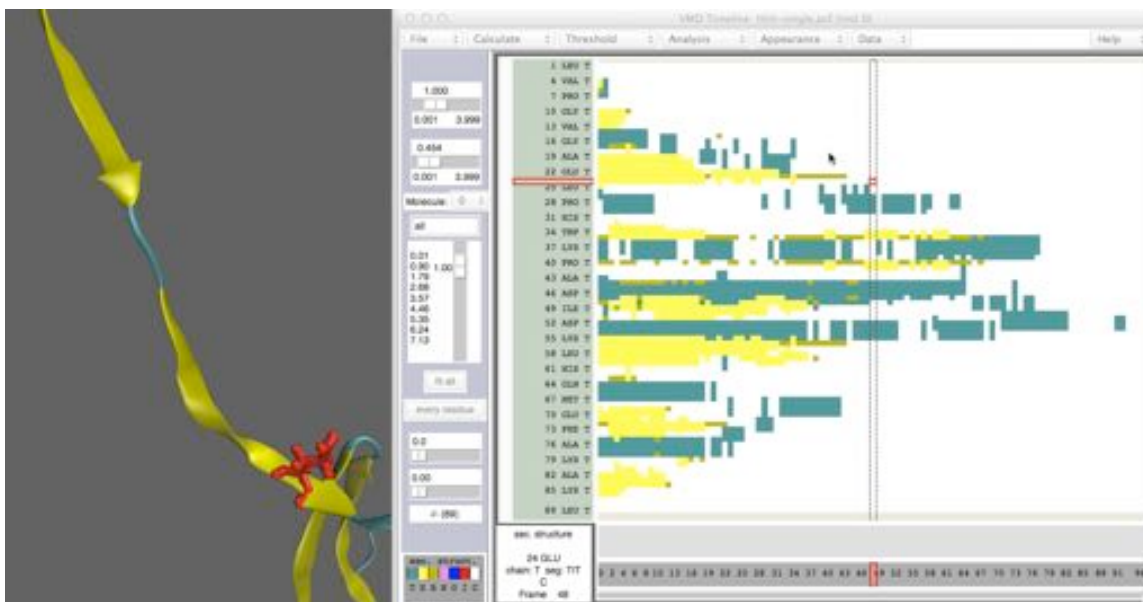


Beta turn
 Extended beta
 Isolated bridge
 None (coil)

5/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory

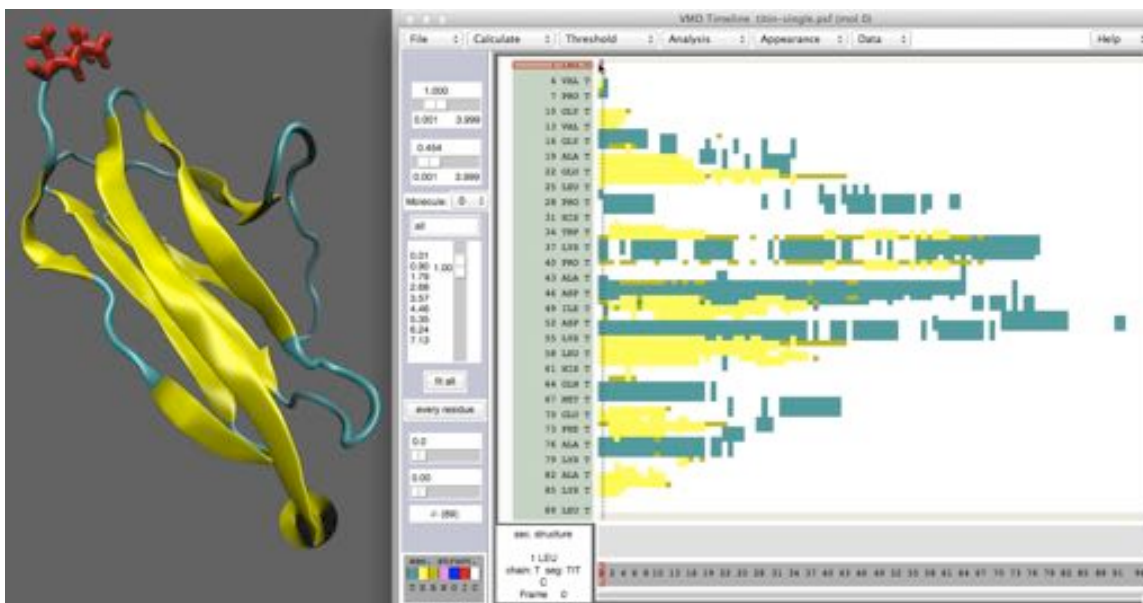


Beta turn
 Extended beta
 Isolated bridge
 None (coil)

6/8

secondary structure during titin domain extension

Timeline: a graphing and analysis tool to identify events in an MD trajectory



■ Beta turn
 ■ Extended beta
 ■ Isolated bridge
 □ None (coil)

7/8

secondary structure during titin domain extension

VMD Plugins: extensible analysis

Modeling Plugins

- Autonize
- AutoPSF
- Chirality
- Cispeptide
- CGTools
- Dowser
- FFTK
- Inorganic Builder
- MDFF
- Membrane Builder
- MergeStructs
- Molefacture
- Mutator
- Nanotube
- Paratool
- Psfgen
- Solvate
- SSRestrains
- Topotools

Analysis Plugins

- APBSRun
- CatDCD
- Contact Map
- GofRGUI
- HBonds
- ILSTools
- IRSpecGUI
- MultiSeq
- NAMDEnergy
- NAMDPLOT
- NetworkView
- NMWiz
- ParseFEP
- PropKaGUI
- RamaPlot
- RMSD Tool
- RMSD Trajectory Tool
- RMSD Visualizer Tool
- Salt Bridges
- Sequence Viewer
- Symmetry Tool
- Timeline
- VolMap

Visualization Plugins

- Clipping Plane Tool
- Clone Rep
- Dipole Watcher
- Intersurf
- Navigate
- NavFly
- MultiMolAnim
- Color Scale Bar
- Remote
- Palette Tool
- ViewChangeRender
- Viewmaster
- Virtual DNA Viewer
- VMDMovie

Simulation Plugins

- AutoIMD
- IMDMenu
- NAMD GUI
- NAMD Server
- QMTool

Data Plugins

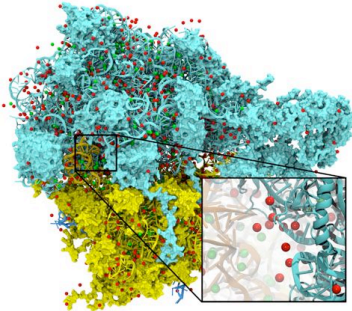
- Data Import
- Multiplot
- PDBtool
- MultiText

Other Plugins

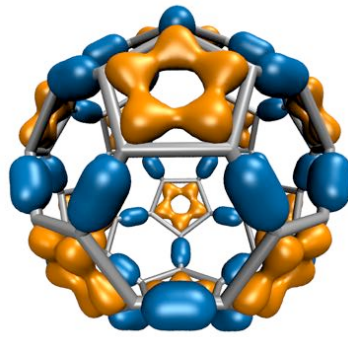
- AtomEdit
- DemoMaster
- ExecTool
- Hesstrans
- Optimization
- PBCTools
- RESPTool
- RNAview
- SignalProc
- TkCon

<http://www.ks.uiuc.edu/Research/vmd/plugins/>

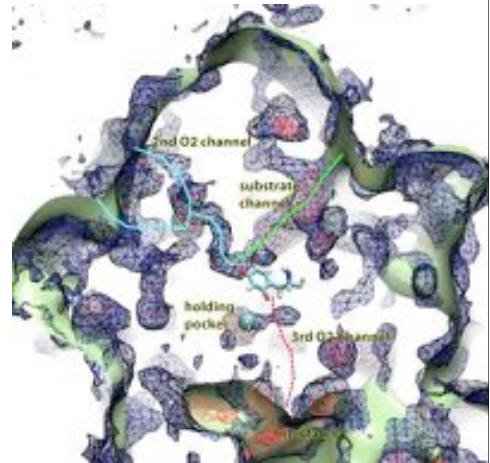
VMD the Compute Engine



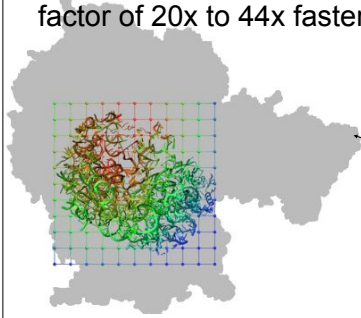
Electrostatic field calculation, ion placement: factor of 20x to 44x faster



Molecular orbital calculation and display: factor of 120x faster



Imaging of gas migration pathways in proteins with implicit ligand sampling: factor of 20x to 30x faster

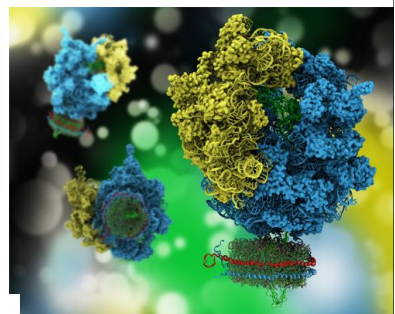
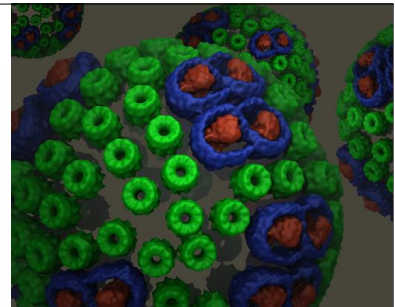


Parallel analysis on GPUs

VMD is first bio-software that is optimized for power consumption!

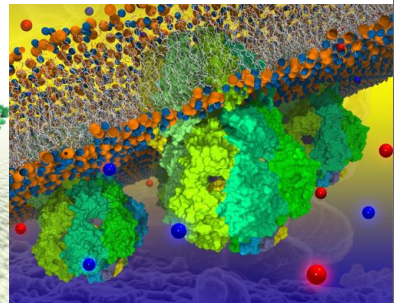
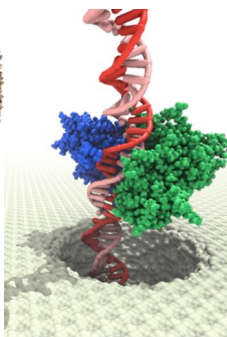
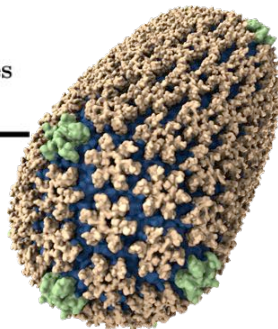
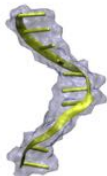
VMD the Artist

Publication-quality images and movies



University of Illinois at Urbana-Champaign
Beckman Institute for Advanced Science and Technology
Theoretical and Computational Biophysics Group
Computational Biophysics Workshop

VMD Images and Movies Tutorial



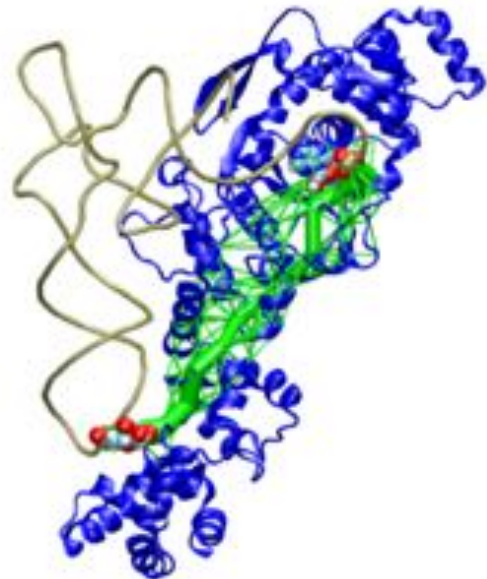
VMD Session 3: *exchanging .vmd file of photosynthetic chromatophore for joint viewing*

VMD 1.9.1 Released Feb. 4, 2012

24

Key Features

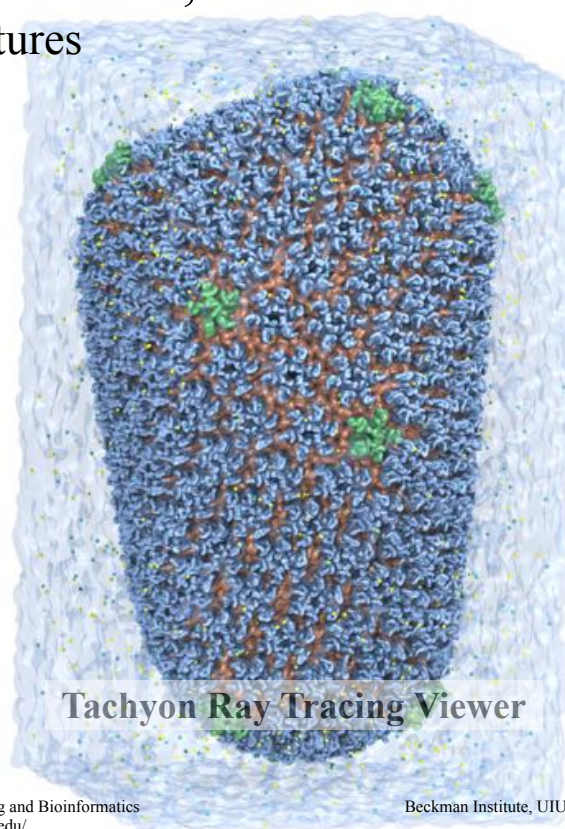
- New **NetworkView** plugin for study of allostery, signaling networks
- New **Force Field Toolkit (ffTK)** assists with CHARMM parameter development
- New “**QuickSurf**” surface representation
- New **user-contributed plugins**:
 - Normal Mode Wizard
 - PropKa interface
 - RMSD Trajectory Tool
 - “Heat map” plotting
 - Many others...



NetworkView: tRNA anti-codon w/
ligand in GluRS active site

Key Features

- New **Tachyon Ray Tracing** plugin for extremely realistic molecular views
- Vastly improved **Force Field Toolkit (ffTK)**: faster charge optimization routine; optimization of bond and angle parameters; projection of missing parameters onto molecular structure; interactive display for analyzing complex dihedral potential energy surfaces within the context of the molecular structure
- Updates **Molecular Dynamics Flexible Fitting (MDFF) Method**: options for MDFF with implicit solvent, xMDFF for low-resolution x-ray crystallography, multi-core CPU and GPU-accelerated analysis
- New **user-contributed plugins** ...



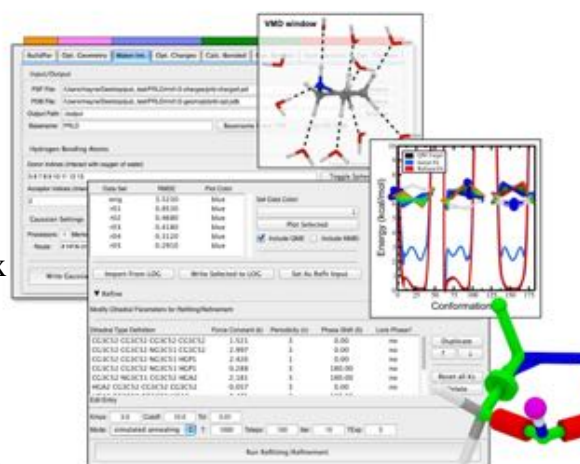
National Center for Research Fluoroscopes

BTRC for Macromolecular Modeling and Bioinformatics
<http://www.ks.uiuc.edu/>

Beckman Institute, UIUC

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Improved Force Field Toolkit



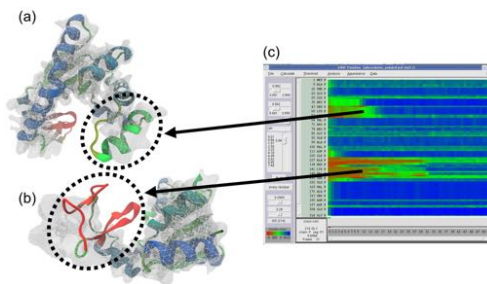
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Improved MDFF Analysis



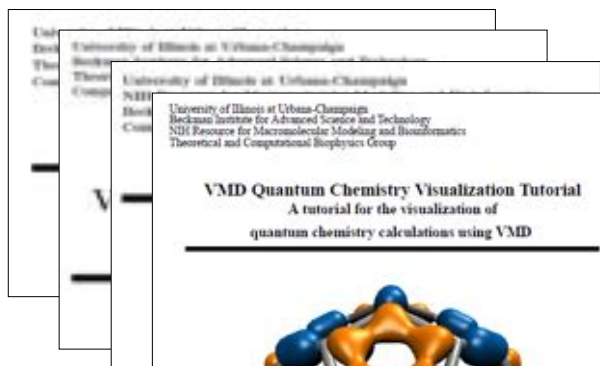
BTRC for Macromolecular Modeling and Bioinformatics
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Beckman Institute, UIUC

VMD and NAMD Work Together



- Over 212,000 registered VMD users
 - 18% (39,000) are NIH-funded
 - Over 49,000 have downloaded multiple VMD releases
- Over 8,000 citations
- User community runs VMD on:
 - MacOS X, Unix, Windows operating systems
 - Laptops, desktop workstations
 - Clusters, supercomputers
- VMD user support efforts:
 - 20,000 emails, 2007-2011
 - Develop and maintain VMD tutorials and topical mini-tutorials; 11 in total
 - Periodic user surveys



The Biomedical Technology Research Center (BTRC) for Macromolecular Achievements Built on People

17

- 5 faculty members (2 physics, 1 chemistry, 1 biochemistry, 1 computer science);
- 8 developers; 1 system admin.; 17 post docs; 46 graduate students; 3 administrative staff (assistant director, grants coordinator, training and dissemination)
- Funding/support from NIH and National Science Foundation



*Beckman
Institute,
Urbana,
Illinois*

1-2