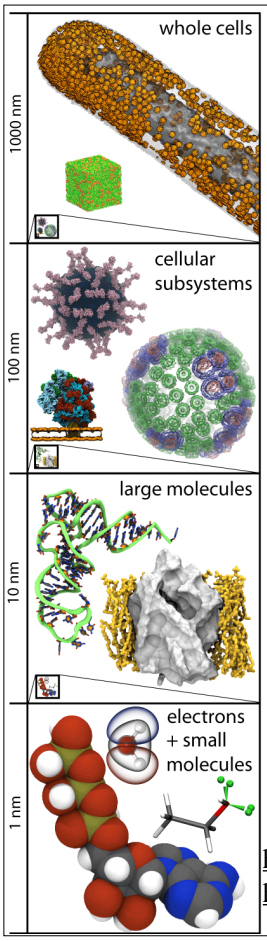
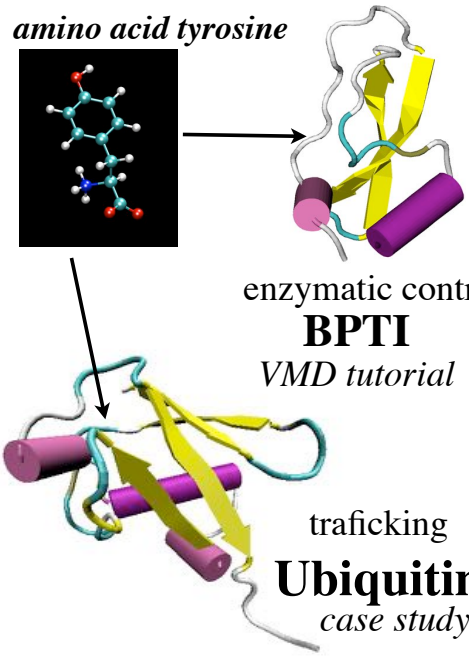


VMD: Visual Molecular Dynamics

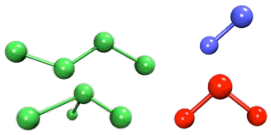
Computational Microscope / Tool to Think



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

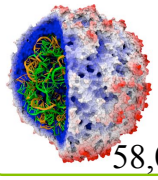
Our Microscope is Made of...

Chemistry

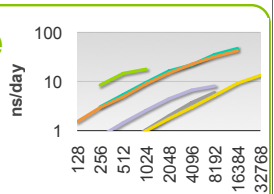


$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} + \underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} + \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}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

NAMD Software



Virus



58,000 registered users

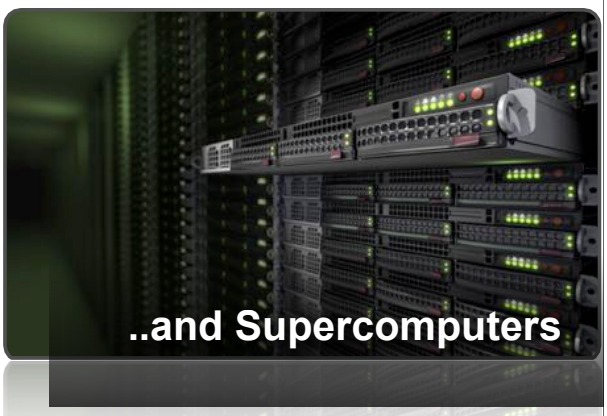
Physics

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

Math

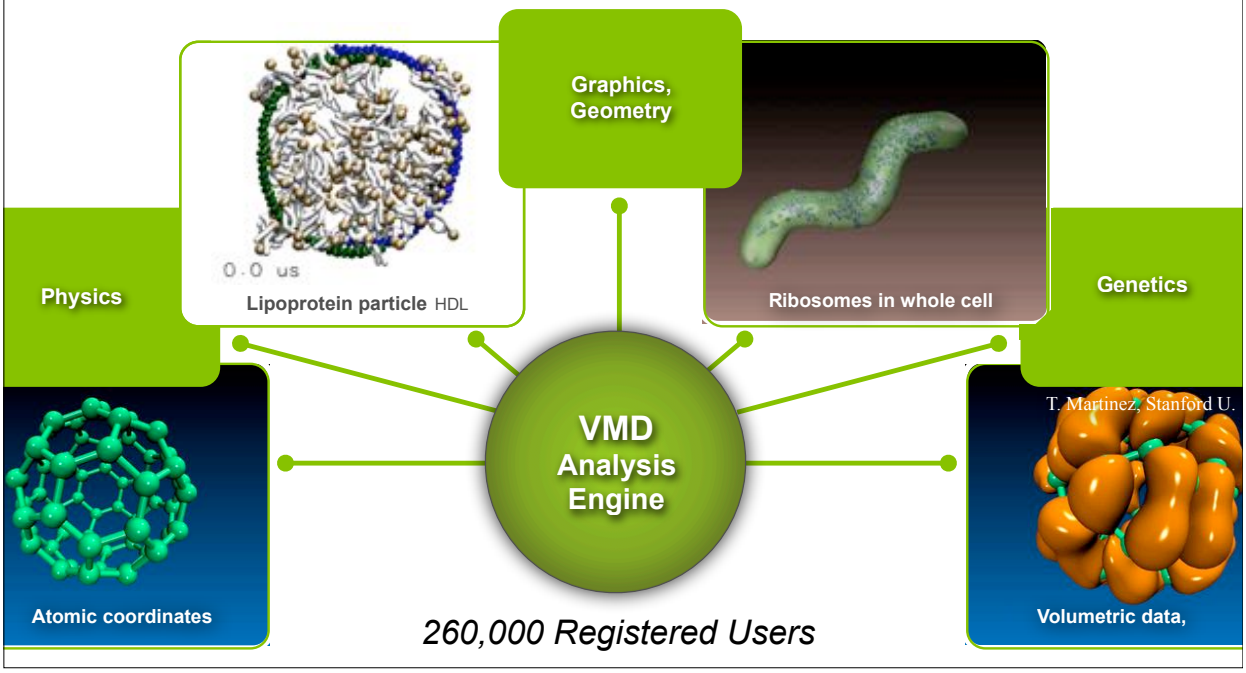
$$\vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \frac{\Delta t^2}{m_i}\vec{F}_i(t)$$

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



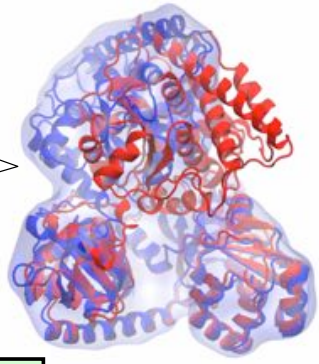
Our Microscope is Made of...

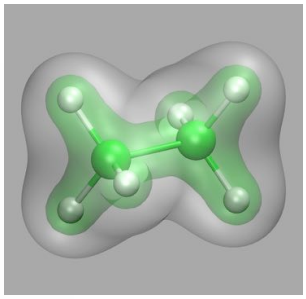
and of...



VMD – A Tool to Think

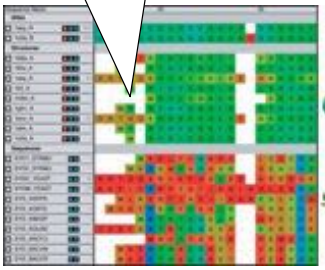
Volumetric Data:
Density maps,
Electron orbitals,
Electrostatic potential,
Time-averaged occupancy, …

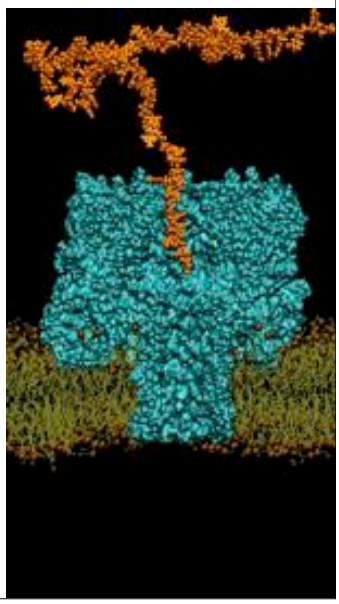




Sequence Data:
Multiple Alignments,
Phylogenetic Trees

VMD

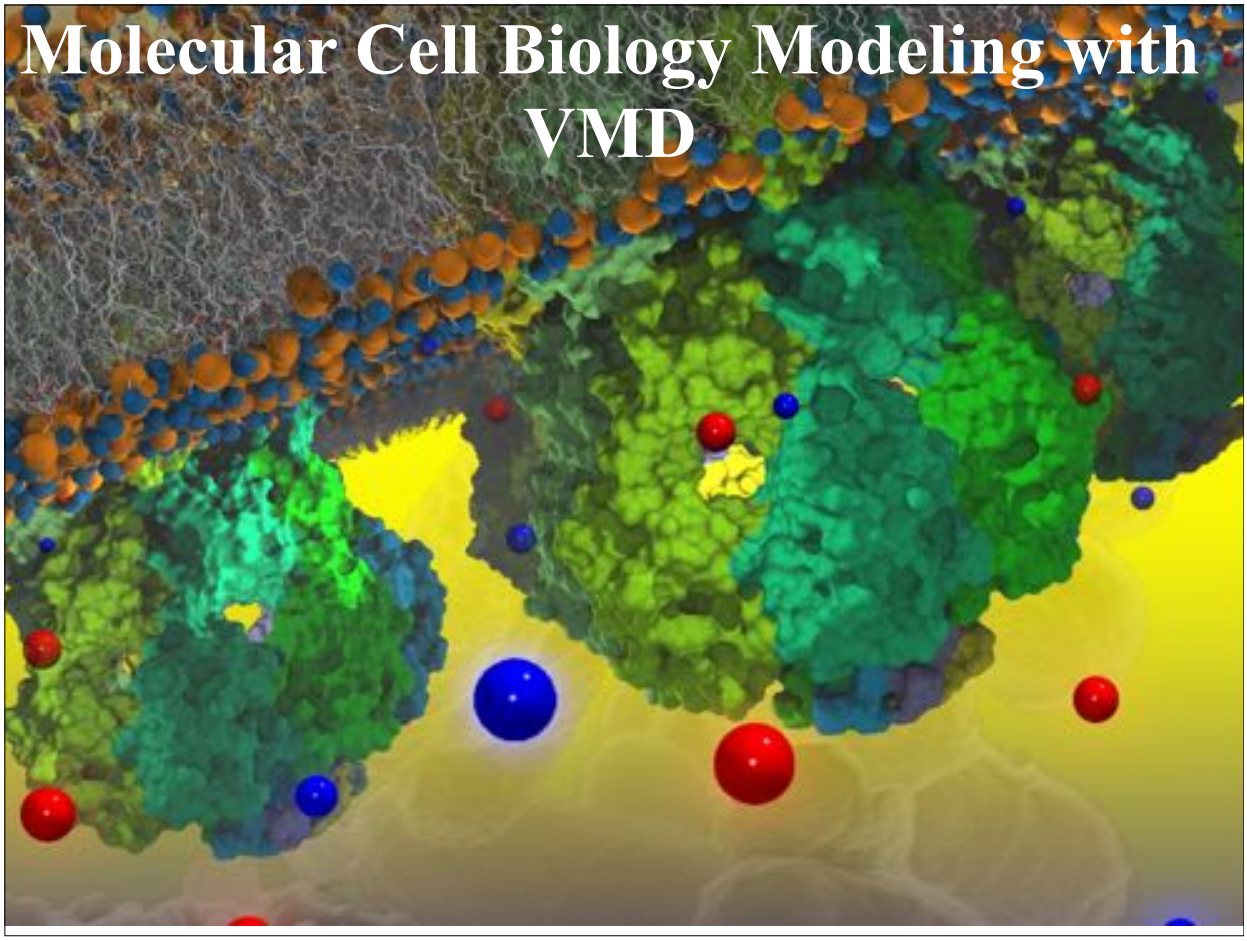




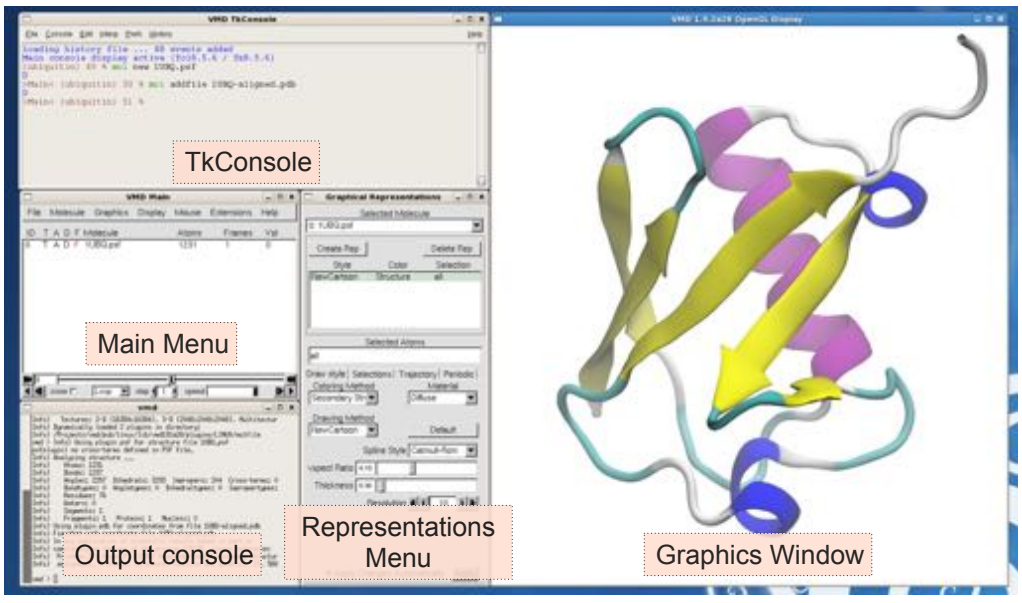
Atomic Data:
Coordinates,
Trajectories,
Energies,
Forces, …

NIH Biotechnology Research Center
for Macromolecular Modeling and Bioinformatics
http://www.ks.uiuc.edu/

Molecular Cell Biology Modeling with VMD



Molecular Graphics with VMD



typical VMD session

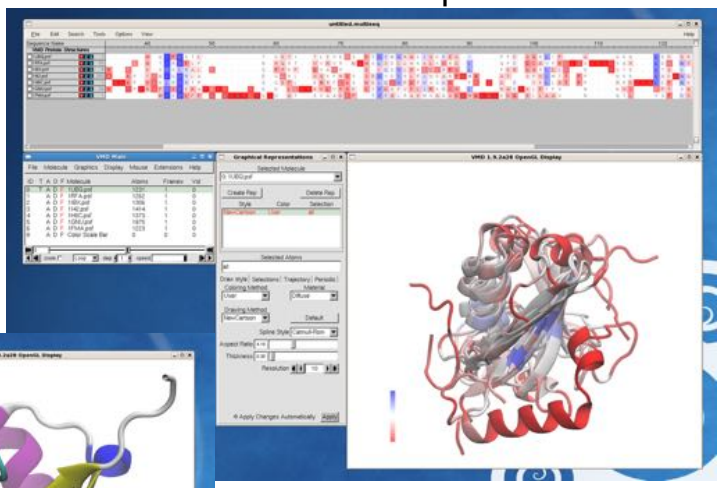
Bioinformatics

Link sequence to structure

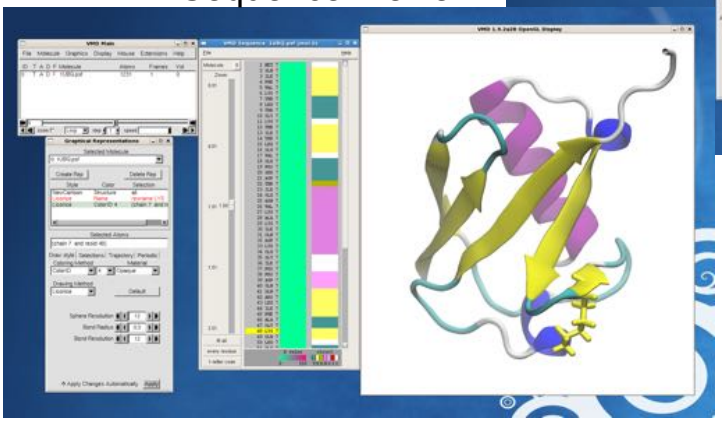
Multiple sequence/
structure alignments

Phylogenetic trees

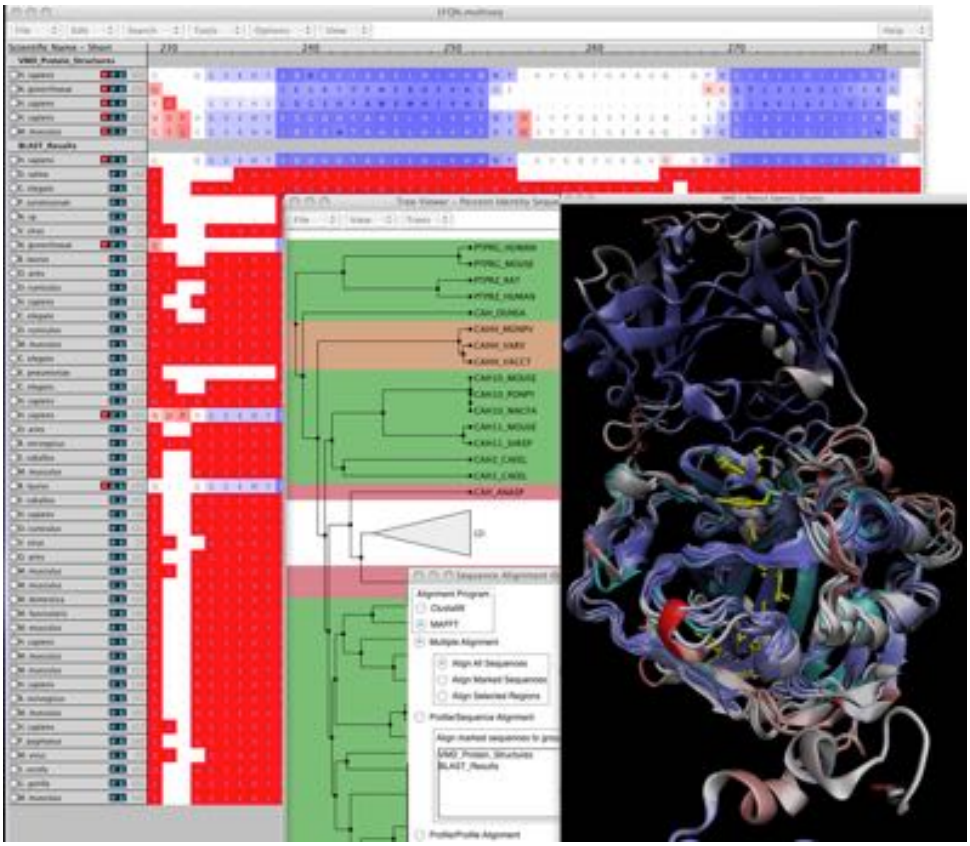
MultiSeq



Sequence Viewer



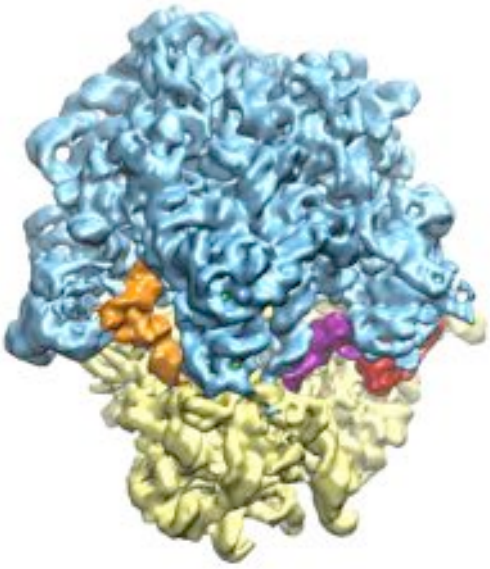
Structure, Sequence and Phylogenetic Analysis with VMD



VMD Handles Volumetric Data

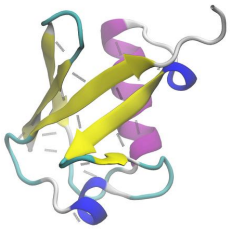
electron density
from QM/MM
calculation
Martinez, Stanford

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

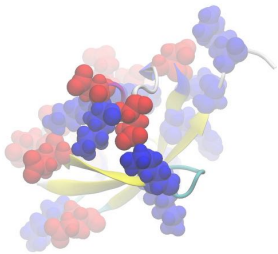


cryo-EM density

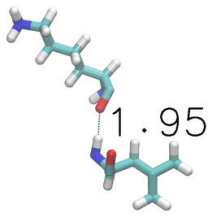
VMD Determines Physical Properties



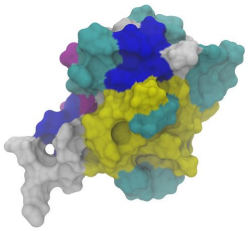
hydrogen bonds



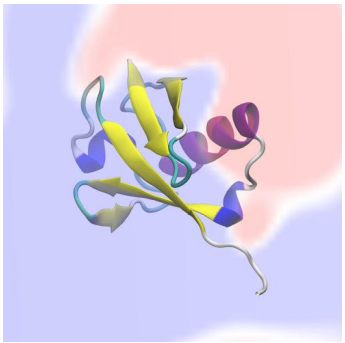
salt bridges



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

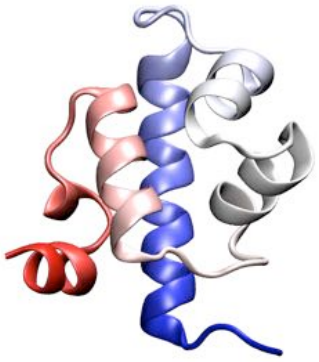
Trajectory Graphics/Analysis with VMD

VMD Plugin: Timeline

plugin to analyze MD trajectories for events

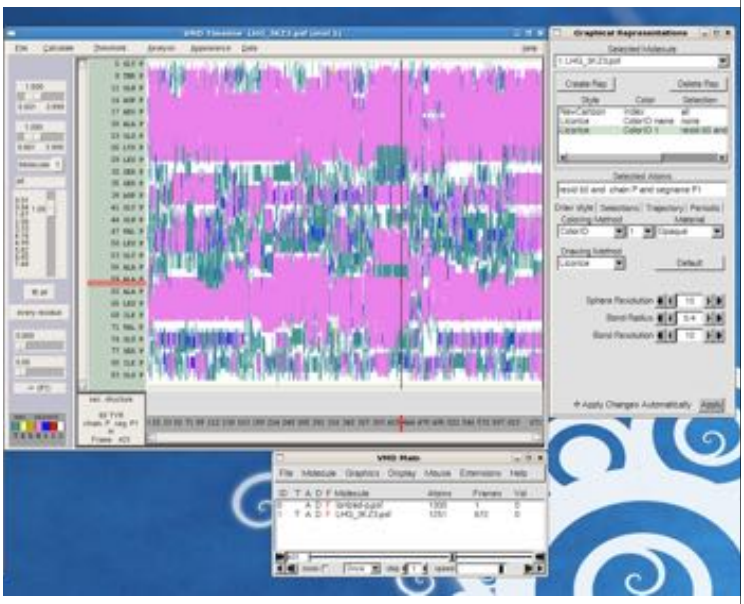
plot properties, e.g. RMSD, secondary structure, hydrogen bonds, for each residue across a trajectory

Example: protein folding



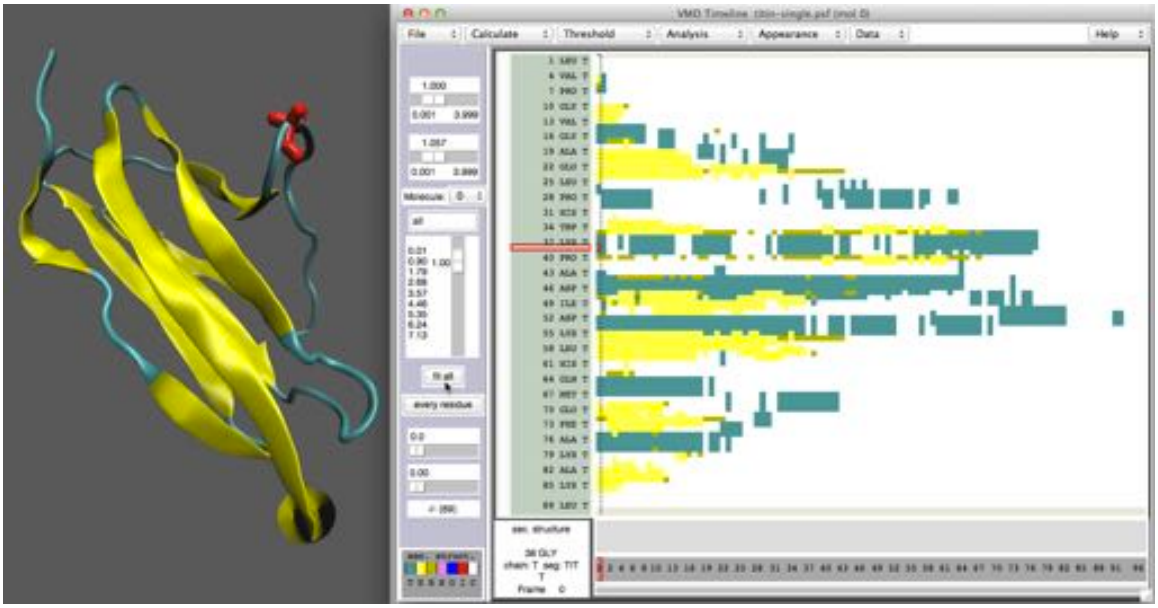
lambda repressor (2012)
80 amino acids, 100 μs

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

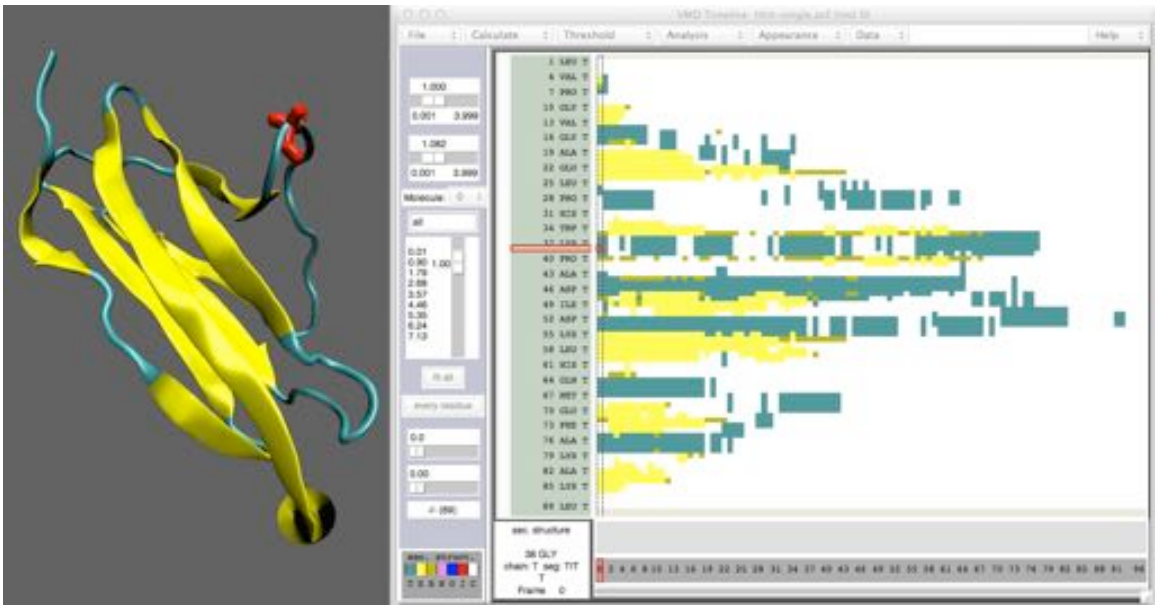
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

secondary structure during titin domain extension

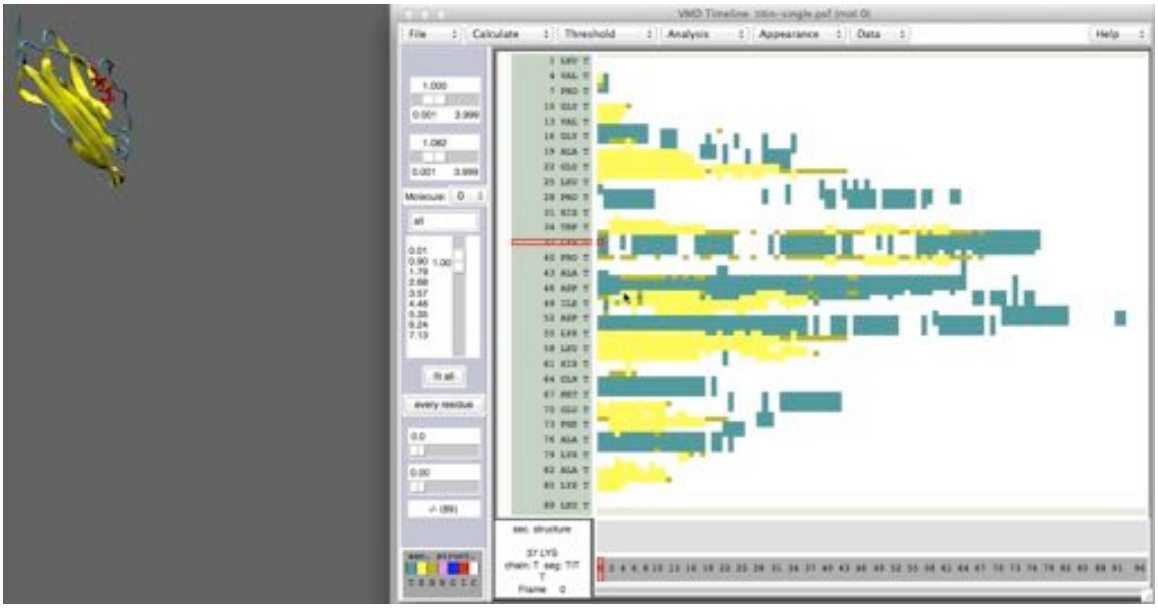
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

secondary structure during titin domain extension

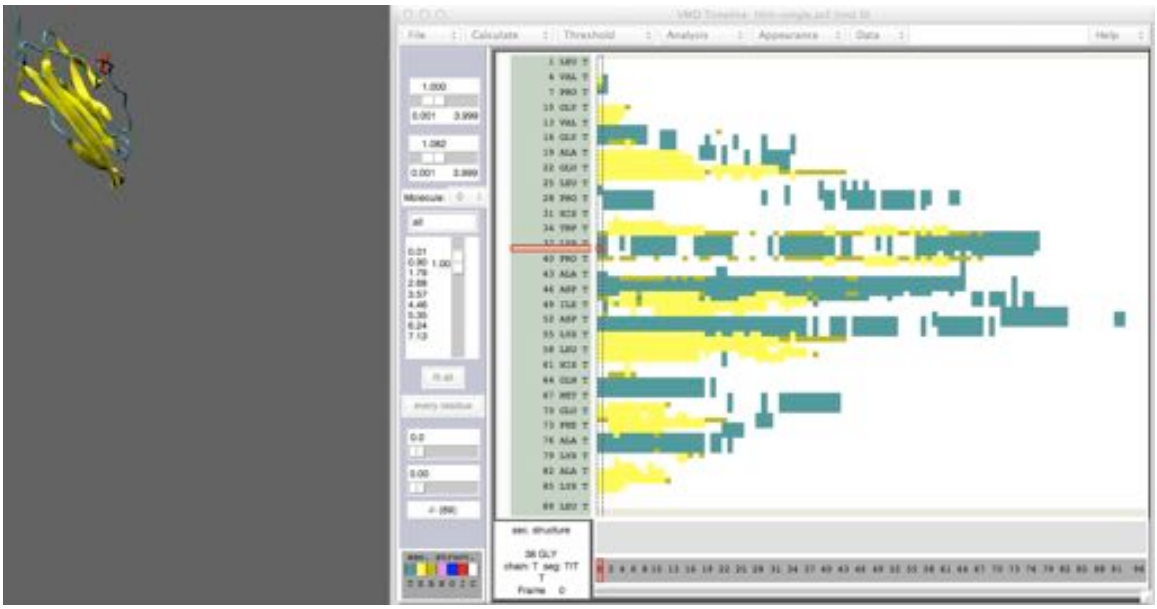
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

secondary structure during titin domain extension

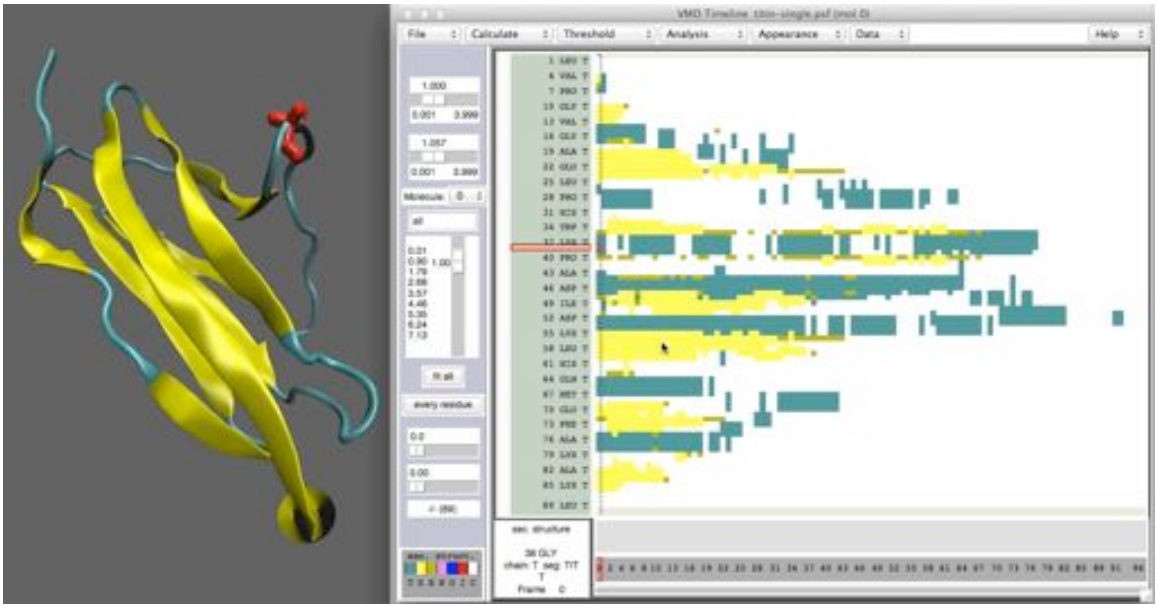
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

secondary structure during titin domain extension

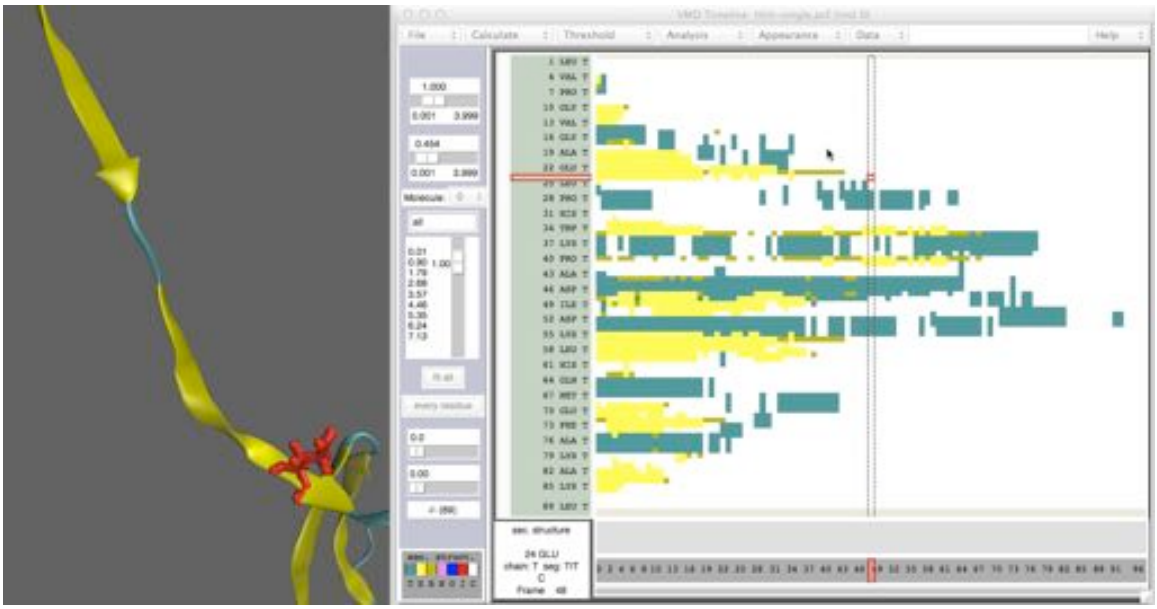
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

secondary structure during titin domain extension

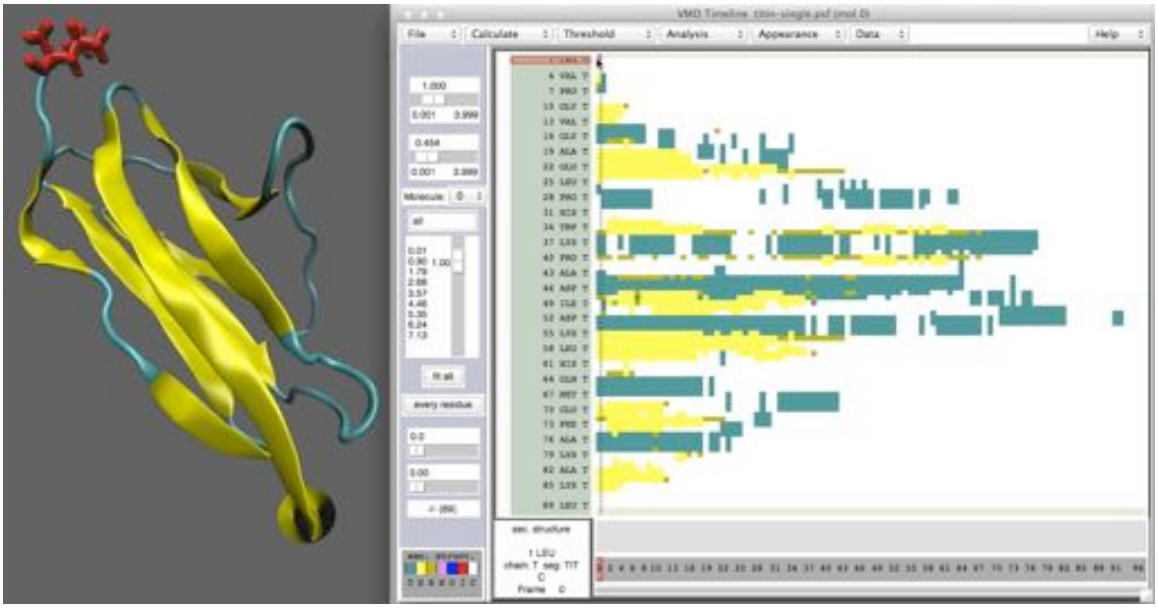
Timeline: a graphing and analysis tool to identify events in an MD trajectory



Beta turn Extended beta Isolated bridge None (coil)

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

- AutoIonize
- AutoPSF
- Chirality
- Cispeptide
- CGTools
- Dowser
- FFTK
- Inorganic Builder
- MDFF
- Membrane Builder
- MergeStructs
- Molefacture
- Mutator
- Nanotube
- Paratool
- Psfgen
- Solvate
- SSRestraints
- 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

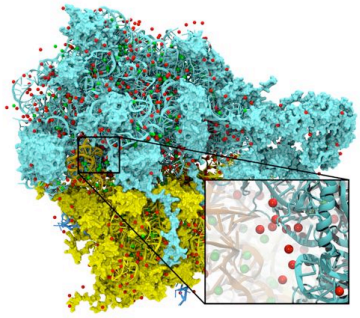
- Data Import
- Multiplot
- PDBtool
- MultiText

Other Plugins

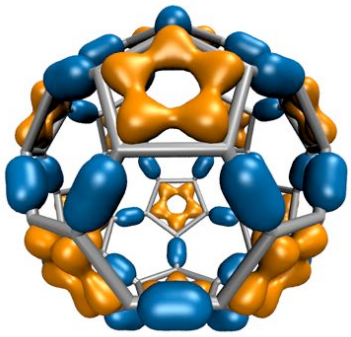
- AtomEdit
- DemoMaster
- ExecTool
- Hesstrans
- Optimization
- PBCTools
- RESPTool
- RNAview
- SignalProc
- TkCon

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

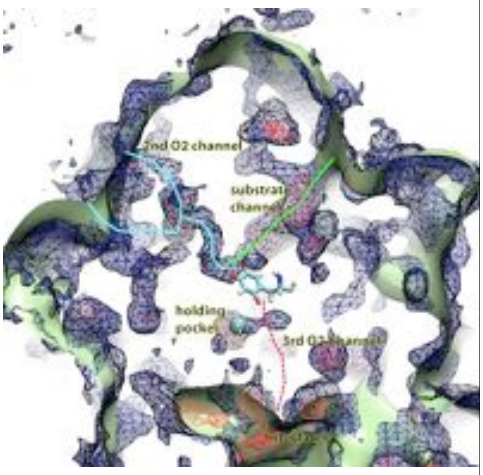
VMD the Compute Engine



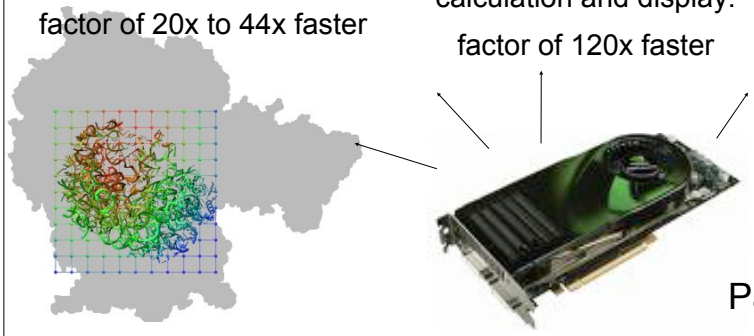
Electrostatic field calculation, ion placement: factor of 20x to 44x faster



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

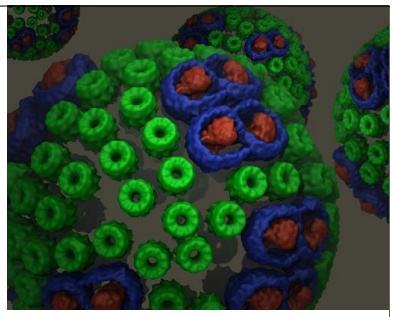


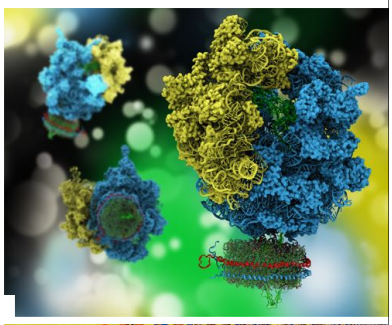
Parallel analysis on GPUs

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

VMD the Artist

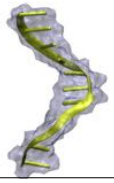
Publication-quality images and movies

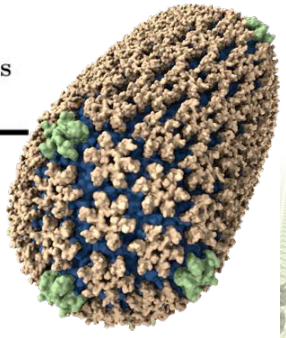


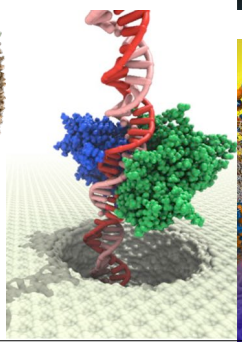


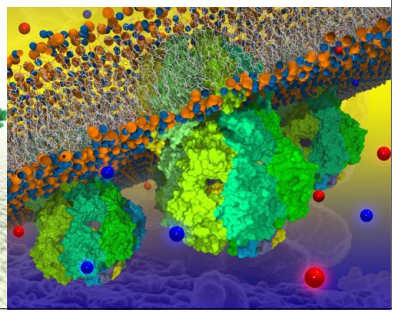
University of Illinois at Urbana-Champaign
Beckman Institute for Advanced Science and Technology
Theoretical and Computational Biophysics Group
Computational Biophysics Workshop

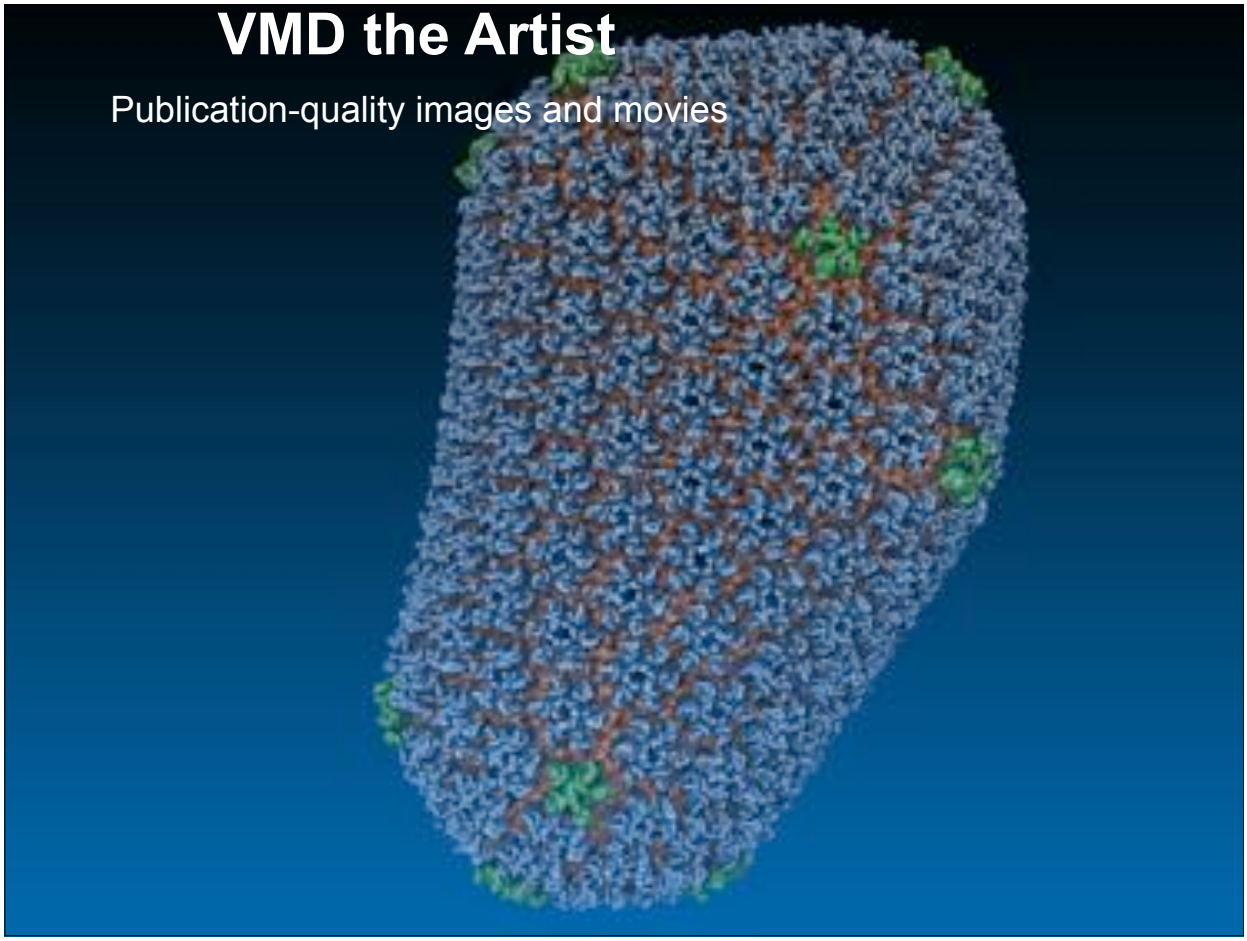
VMD Images and Movies Tutorial









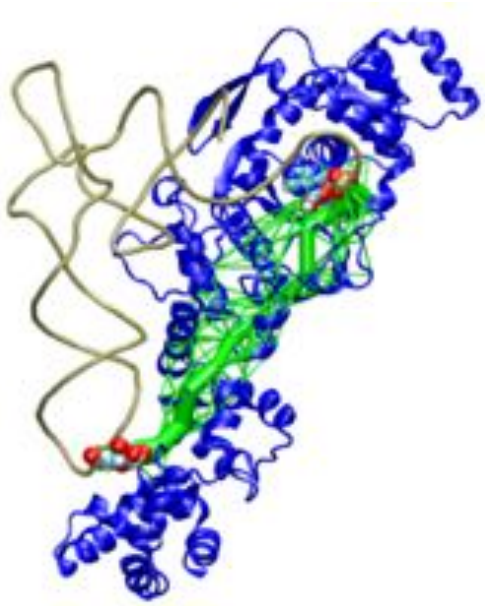


VMD Session 3:
exchanging .vmd file of photosynthetic chromatophore for joint viewing

VMD 1.9.1 Released Feb. 4, 2012

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…

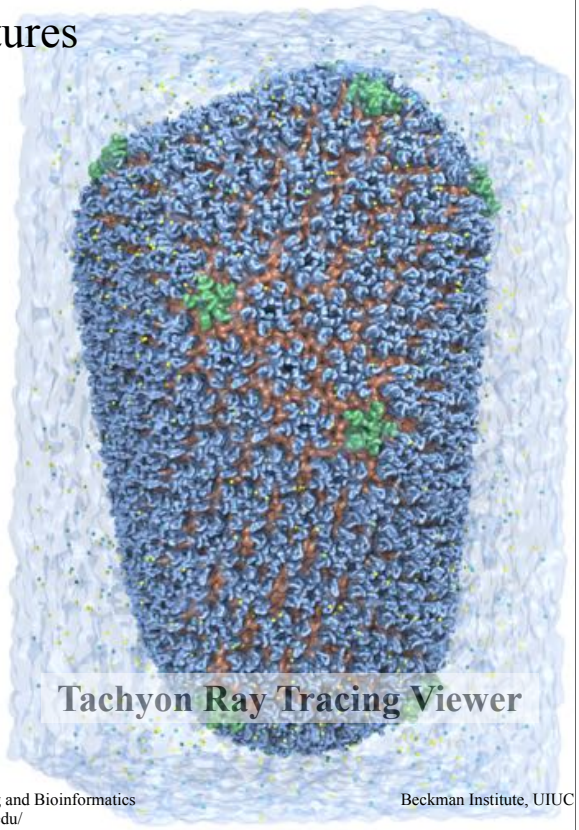


NetworkView: tRNA anti-codon w/ ligand in GluRS active site

VMD 1.9.2 Release Dec, 2014

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** …



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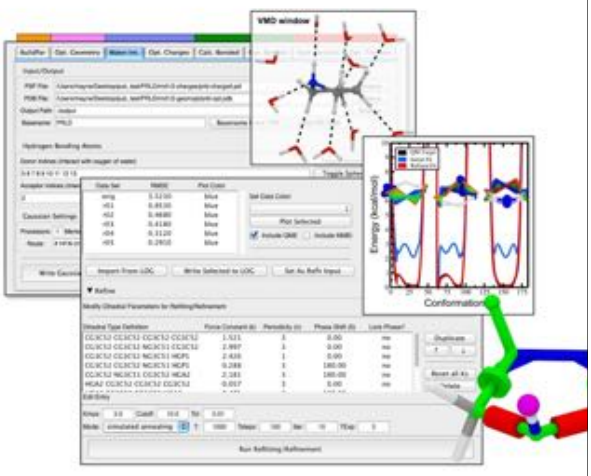

Improved Force Field Toolkit

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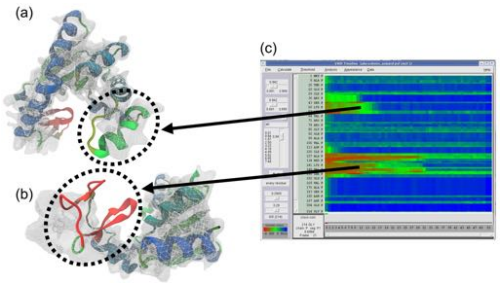


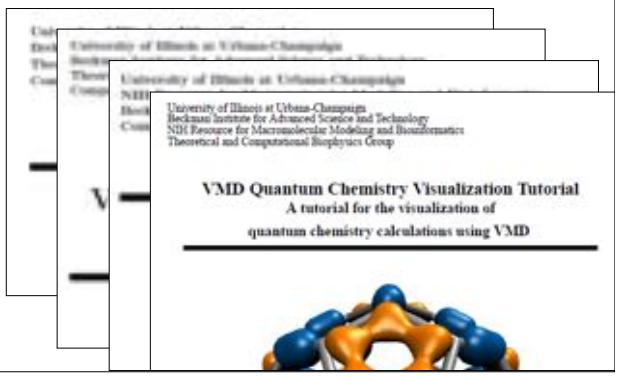
Improved MDFF Analysis

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