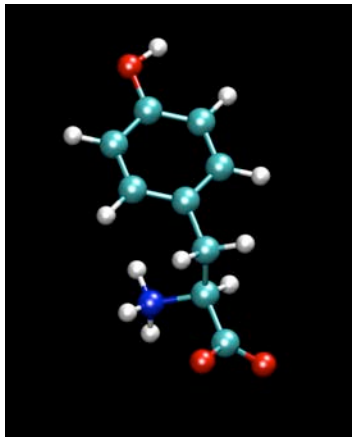
Lecture 1a

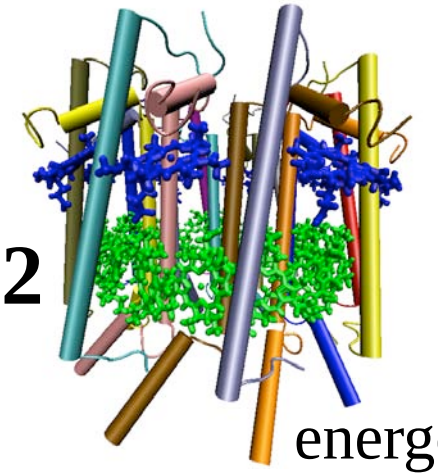
Introduction to Protein Structures - Molecular Graphics Tool



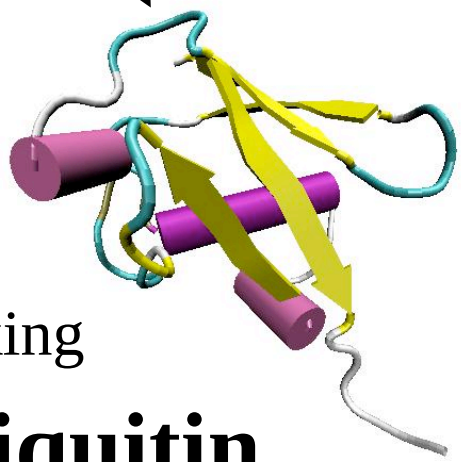
amino acid

tyrosine

LH2

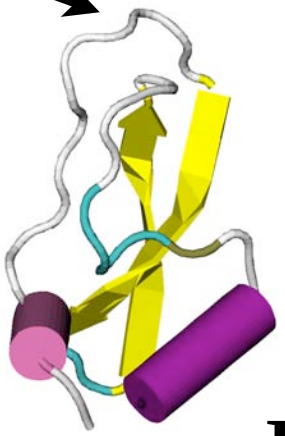


energetics



traficking

Ubiquitin

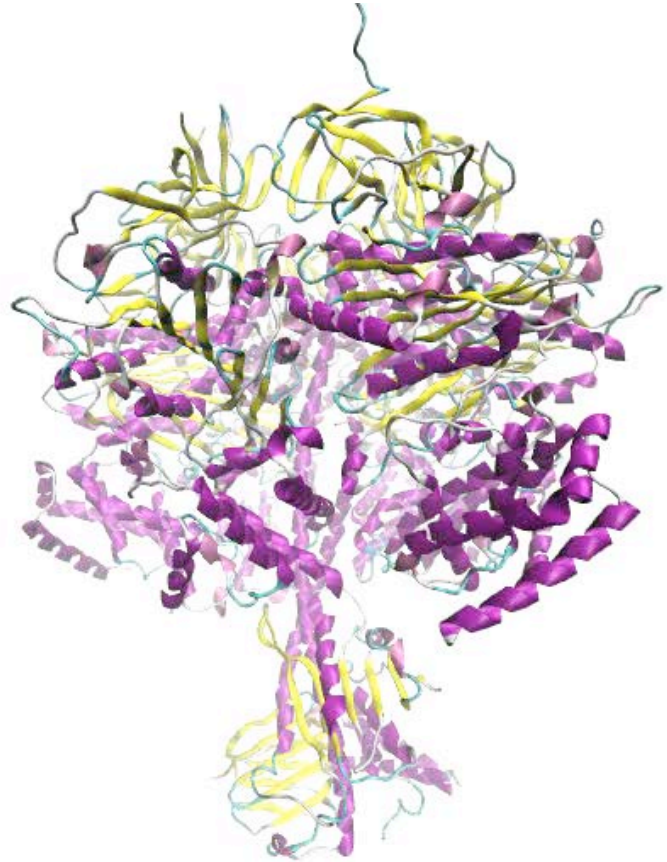


enzymatic control

BPTI

Highlights of the VMD Molecular Graphics Program

- > 120,000 registered users
- Platforms:
  - Unix / Linux
  - Windows
  - MacOS X
- Display of large biomolecules and simulation trajectories
- Sequence browsing and structure highlighting
- Multiple sequence - structure analysis
- User-extensible scripting interfaces for analysis and customization

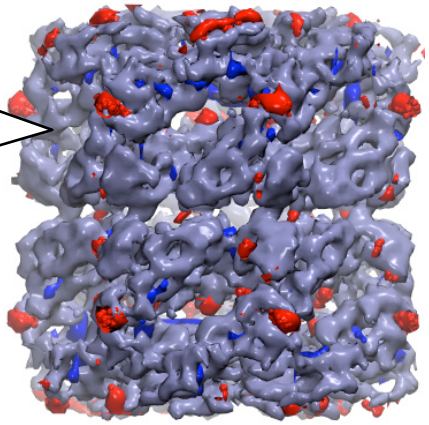


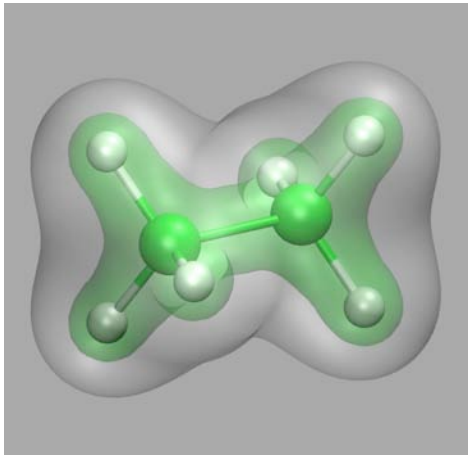
The program is used today more for preparation and analysis of modeling than for graphics

VMD – A Tool to Think

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

23,000 Users

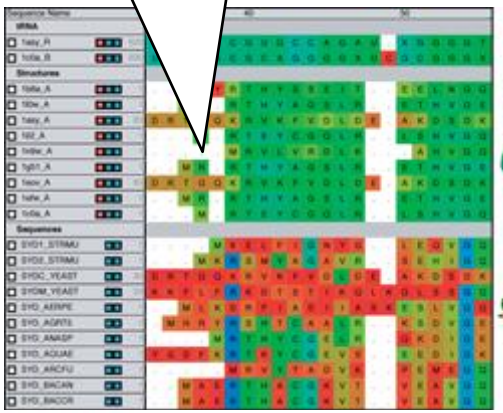


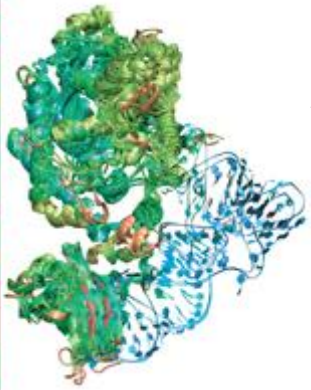


Sequence Data:
Multiple Alignments,
Phylogenetic Trees

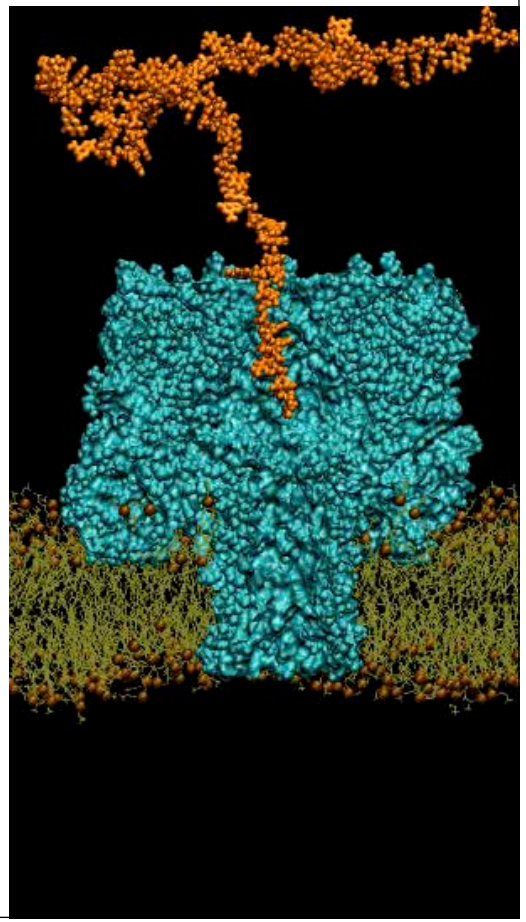
VMD

Annotations





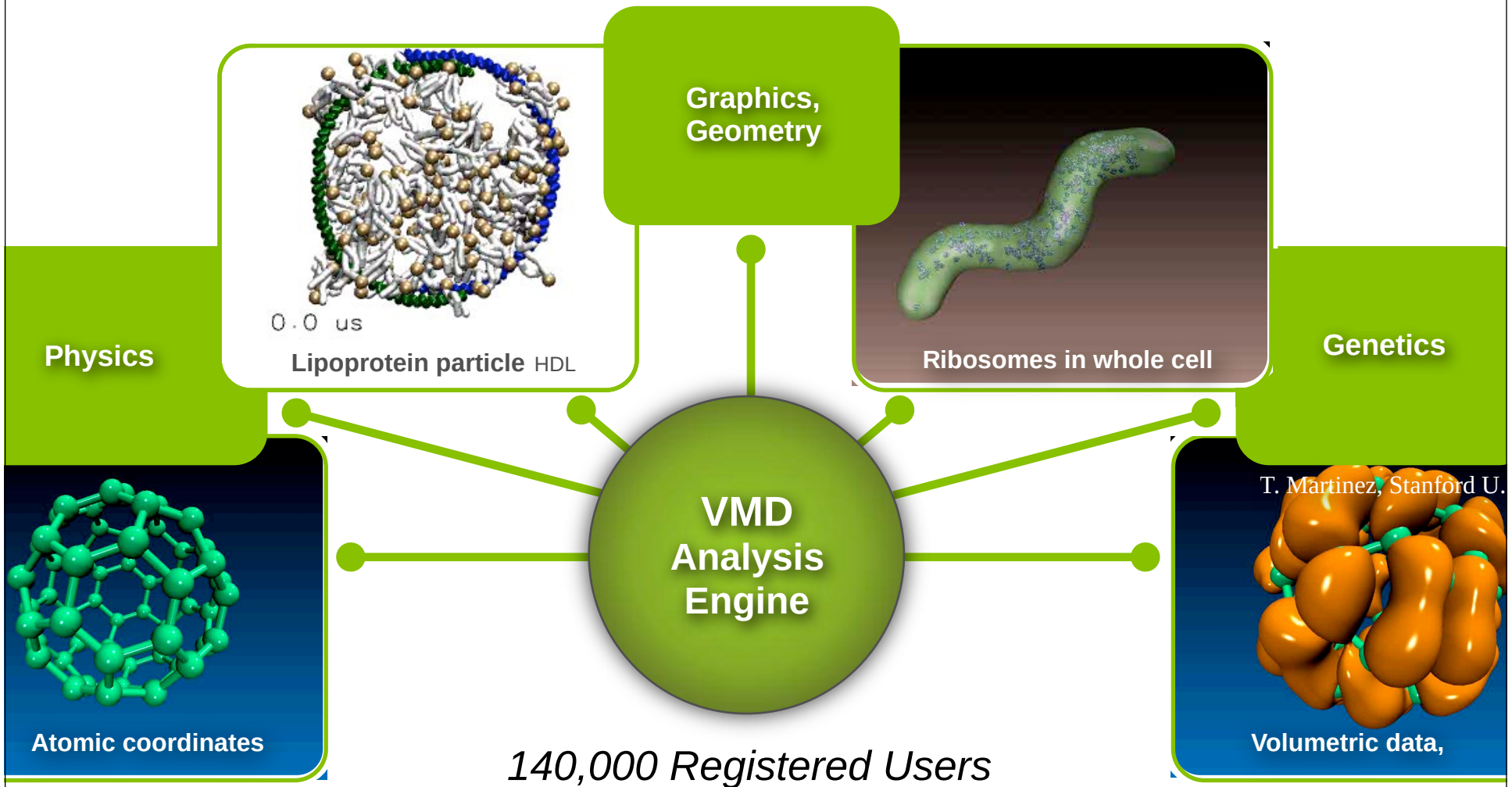
Atomic Data:
Coordinates,
Trajectories,
Energies,
Forces, …



National Center for Research Resources

VMD a “Tool to Think”

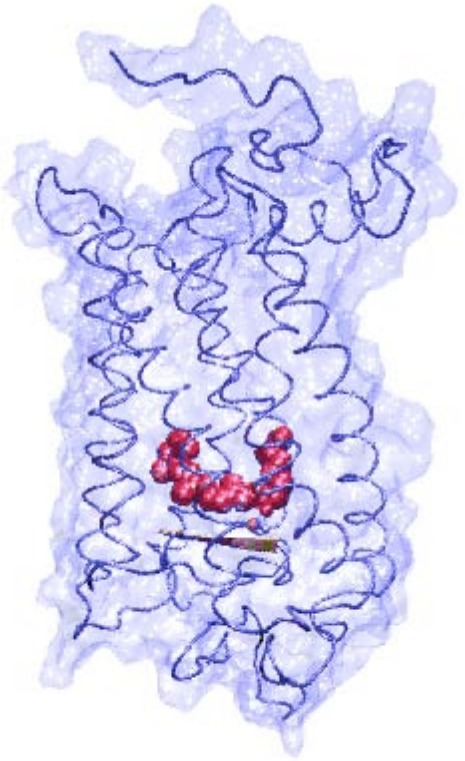
Carl Woese

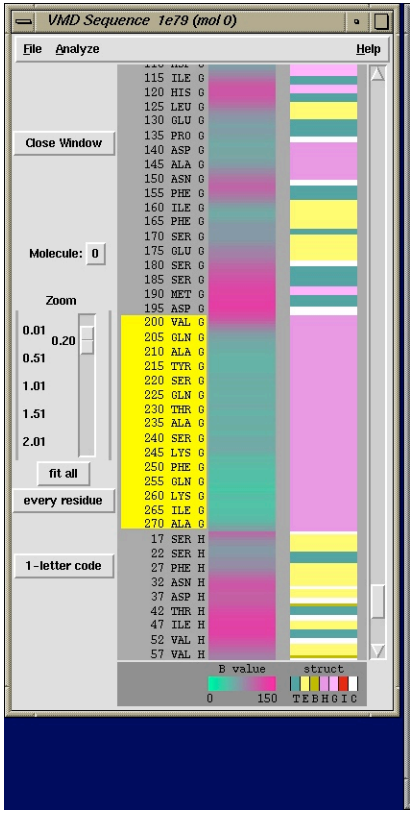


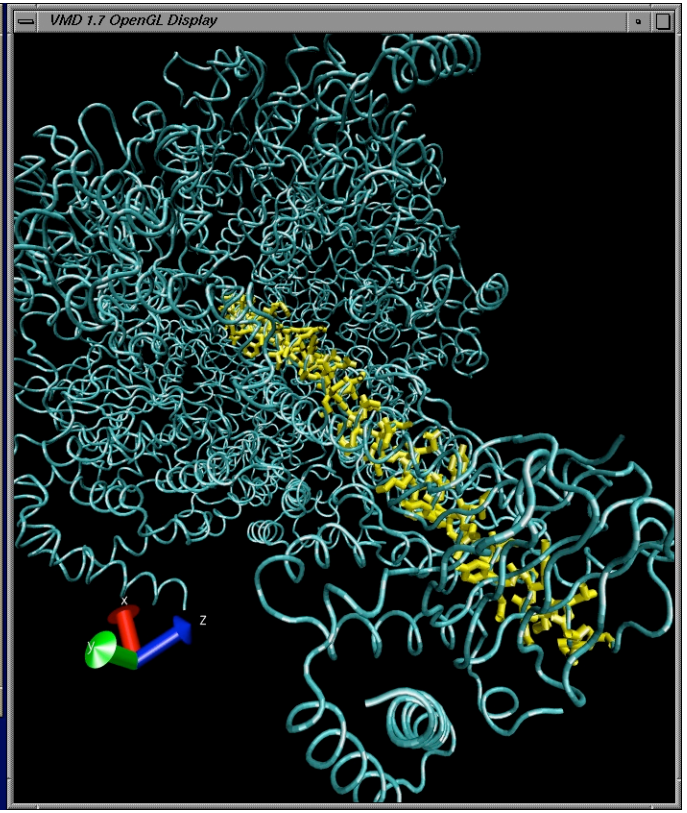
140,000 Registered Users

Molecular Graphics Perspective of Protein Structure and Function

see tutorial at http://www.ks.uiuc.edu/Training/Tutorials/



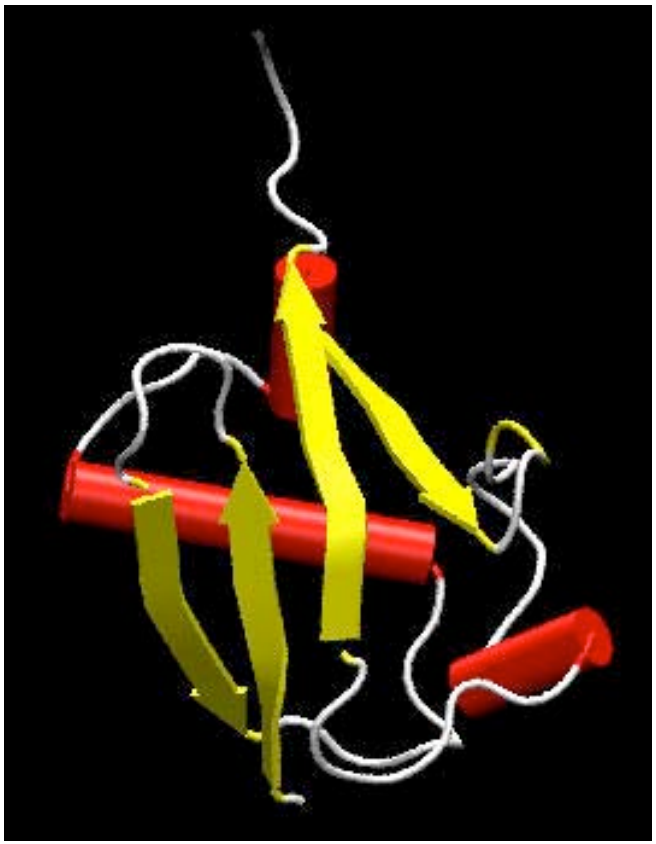




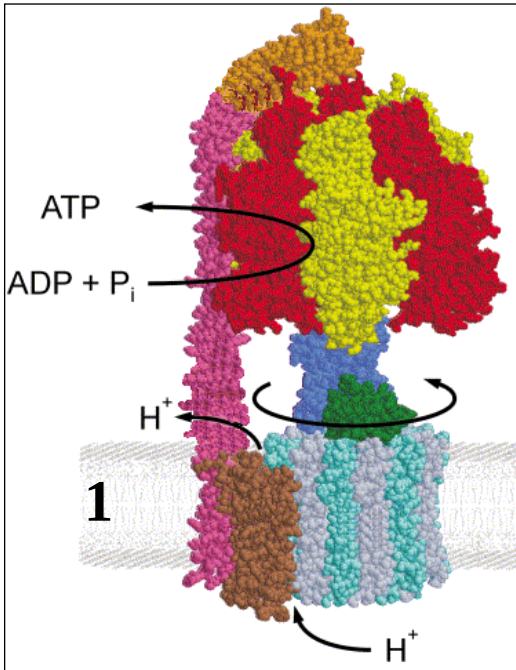
animation sequence structure

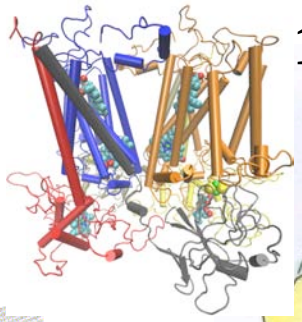
Ubiquitin

- 76 amino acids
- highly conserved
- covalently attaches to proteins and tags them for degradation
- other cell traficking



The proteins that make up the chromatophore of photosynthetic bacteria

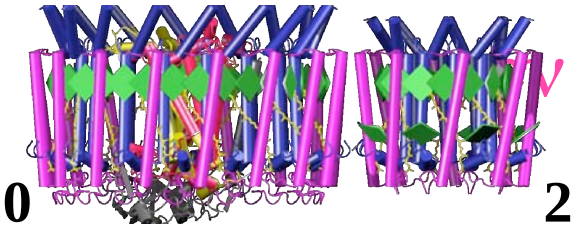




10

1

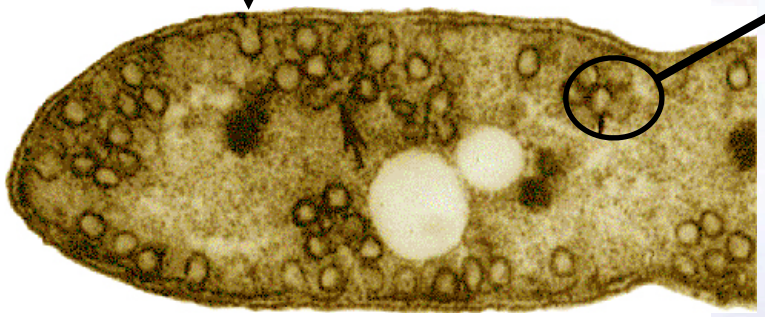
5



20

200

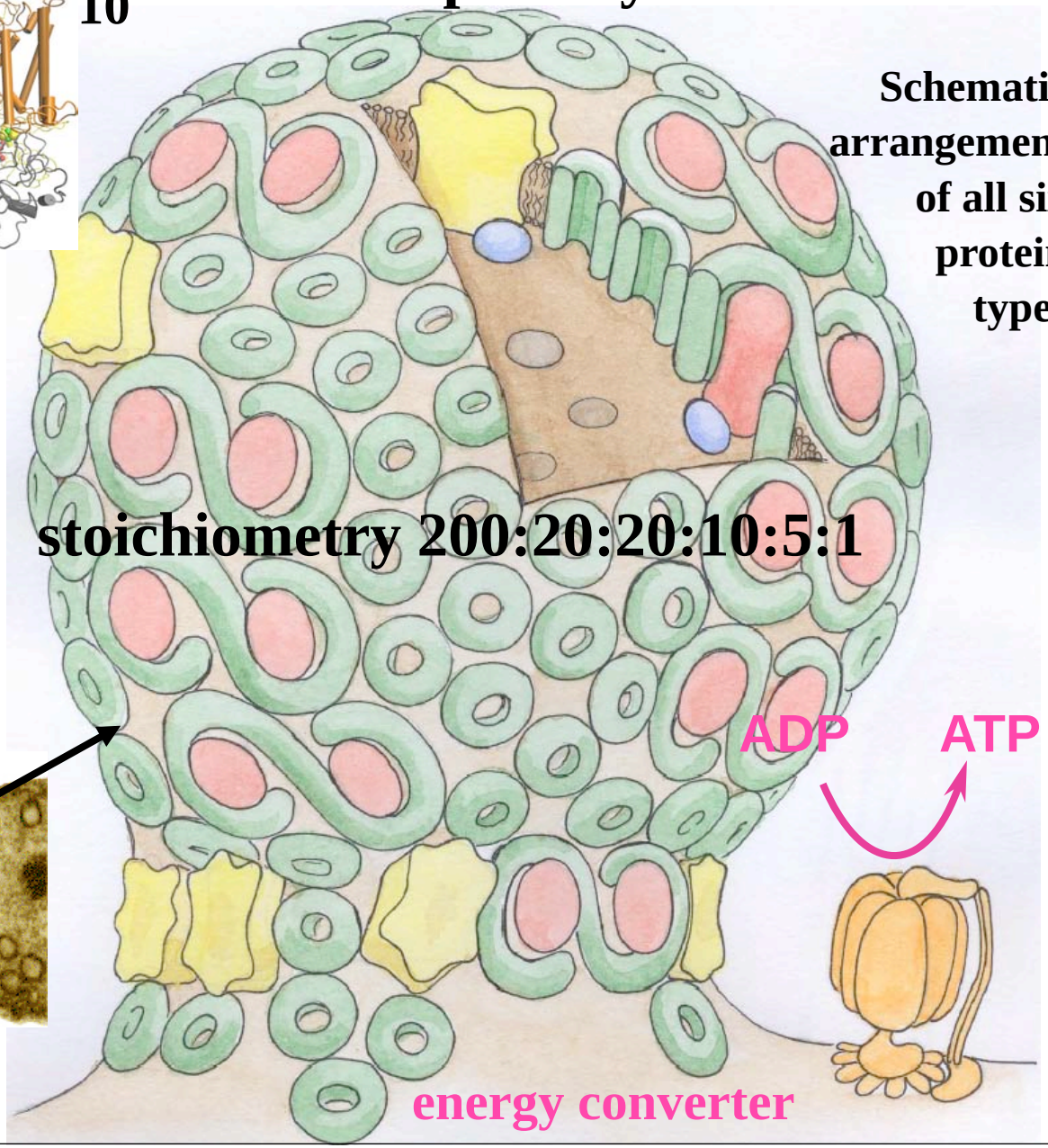
photosynthetic unit



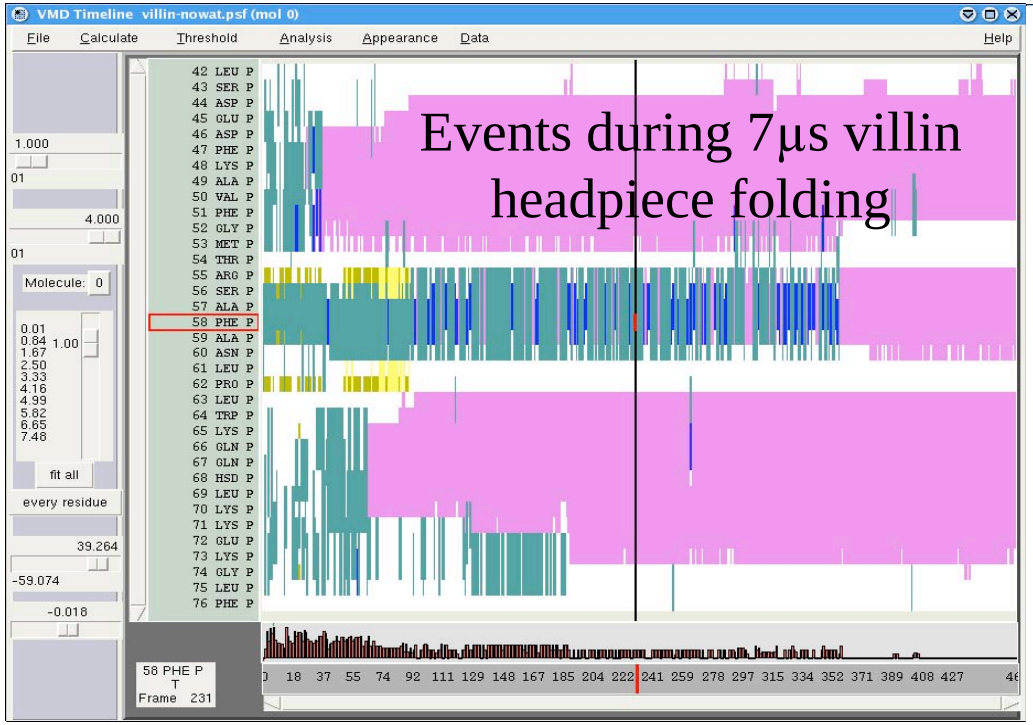
purple bacterium cell

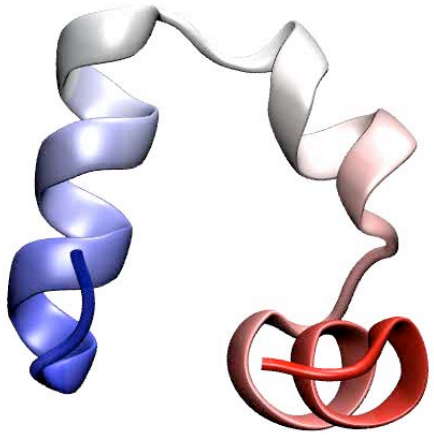
Schematic arrangement of all six protein types

stoichiometry 200:20:20:10:5:1



VMD New Timeline plug-in





Alpha helix Extended beta Isolated bridge 3-10 helix Beta turn None (coil)

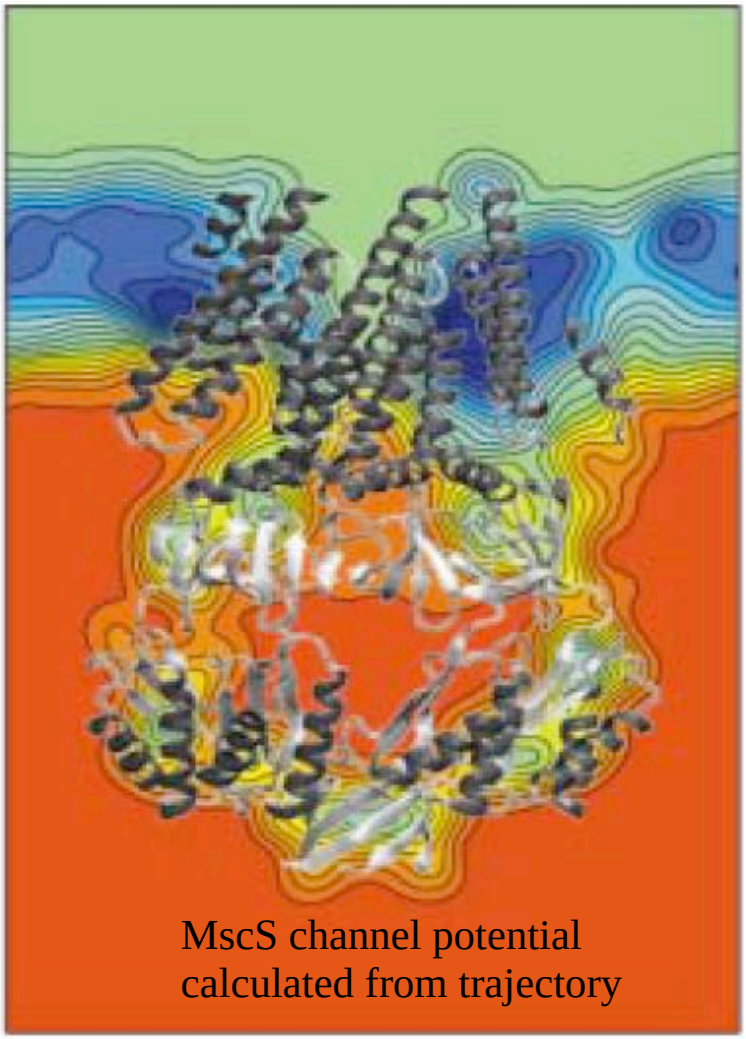
Per-residue secondary structure: villin headpiece folding from a fully denatured state.
7μs simulation; 654 atoms; over 1 million frames to examine

VMD **Timeline plug-in**: graphing and analysis tool to identify events in an MD trajectory
- a single picture shows changing properties across entire structure, entire trajectory.
- explore time vs. attribute (per-residue or per-selection) linked to molecular structure
- many analysis methods available; user-extendable

Electrostatic Potential Maps

New VMD features made possible through GPU computing

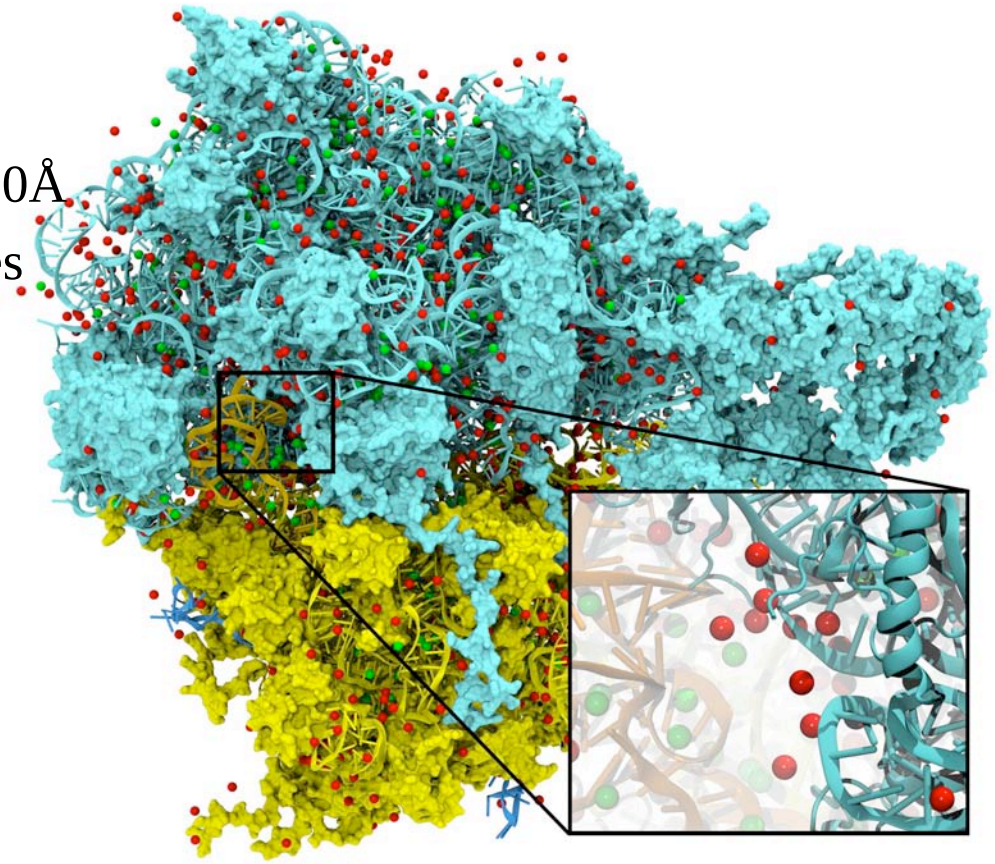
- Electrostatic potentials evaluated on 3-D lattice
- Applications include:
  - Ion placement for structure building
  - Time-averaged potentials for simulation
  - Visualization and analysis



MscS channel potential calculated from trajectory

Time-averaged Electrostatic Potential Calculation for the Ribosome with VMD

- Direct Coulomb summation ~580,000 atoms
  - Lattice spacing 1.0Å, padding 10Å
  - Time-average from 1,000 frames
- 3 GPUs: 49 hours
- 3 CPUs: 0.23 years (est.)

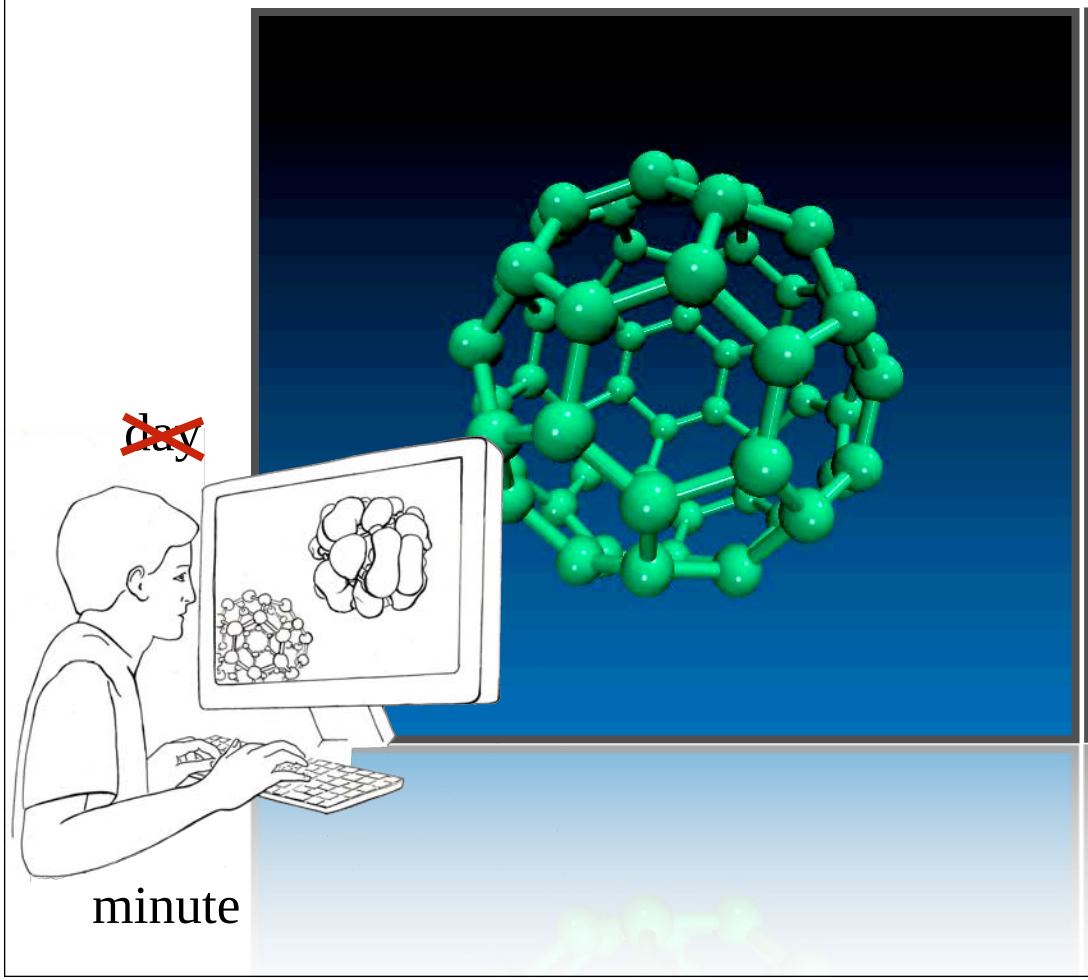


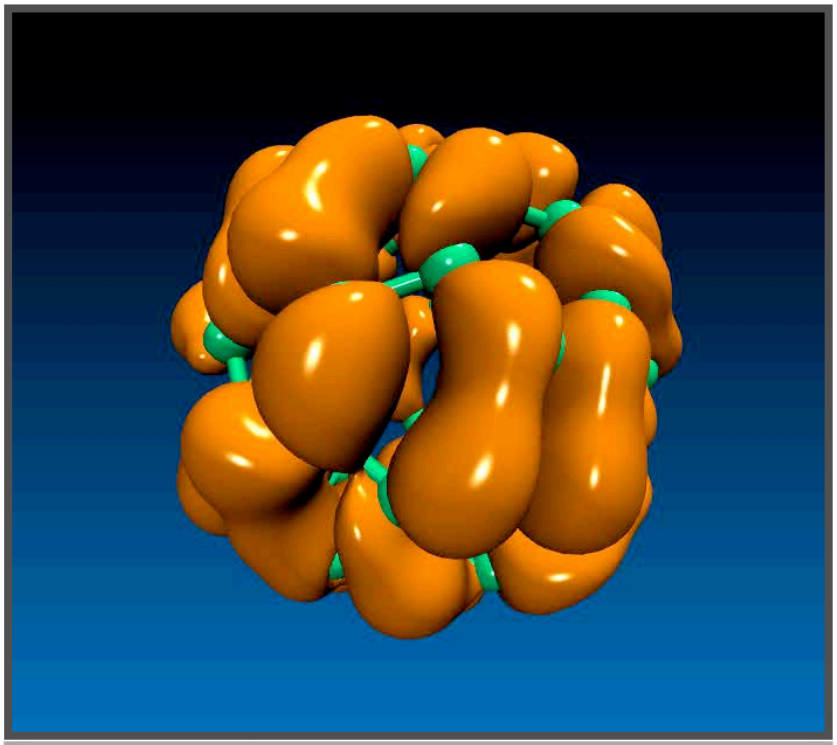
This was one of our early results, using the multi-GPU direct Coulomb summation algorithm, showing the benefit it gave at the time. Now that we have MSM (multilevel summation) we would get much faster performance since it is a linear-time algorithm, but we haven't yet re-run these tests using MSM.

Stone et al. (2007) *J Comp Chem* 28:2618-2640

Quantum Chemistry Visualization

Rendering of electron “clouds” achieved on GPUs as quickly as you see this movie! CPUs: One working day!





Simulation: Terachem Interactive Visualization: VMD
Courtesy T. Martinez, Stanford

Acknowledgements

VMD team

J. Stone (leader)
D. Hardy
B. Isralewitz
J. Saam
K. Vandivoort
R. Brunner

Funding: NIH, NSF

National Center for Research Resources

DOE - Incite