

VMD: Visual Molecular Dynamics

Computational Microscope / Tool to Think

amino acid tyrosine

enzymatic control
BPTI
VMD tutorial

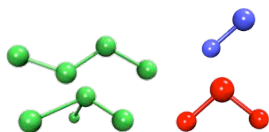
trafficking
Ubiquitin
case study

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

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

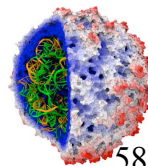
Our Microscope is Made of...

Chemistry



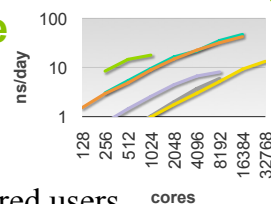
$$U(\vec{R}) = \underbrace{\sum_{\text{bonds}} k_i^{\text{bond}} (r_i - r_0)^2}_{U_{\text{bond}}} + \underbrace{\sum_{\text{angles}} k_i^{\text{angle}} (\theta_i - \theta_0)^2}_{U_{\text{angle}}} + \underbrace{\sum_{\text{dihedrals}} k_i^{\text{dih}} [1 + \cos(n_i \phi_i + \delta_i)]}_{U_{\text{dihedral}}}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

NAMD Software



Virus

58,000 registered users



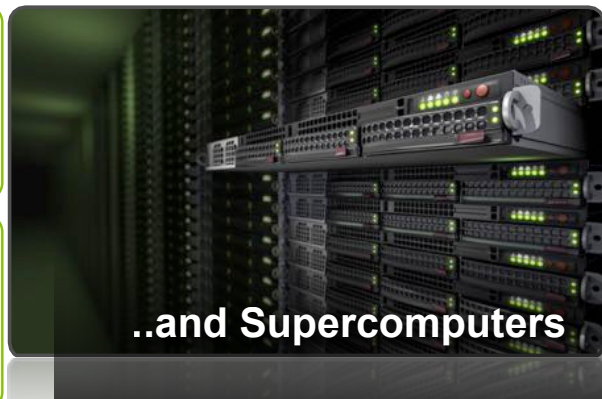
Physics

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

Math

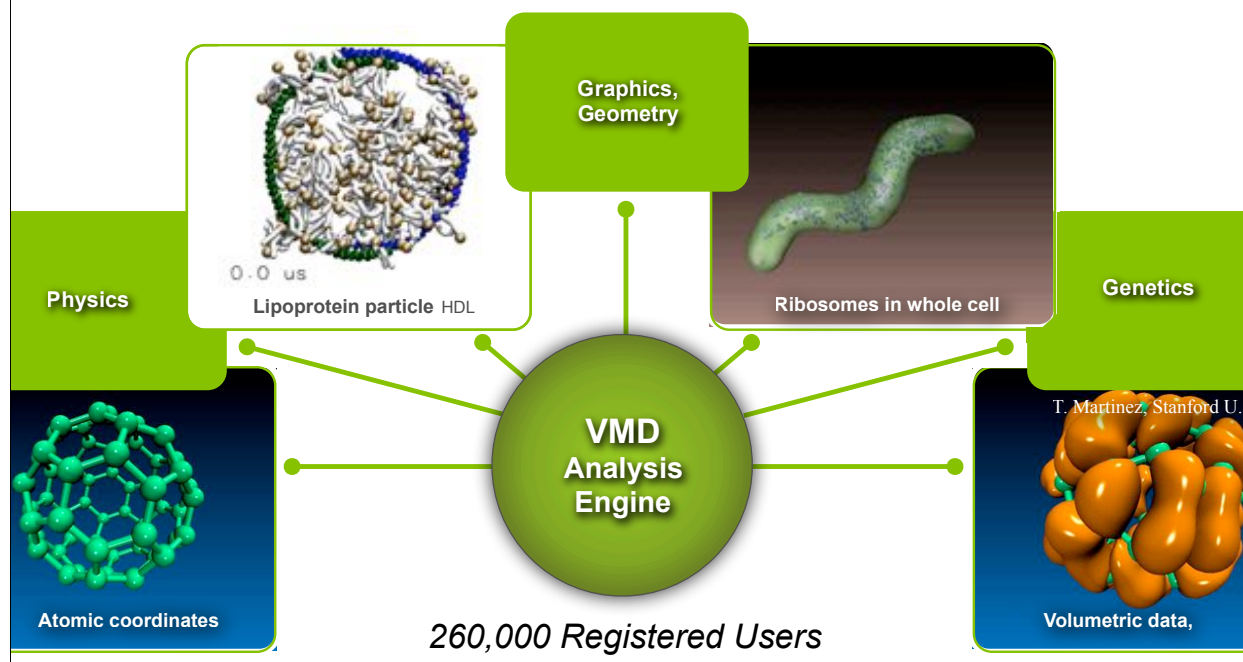
$$\vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \frac{\Delta t^2}{m_i} \vec{F}_i(t)$$

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



..and Supercomputers

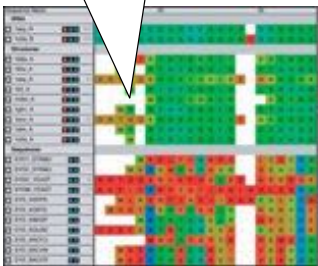
Our Microscope is Made of... and of...



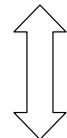
VMD – A Tool to Think

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

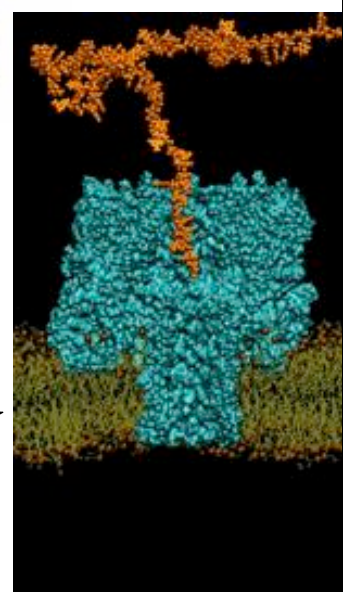
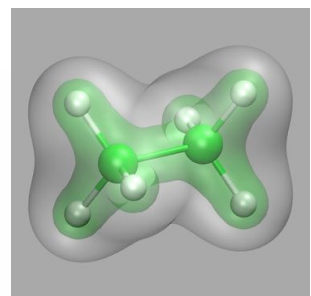
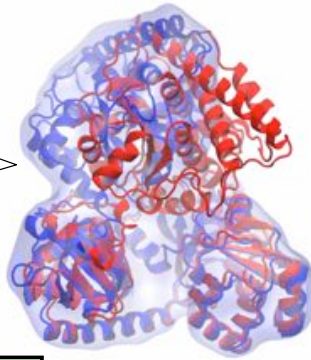
Sequence Data:
Multiple Alignments,
Phylogenetic Trees



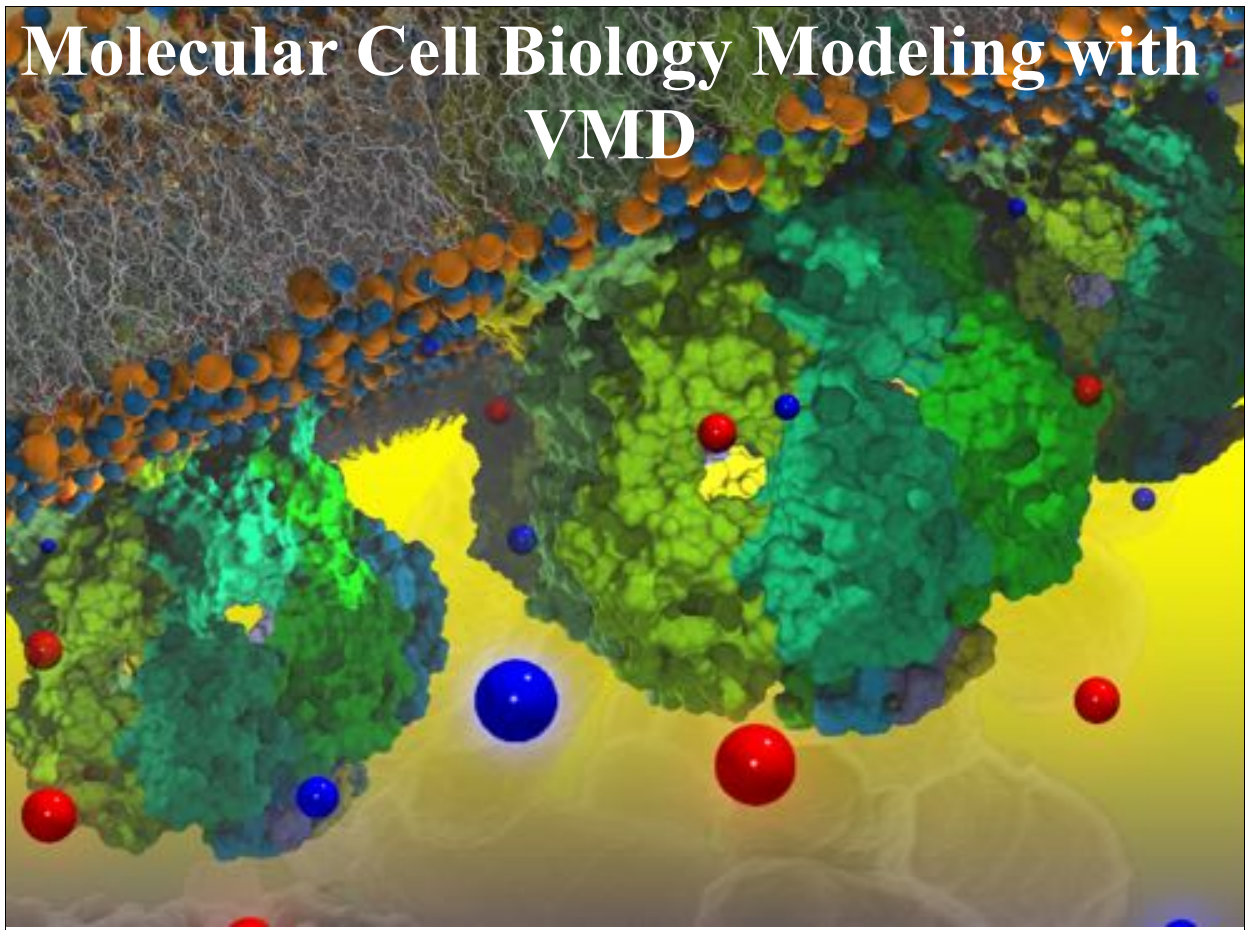
VMD



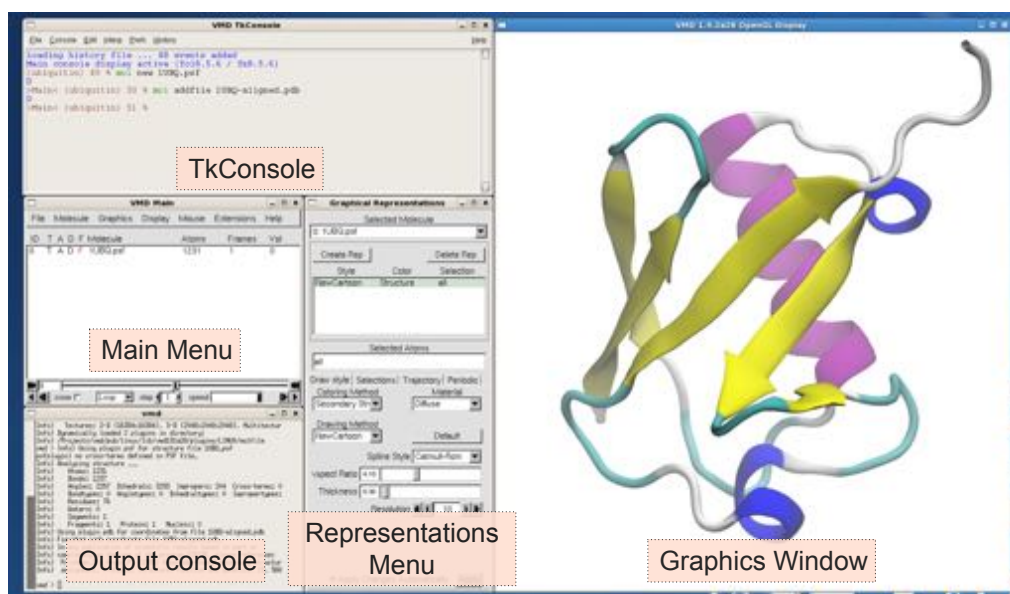
Atomic Data:
Coordinates,
Trajectories,
Energies,
Forces, ...



Molecular Cell Biology Modeling with VMD



Molecular Graphics with VMD



typical VMD session

Bioinformatics

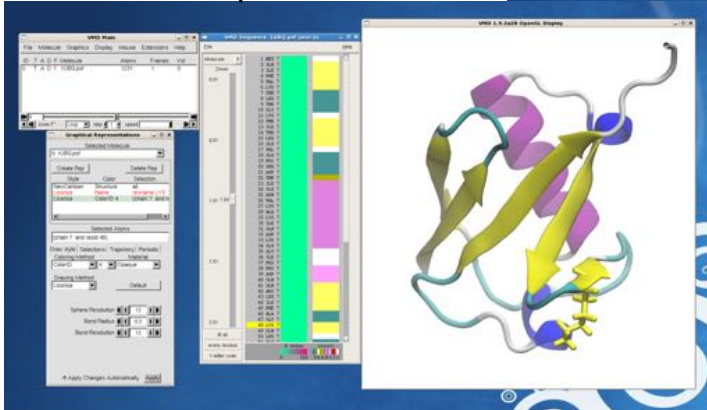
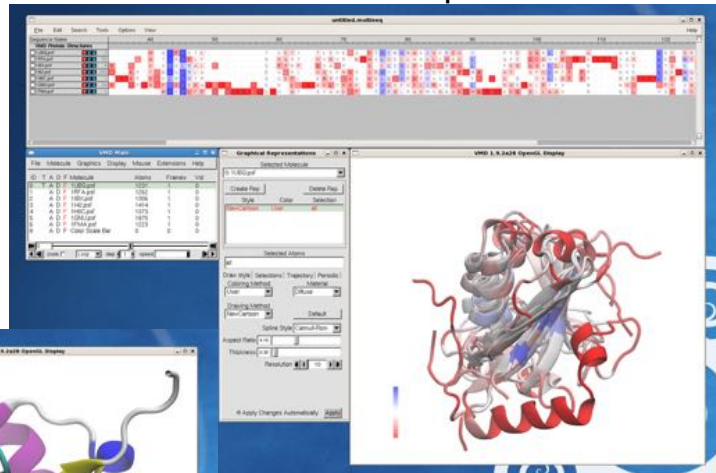
MultiSeq

Link sequence to structure

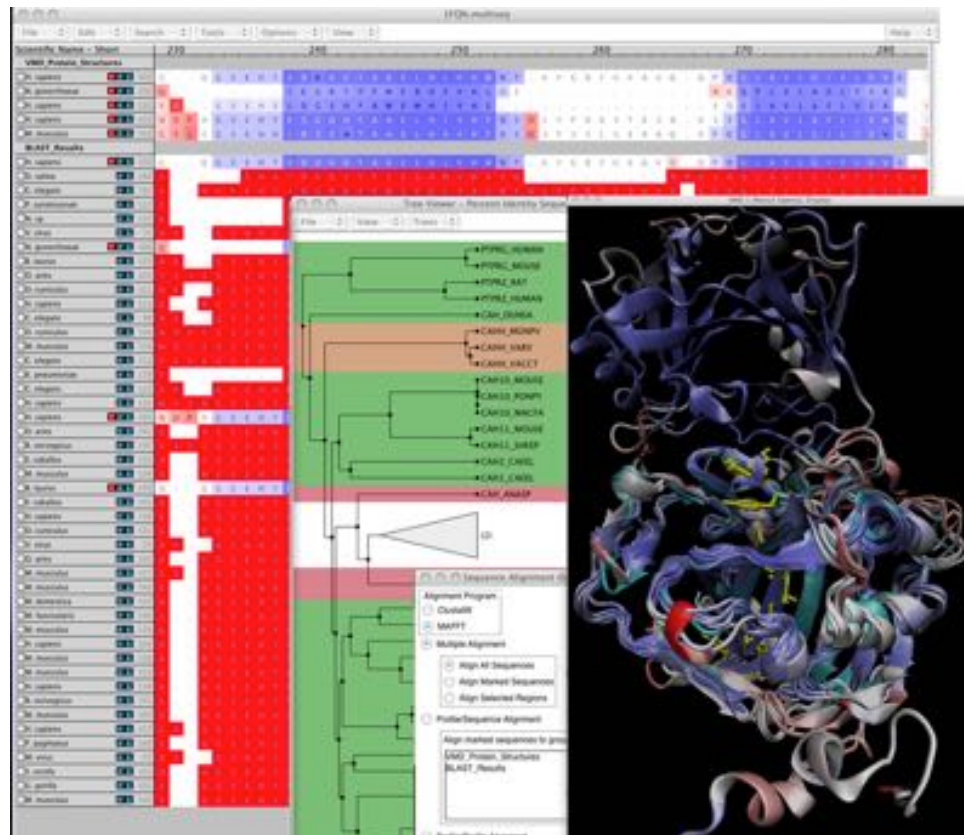
Multiple sequence/
structure alignments

Phylogenetic trees

Sequence Viewer

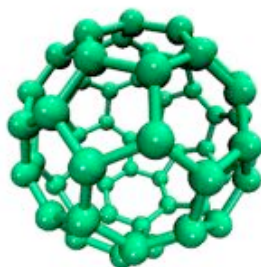


Structure, Sequence and Phylogenetic Analysis with VMD



VMD Handles Volumetric Data

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

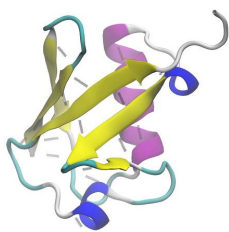


electron density
from QM/MM
calculation
Martinez, Stanford

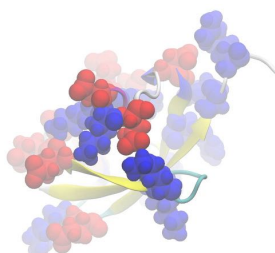


cryo-EM density

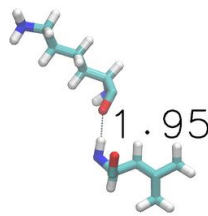
VMD Determines Physical Properties



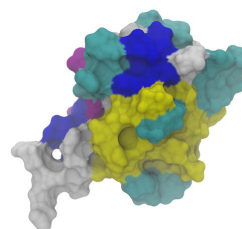
hydrogen bonds



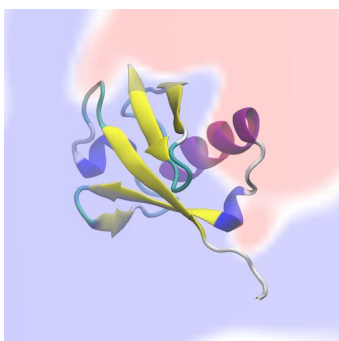
salt bridges



distances



SASA



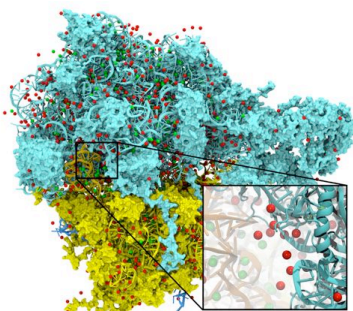
electrostatics

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

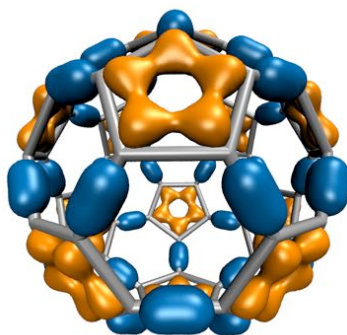
Insertion: VMD tool to think and VMD plugins

VMD Session Folding of Villin Head Piece

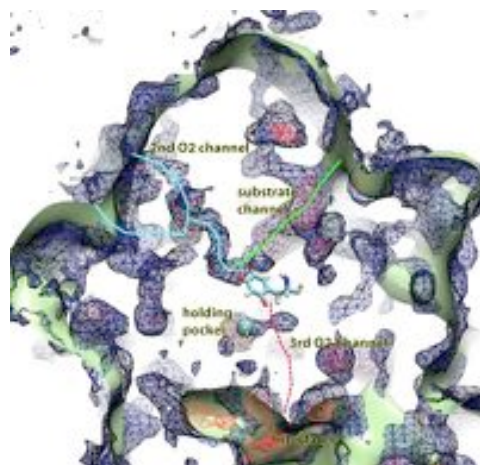
VMD the Compute Engine



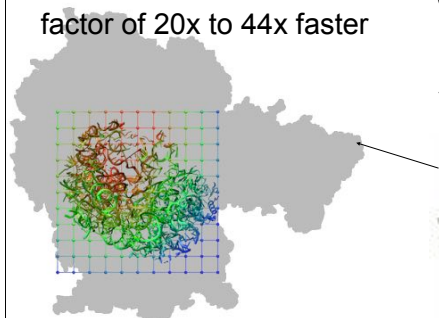
Electrostatic field
calculation, ion placement:
factor of 20x to 44x faster



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

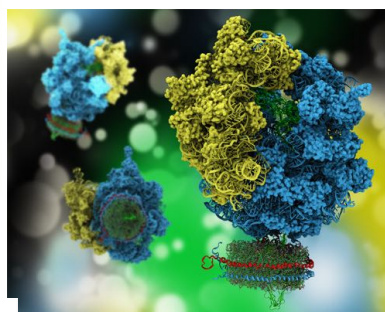
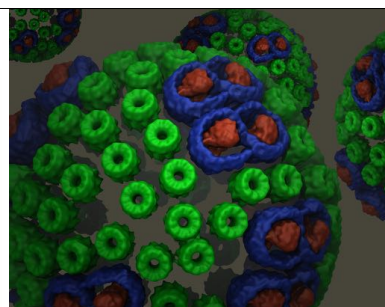


Parallel analysis on GPUs

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

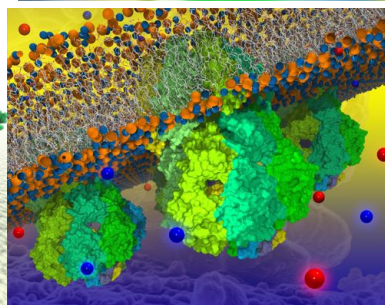
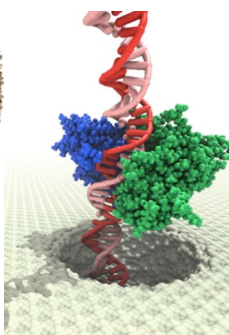
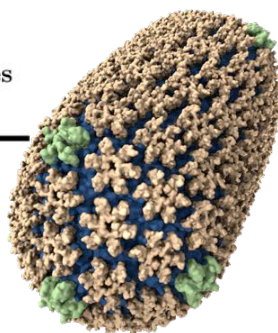
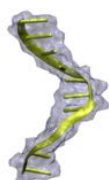
VMD the Artist

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



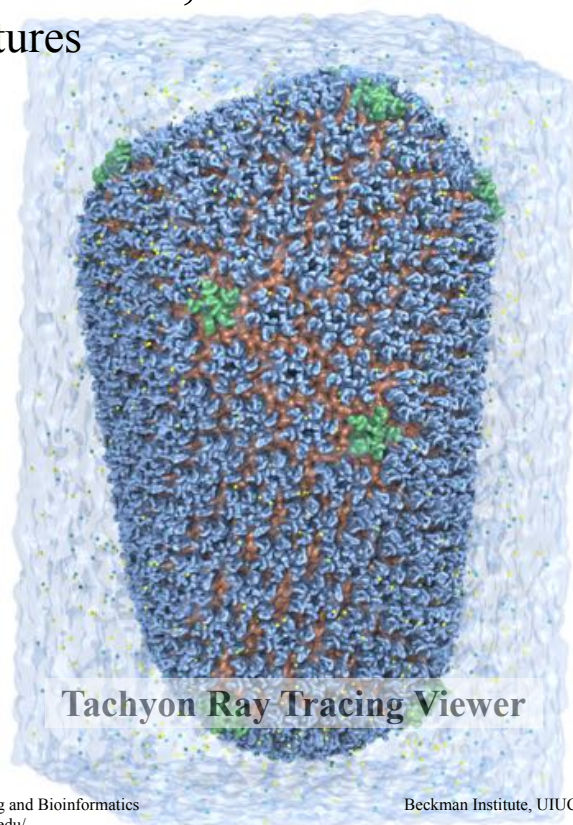
VMD Session 3: *exchanging .vmd file of photosynthetic chromatophore for joint viewing*

VMD 1.9.2 Release Dec, 2014

16

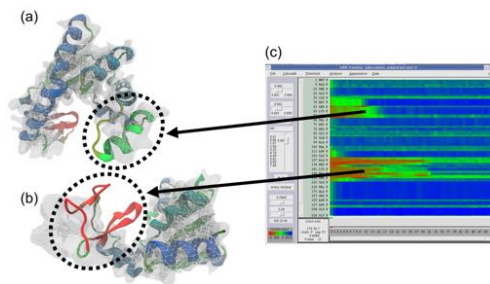
Key Features

- 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 MDFF Analysis



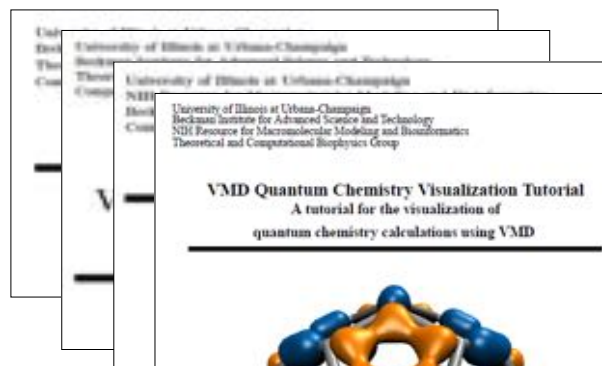
BTRC for Macromolecular Modeling and Bioinformatics
<http://www.ks.uiuc.edu/>

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*

1-2