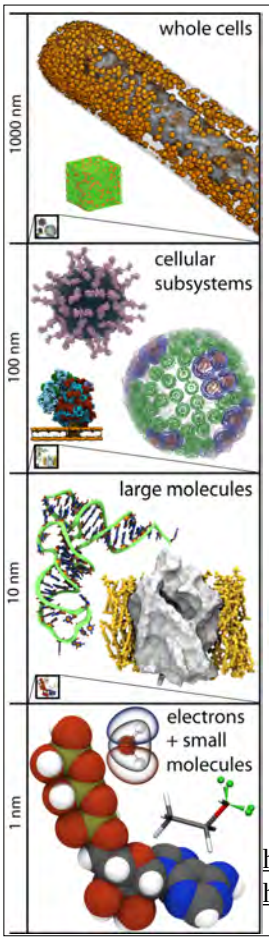
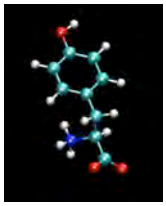
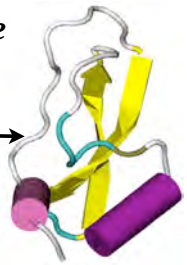


VMD: Visual Molecular Dynamics

Computational Microscope / Tool to Think

amino acid tyrosine

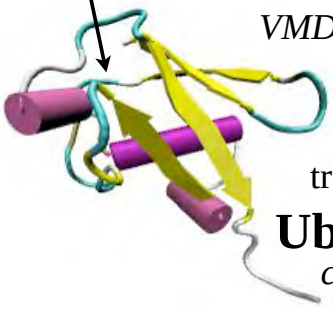




enzymatic control

BPTI

VMD tutorial



traficking

Ubiquitin

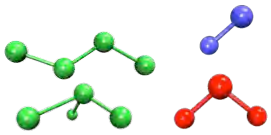
case study

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

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

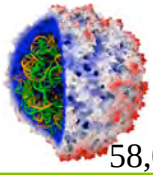
Our Microscope is Made of...

Chemistry

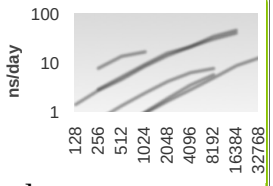


$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond}(r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle}(\theta_i - \theta_0)^2}_{U_{angle}} + \underbrace{\sum_{dihedrals} k_i^{dihe}[1 + \cos(n_i\phi_i + \delta_i)]}_{U_{dihedral}} + \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12}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

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

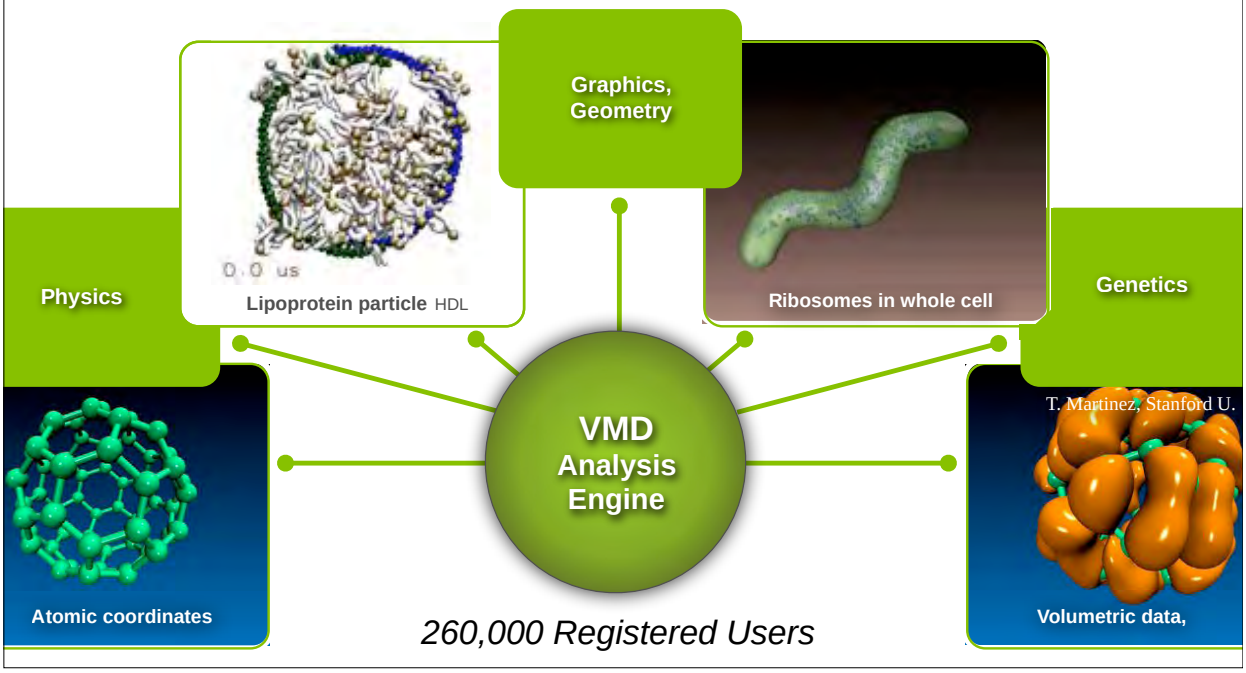
$$\vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \frac{\Delta t^2}{m_i}\vec{F}_i(t)$$

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

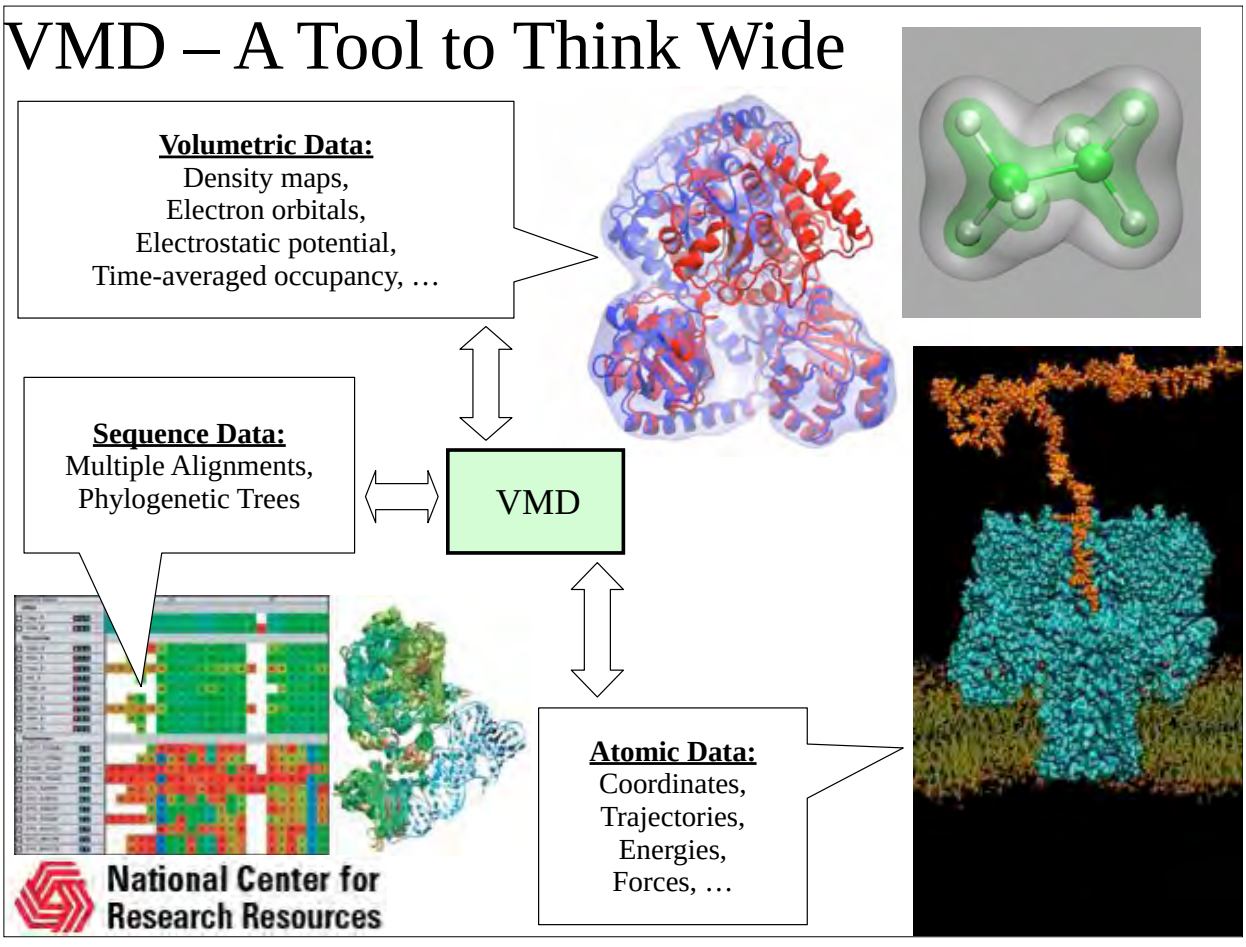
..and Supercomputers

Our Microscope is Made of...

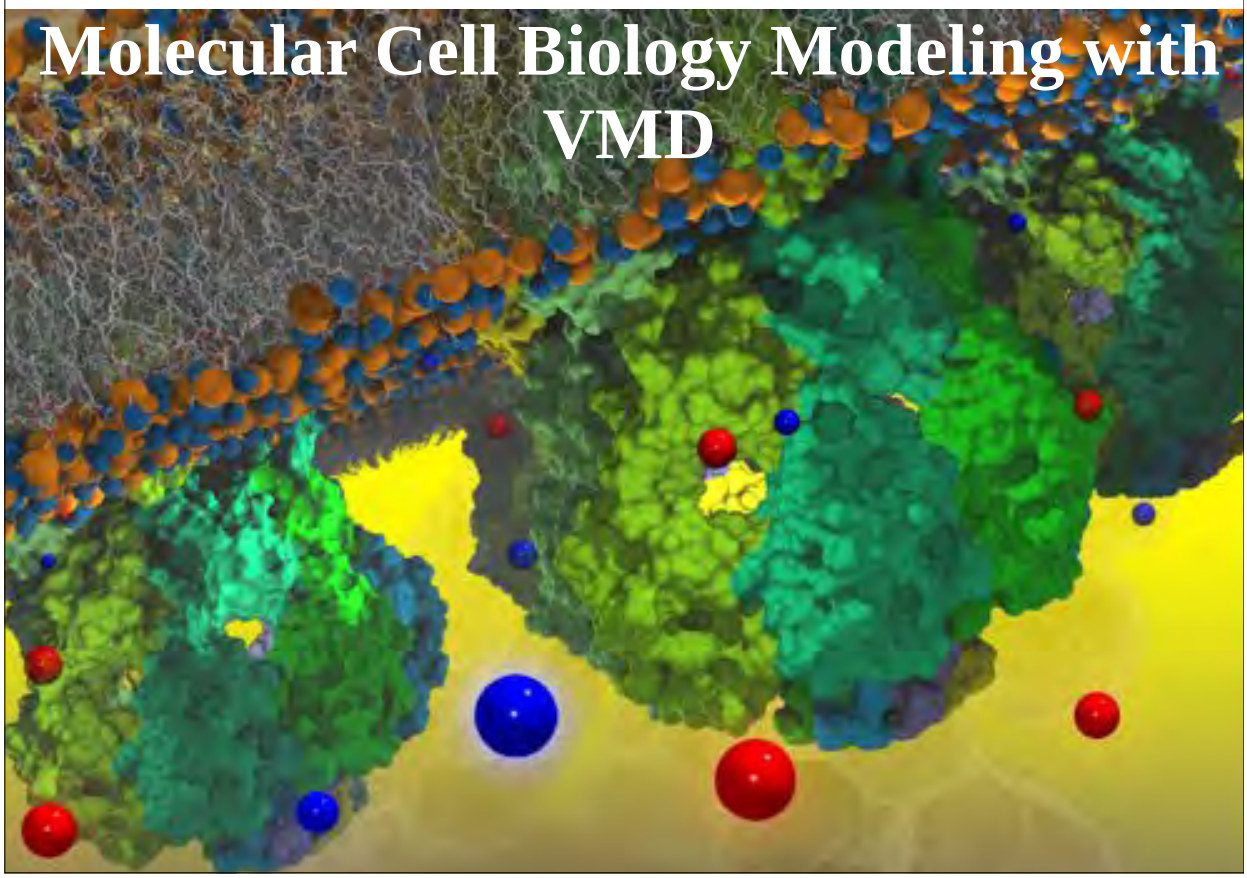
and of...



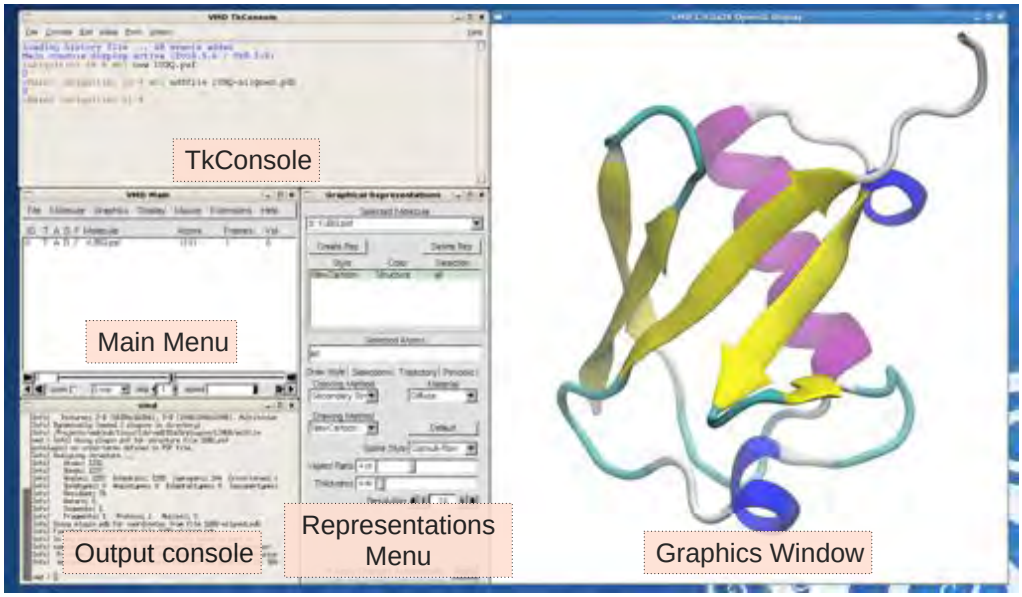
VMD – A Tool to Think Wide



Molecular Cell Biology Modeling with VMD



Molecular Graphics with VMD



typical VMD session

An Example: Ubiquitin and the Proteosome

Ubiquitin: a small protein of 76 amino acids

Present in all eukaryotes, and highly conserved

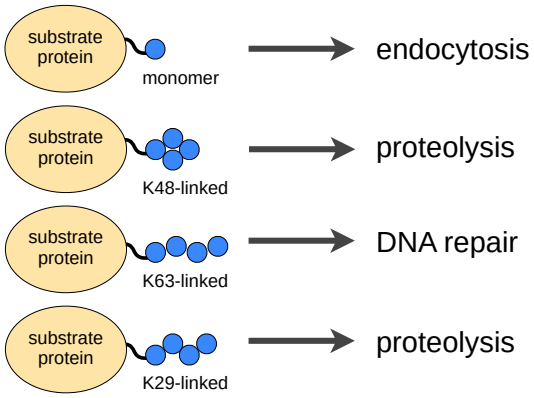
Regulates key cellular processes such as cell division, gene expression, cell trafficking, and protein degradation

Deficiency in ubiquitin expression can lead to neurodegenerative disorders

Tags misfolded proteins to be degraded in the proteosome ("kiss of death" protein)

Ubiquitin Chains

Ubiquitins monomers attach to others to make a poly-ubiquitin chain



7 conserved lysine residues can form differently shaped chains depending on which lysine is used to connect the monomers

A Glycine at C-terminal attaches to a lysine on the protein by an isopeptide bond

A chain of at least four ubiquitins is needed to be recognized by the proteosome for protein degradation

VMD Session 1:
ubiquitin

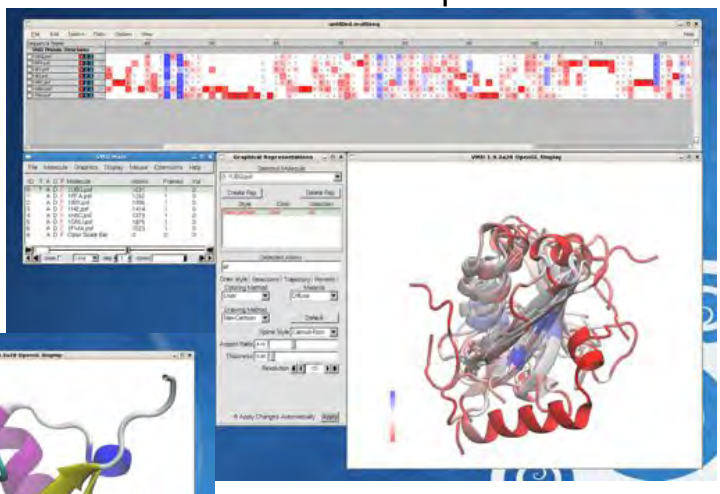
Bioinformatics

Link sequence to structure

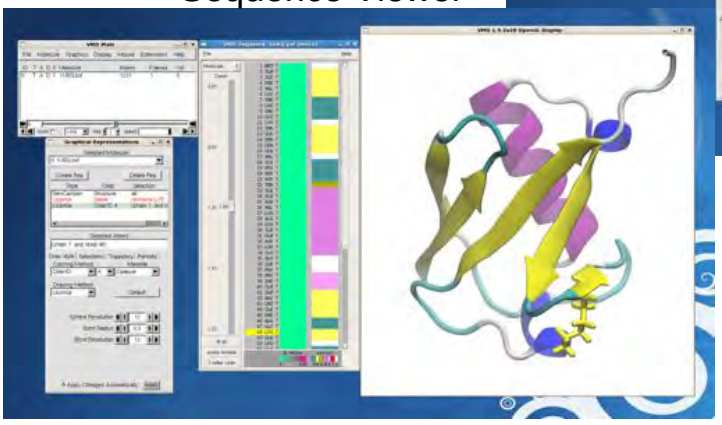
Multiple sequence/
structure alignments

Phylogenetic trees

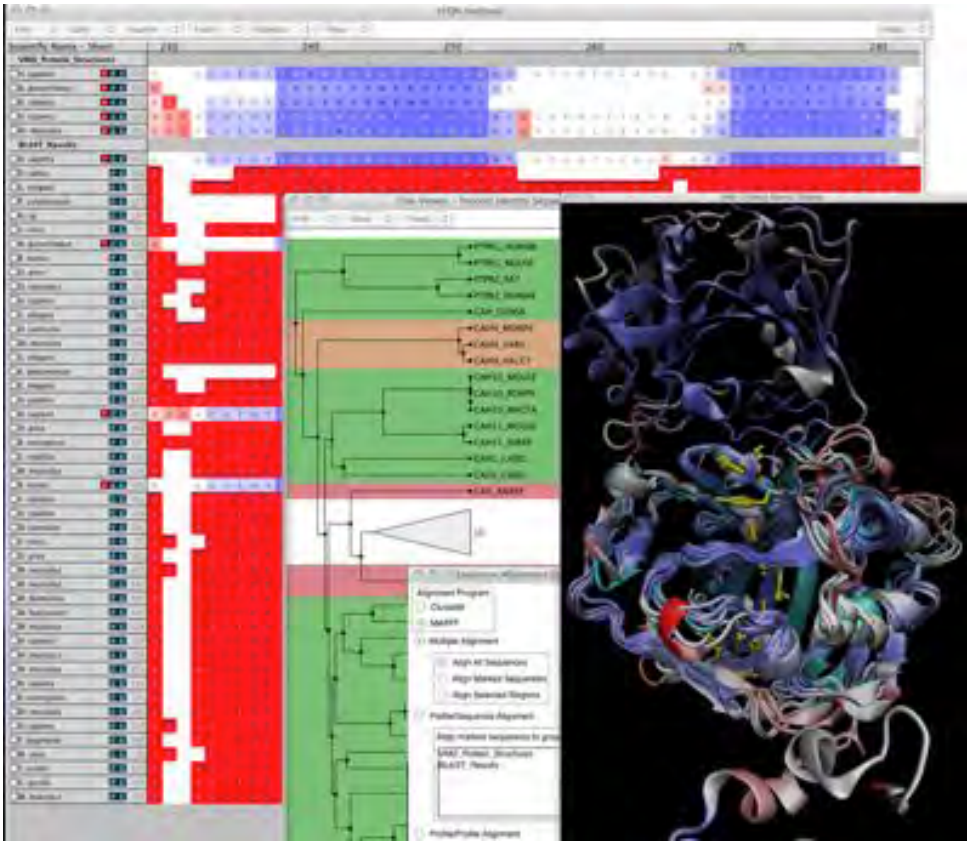
MultiSeq



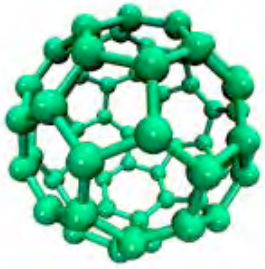
Sequence Viewer



Structure, Sequence and Phylogenetic Analysis with VMD



VMD Handles Volumetric Data



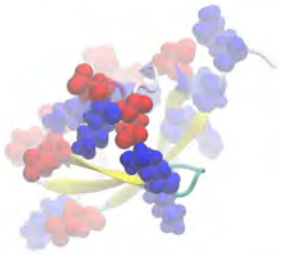
electron density
from QM/MM
calculation
Martinez, Stanford

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

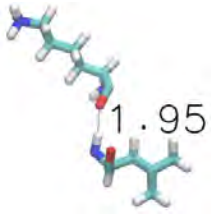
cryo-EM density

VMD Deternines Physical Properties

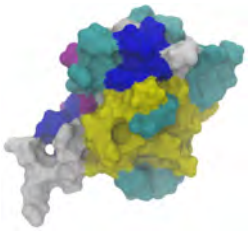
hydrogen bonds



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

Example: protein folding

lambda repressor (2012)
80 amino acids, 100 μs

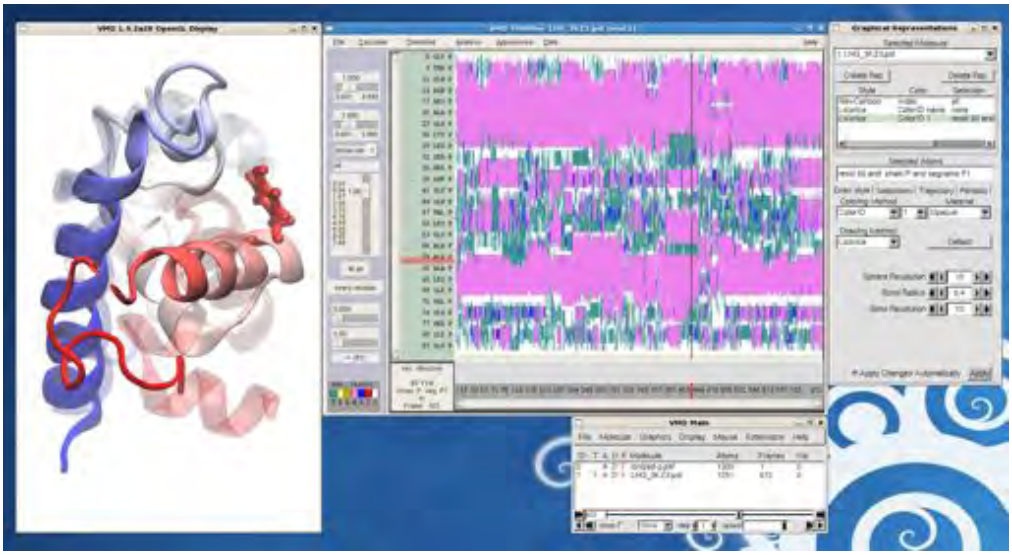
Journal of Physical Chemistry Letters, 3:1117-1123, 2012.
Proceedings of the National Academy of Sciences, USA, In press, 2013.

VMD Plugins

Featured example: Timeline

plugin to analyze MD trajectories for events

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



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

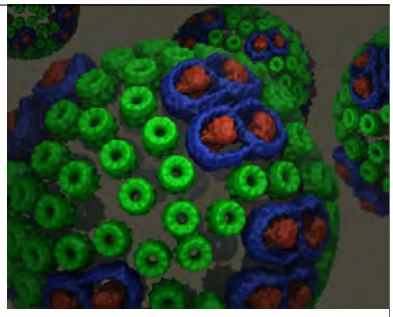
Other Plugins

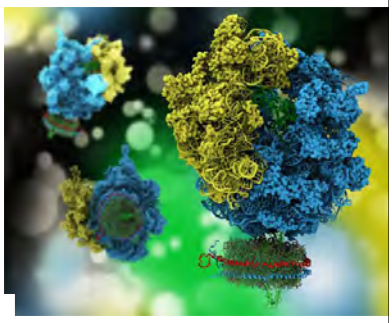
- AtomEdit
- DemoMaster
- ExecTool
- Hesstrans
- Optimization
- PBCTools
- RESPTool
- RNAview
- SignalProc
- TkCon

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

VMD the Artist

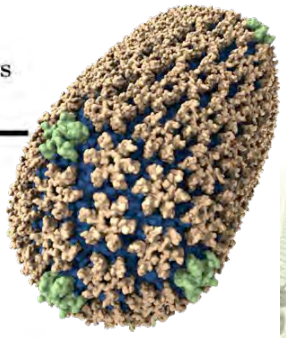
Publication-quality images and movies

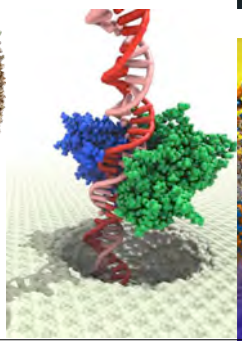


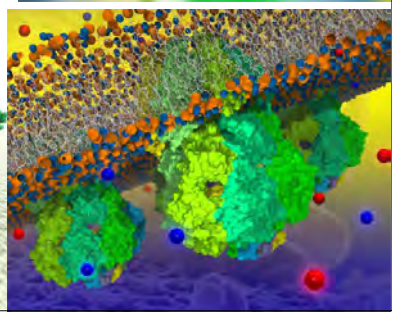


University of Illinois at Urbana-Champaign
Beckman Institute for Advanced Science and Technology
Theoretical and Computational Biophysics Group
Computational Biophysics Workshop

VMD Images and Movies
Tutorial



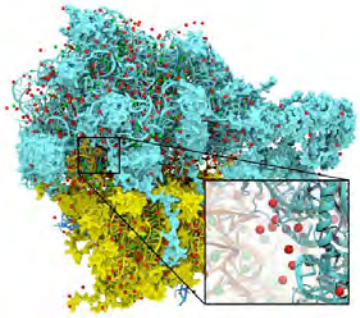




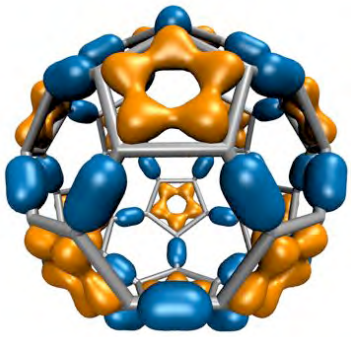
VMD the Artist

Publication-quality images and movies

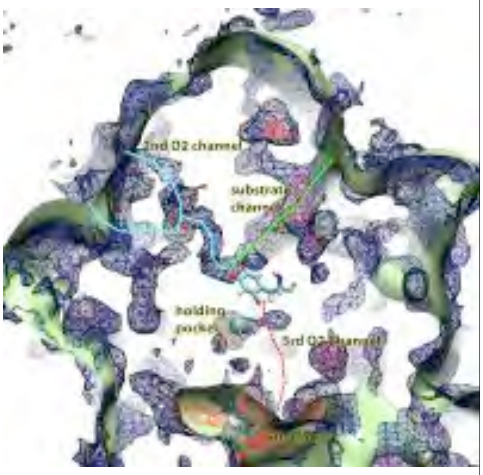
VMD the Compute Engine



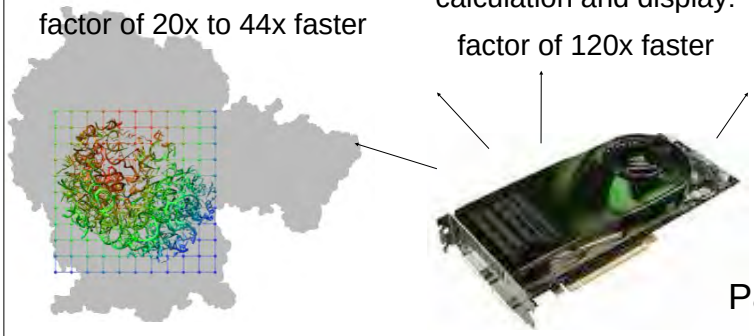
Electrostatic field calculation, ion placement: factor of 20x to 44x faster



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 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