Visualization of Petascale Molecular Dynamics Simulations

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

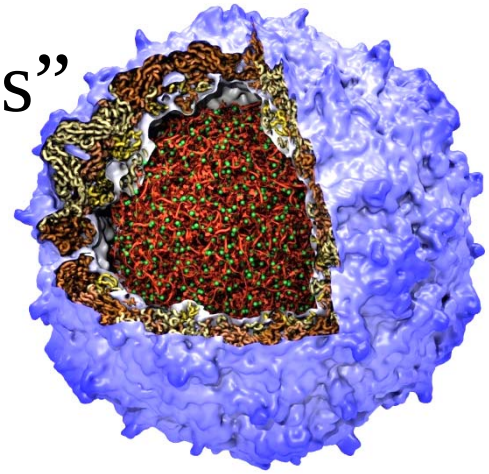
Imaging at Illinois:

Computational Imaging and Visualization

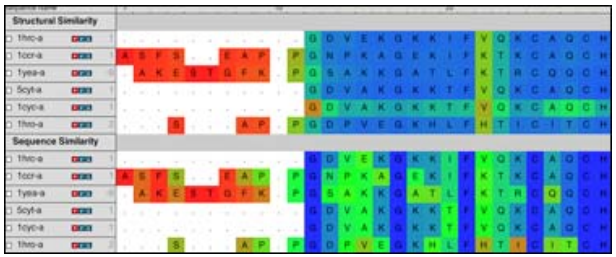
Beckman Institute, University of Illinois, June 1, 2012

VMD – “Visual Molecular Dynamics”

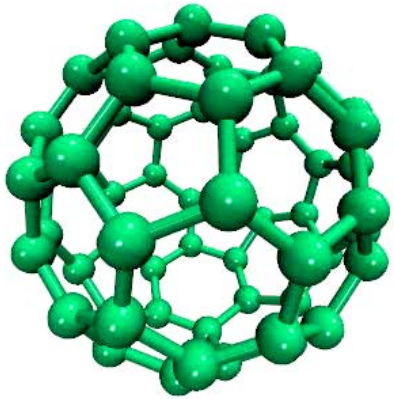
- Visualization and analysis of:
  - molecular dynamics simulations
  - quantum chemistry calculations
  - particle systems and whole cells
  - sequence data
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



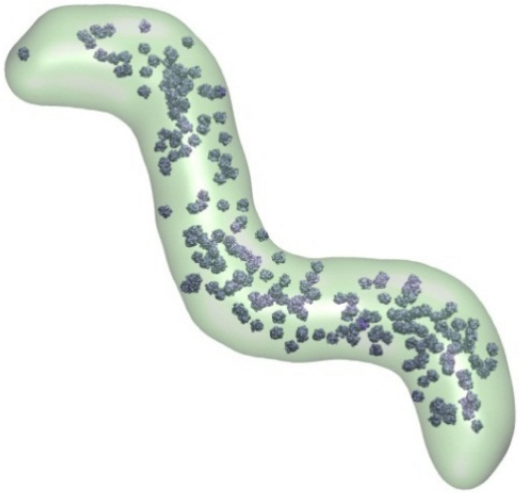
Poliovirus



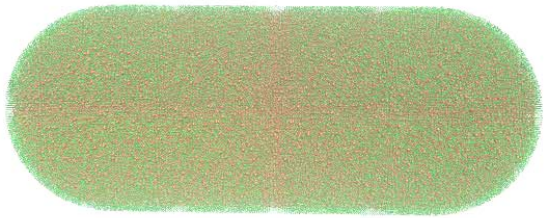
Ribosome Sequences



Electrons in
Vibrating Buckyball



Cellular Tomography,
Cryo-electron Microscopy

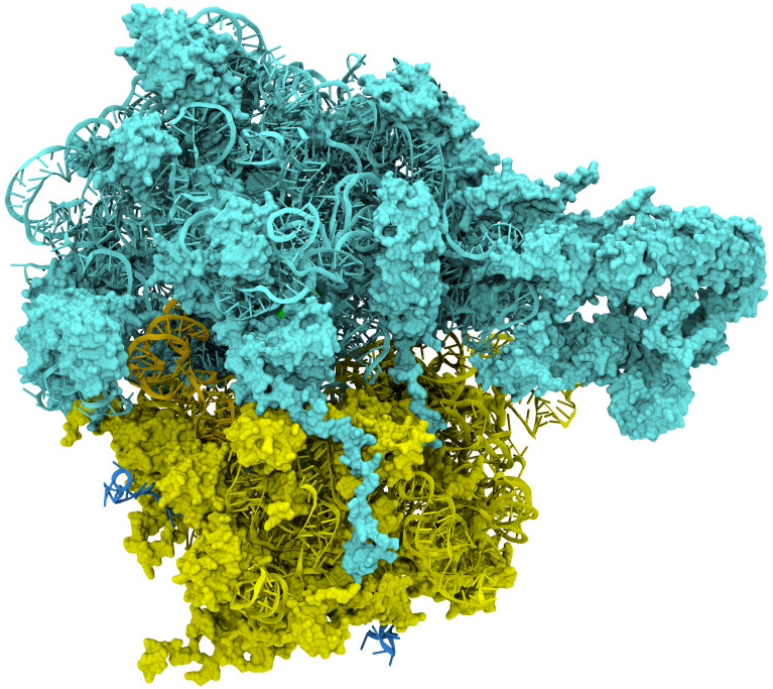


Whole Cell Simulations

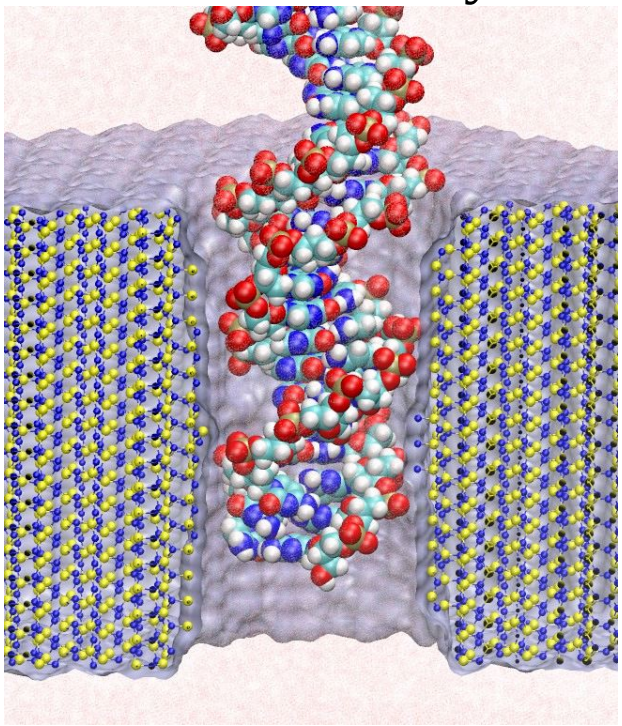
Goal: A Computational Microscope

- Study the molecular machines in living cells

Ribosome: synthesizes proteins from genetic information, target for antibiotics



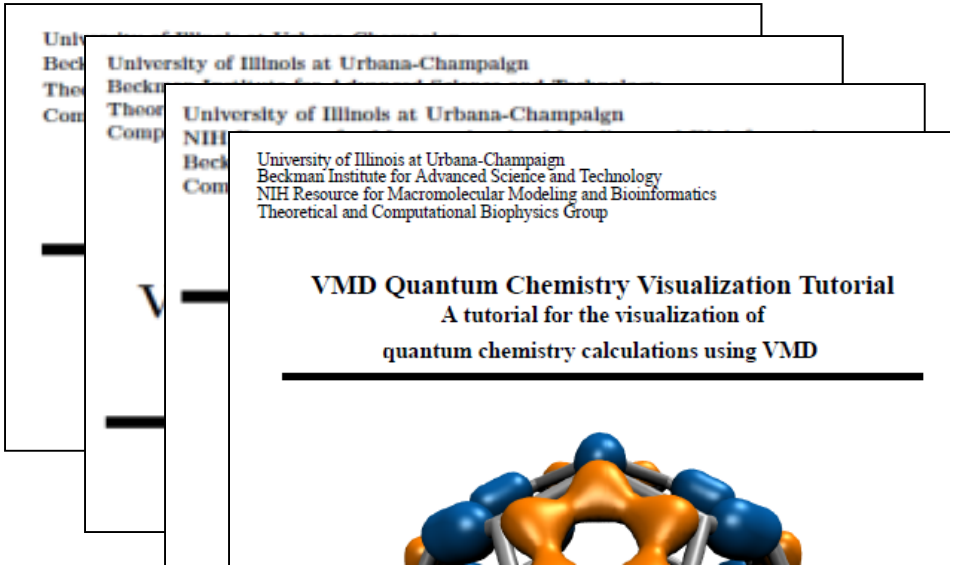
Silicon nanopore: bionanodevice for sequencing DNA efficiently



Meeting the Diverse Needs of the Molecular Modeling Community

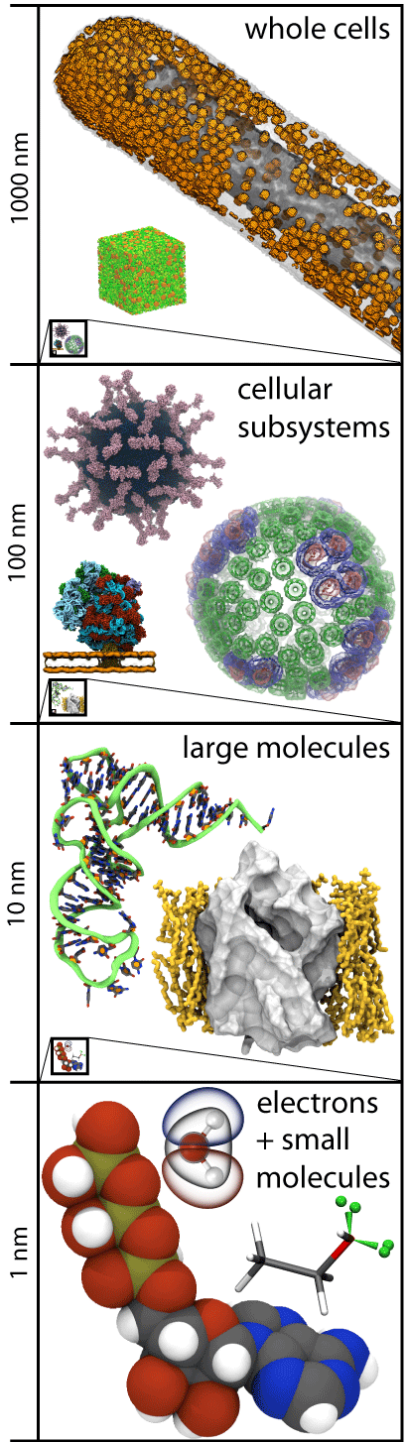
- Over 212,000 registered users
  - 18% (39,000) are NIH-funded
  - Over 49,000 have downloaded multiple VMD releases
- Over 6,600 citations
- User community runs VMD on:
  - MacOS X, Unix, Windows operating systems
  - Laptops, desktop workstations
  - Clusters, supercomputers

- VMD user support and service efforts:
  - 20,000 emails, 2007-2011
  - Develop and maintain VMD tutorials and topical mini-tutorials; 11 in total
  - Periodic user surveys



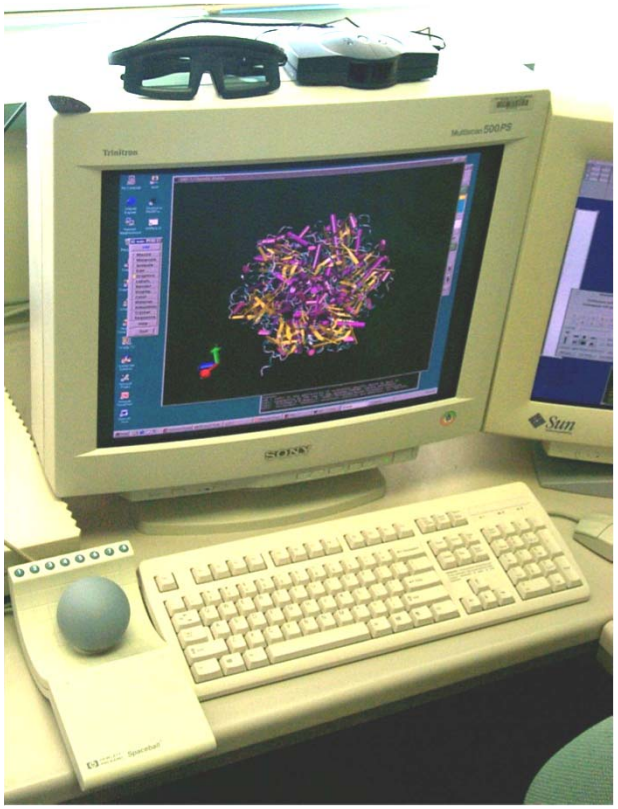
VMD Interoperability – Linked to Today's Key Research Areas

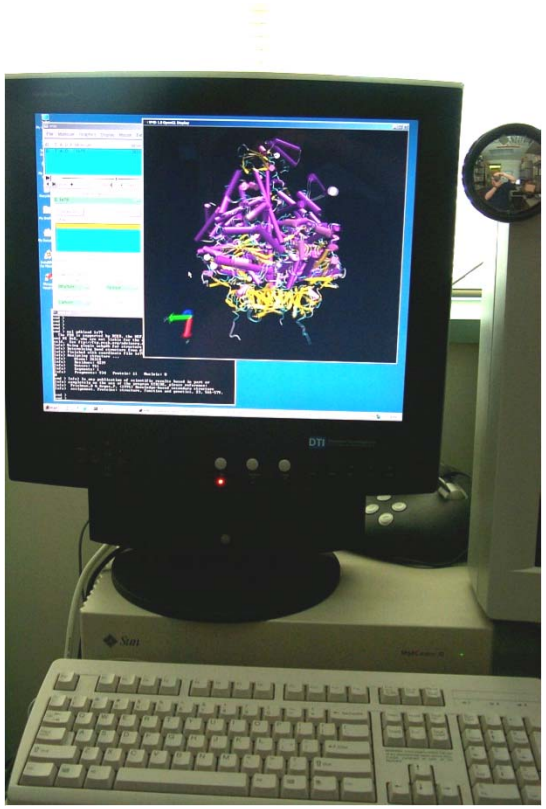
- Unique in its interoperability with a broad range of modeling tools: AMBER, CHARMM, CPMD, DL_POLY, GAMESS, GROMACS, HOOMD, LAMMPS, NAMD, and many more …
- Supports key data types, file formats, and databases, e.g. electron microscopy, quantum chemistry, MD trajectories, sequence alignments, super resolution light microscopy
- Incorporates tools for simulation preparation, visualization, and analysis

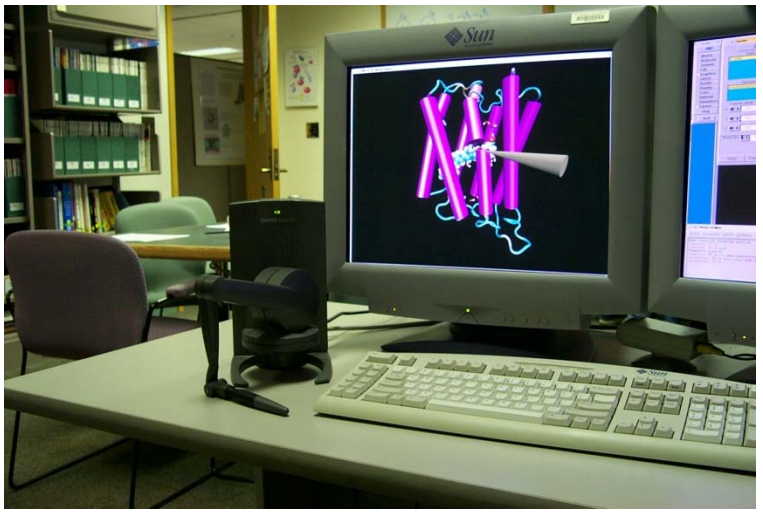


Support for Diverse Display Hardware:

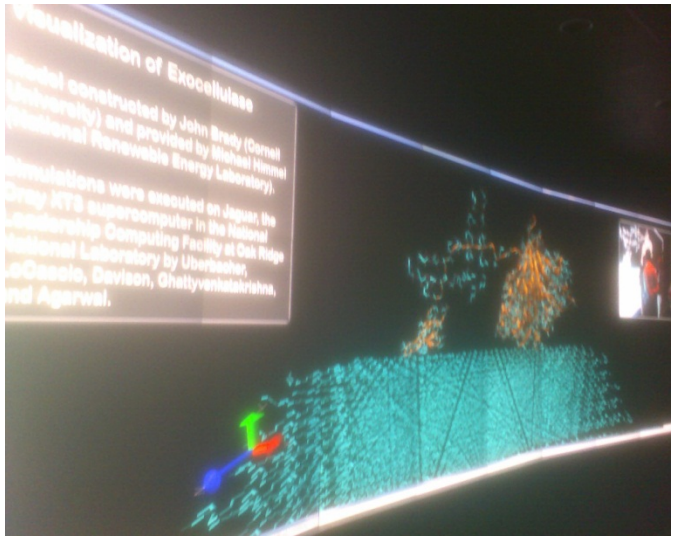
Stereoscopic Displays, 6-DOF Input



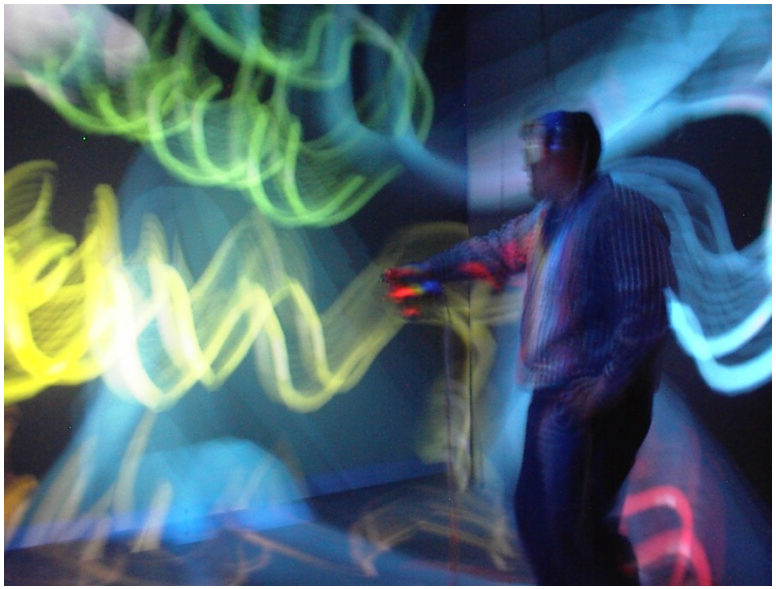


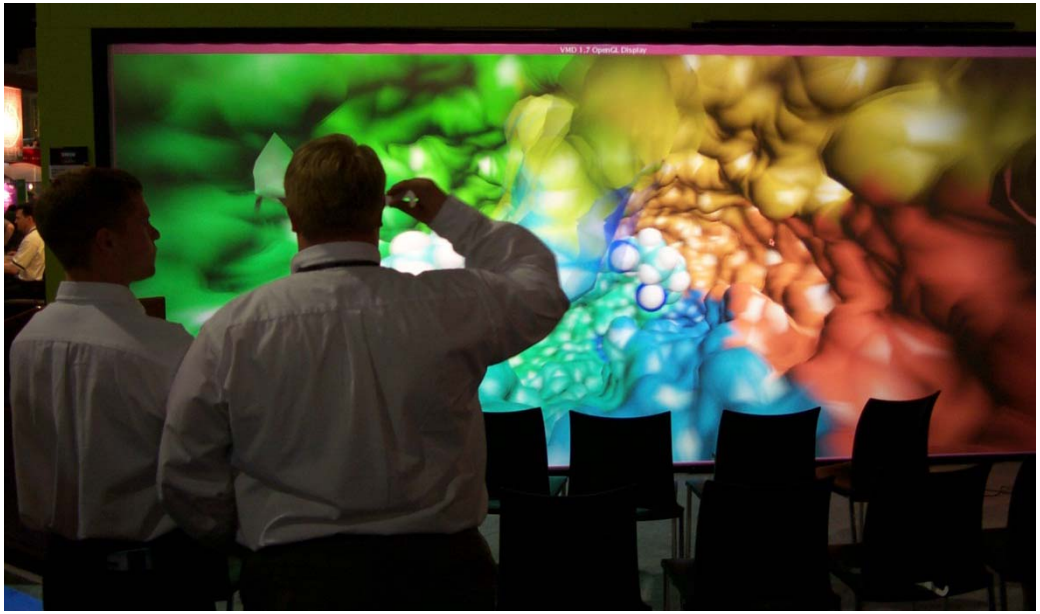


Support for Diverse Display Hardware:
Stereoscopic Projection for Presentations to Large Groups

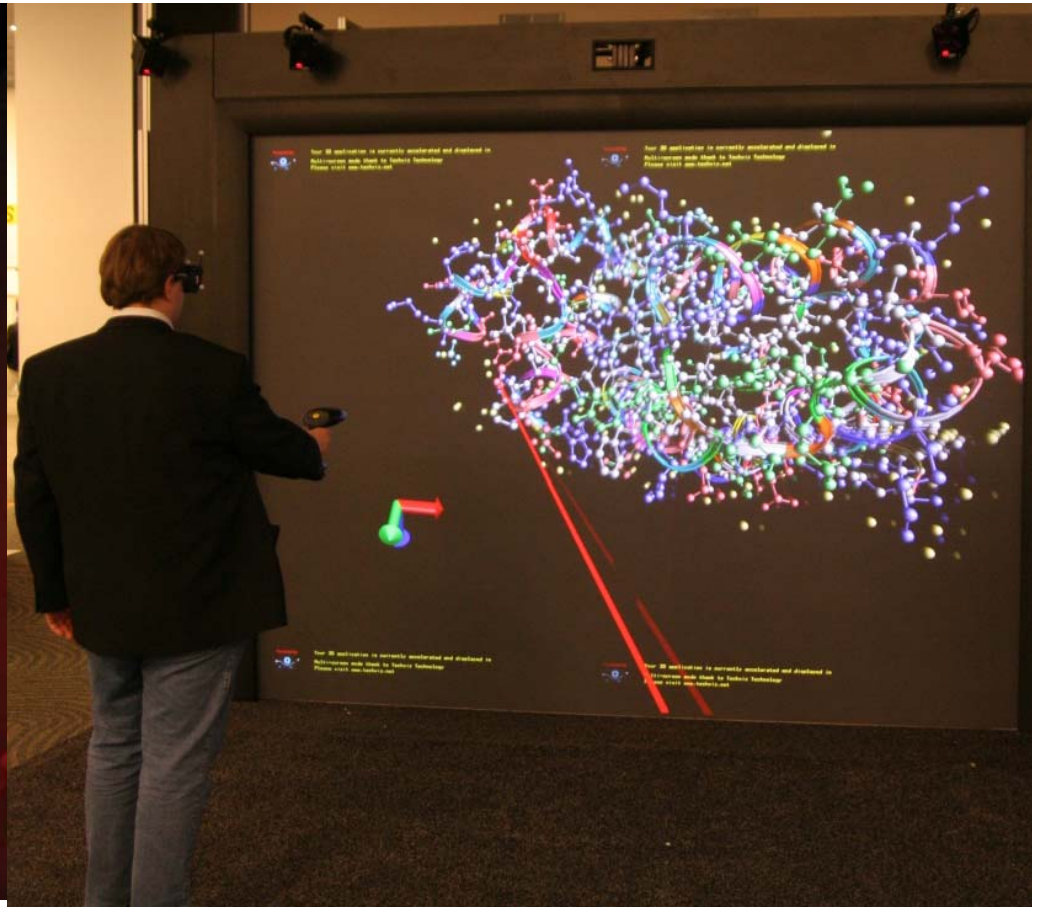


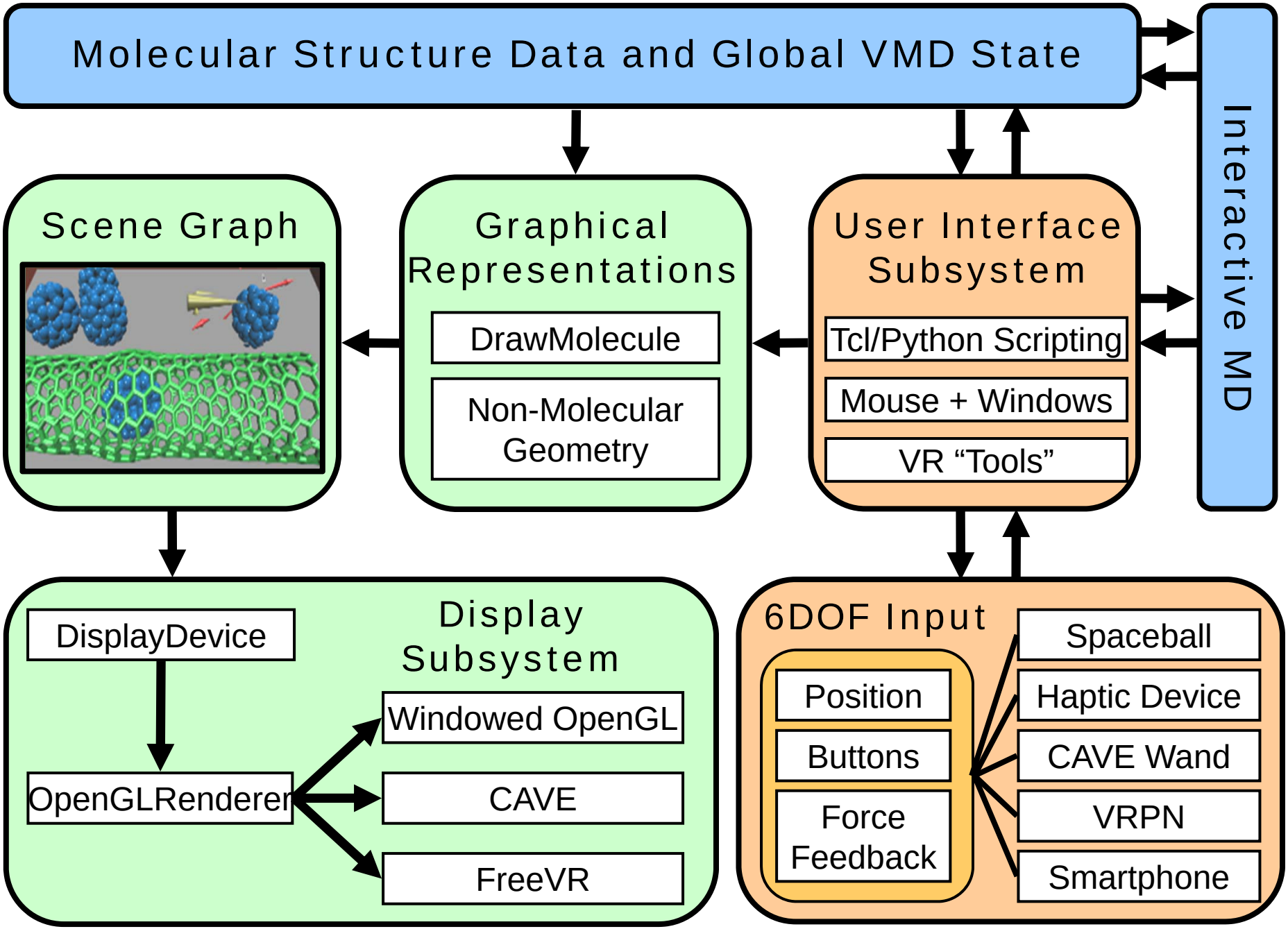
Support for Diverse Display Hardware:
CAVE, 3-D Workbench, Tiled Projector Arrays





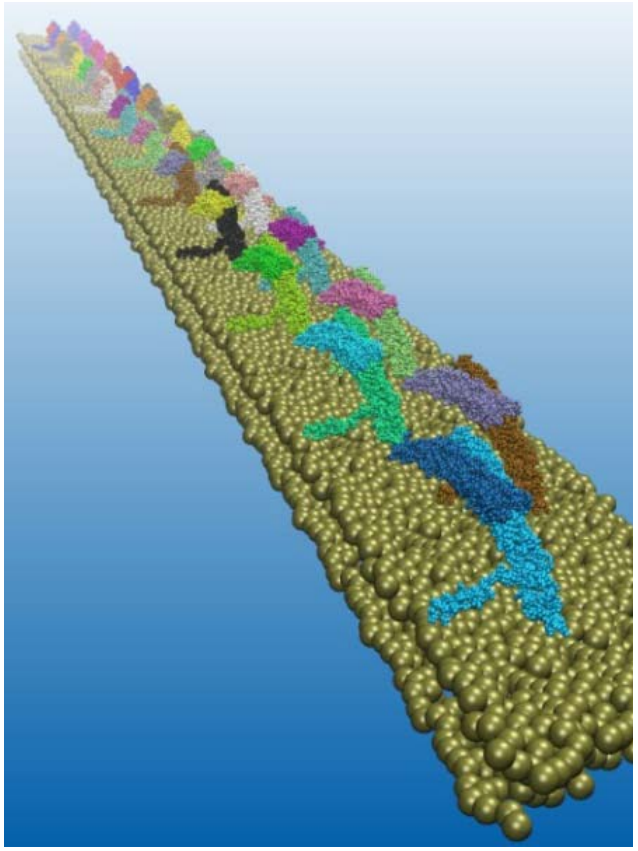
Immersive Visualization in VMD: CAVE, 6-DOF Input w/ Stereo Display




Molecular Structure Data and Global VMD State
Interactive MD
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR “Tools”
DisplayDevice
OpenGLRenderer
Display Subsystem
Windowed OpenGL
CAVE
FreeVR
6DOF Input
Position
Buttons
Force Feedback
Spaceball
Haptic Device
CAVE Wand
VRPN
Smartphone

Challenges for Immersive Visualization of Dynamics of Large Structures

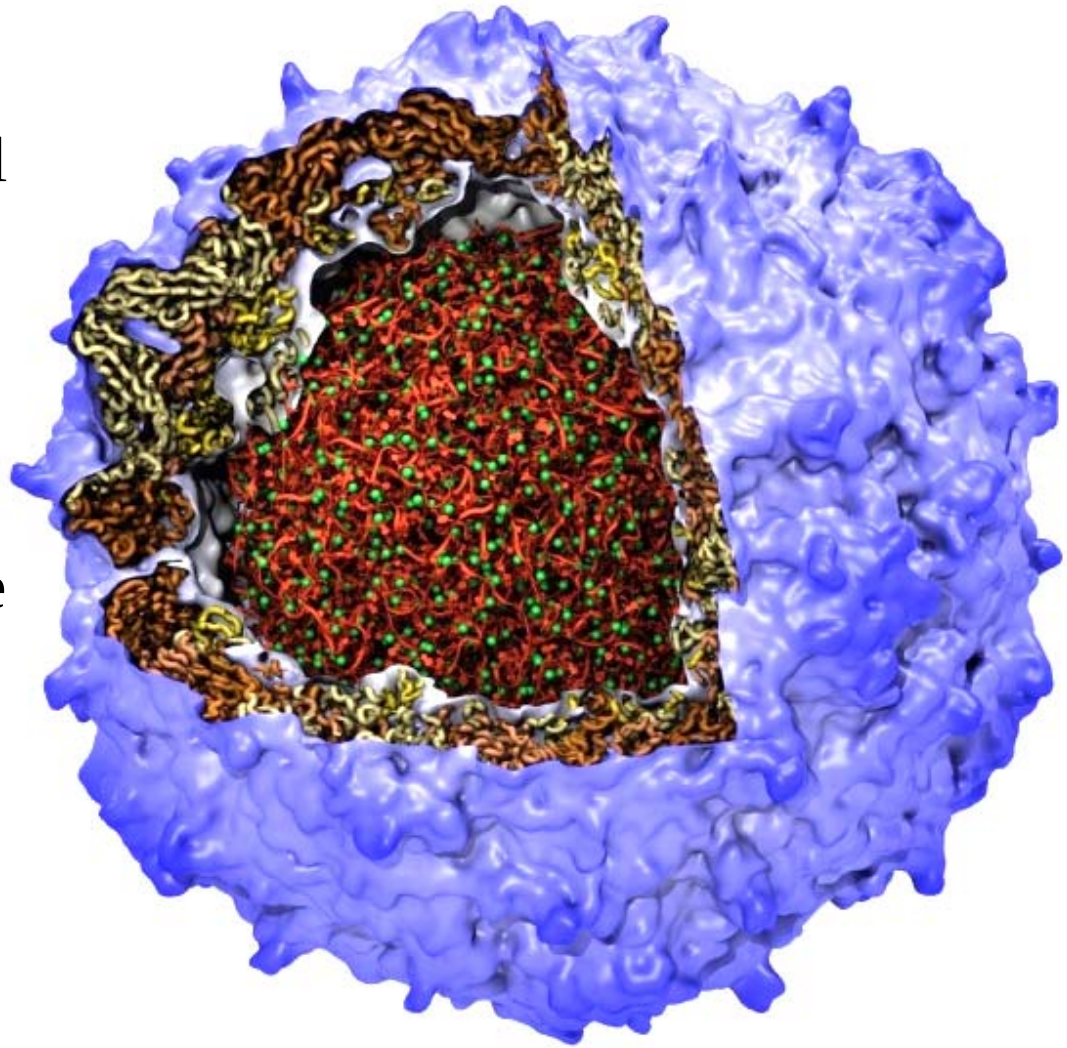
- Graphical representations re-generated for each animated simulation trajectory frame:
  - Dependent on user-defined atom selections
- Although visualizations often focus on interesting regions of substructure, fast display updates require rapid traversal of molecular data structures
- Optimized atom selection traversal:
  - Increased performance of per-frame updates by ~10x for 116M atom BAR case with 200,000 selected atoms
- New GLSL point sprite sphere shader:
  - Reduce host-GPU bandwidth for displayed geometry
  - Over 20x faster than old GLSL spheres drawn using display lists — drawing time is now inconsequential
- Optimized all graphical representation generation routines for large atom counts, sparse selections



116M atom BAR domain test case:
200,000 selected atoms,
stereo trajectory animation 70 FPS,
static scene in stereo 116 FPS

VMD “QuickSurf” Representation

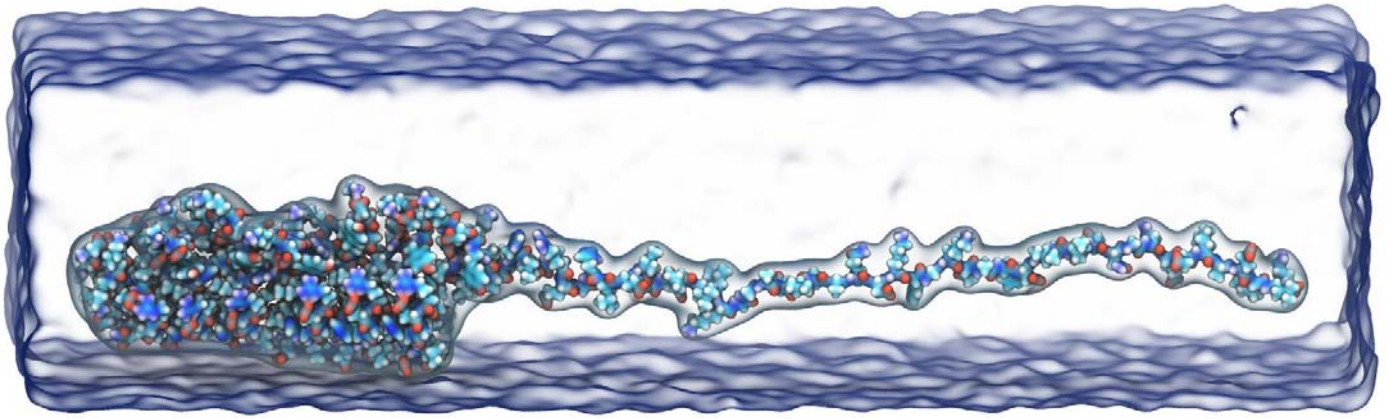
- Large biomolecular complexes are difficult to interpret with atomic detail graphical representations
- Even secondary structure representations become cluttered
- Surface representations are easier to use when greater abstraction is desired, but are computationally costly
- Existing surface display methods incapable of animating dynamics of large structures



Poliovirus

VMD “QuickSurf” Representation

- Displays continuum of structural detail:
  - All-atom models
  - Coarse-grained models
  - Cellular scale models
  - Multi-scale models: All-atom + CG, Brownian + Whole Cell
  - Smoothly variable between full detail, and reduced resolution representations of very large complexes

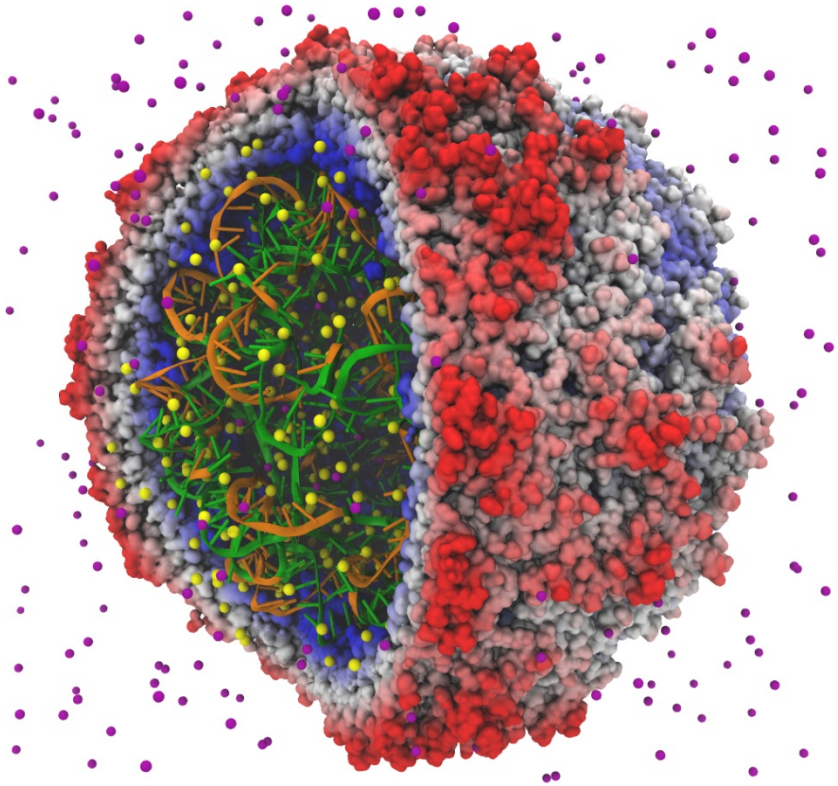


Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.

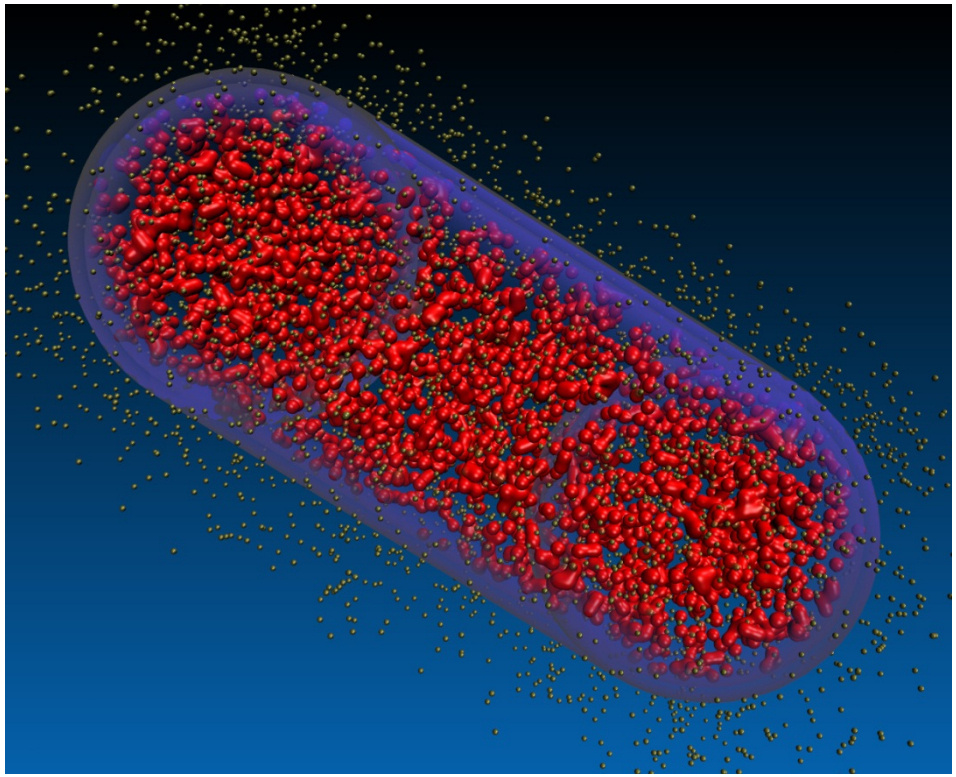
M. Krone, J. Stone, T. Ertl, K. Schulten. *EuroVis* 2012. (*In-press*)

VMD “QuickSurf” Representation

- Uses multi-core CPUs and GPU acceleration to enable **smooth real-time animation** of MD trajectories
- Linear-time algorithm, scales to millions of particles, as limited by memory capacity

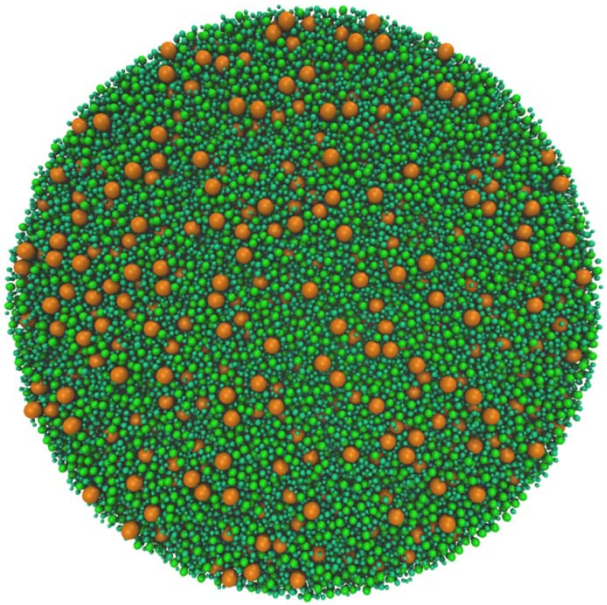


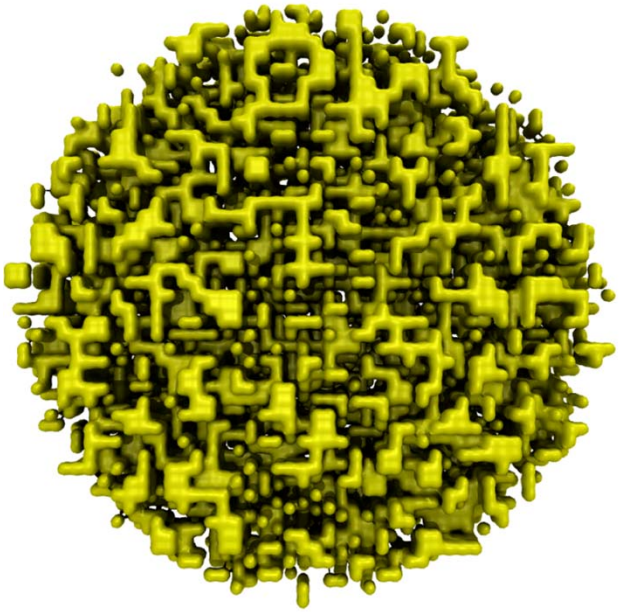
Satellite Tobacco Mosaic Virus

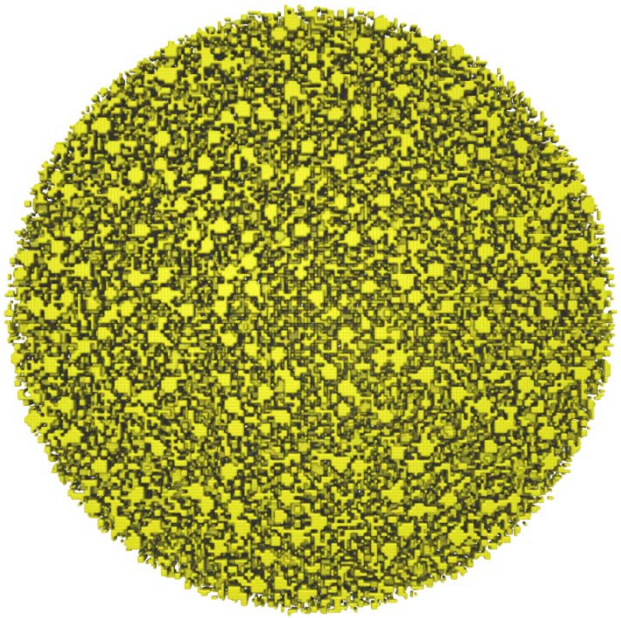


Lattice Cell Simulations

QuickSurf Representation of Lattice Cell Models







Continuous particle based model – often 70 to 300 million particles

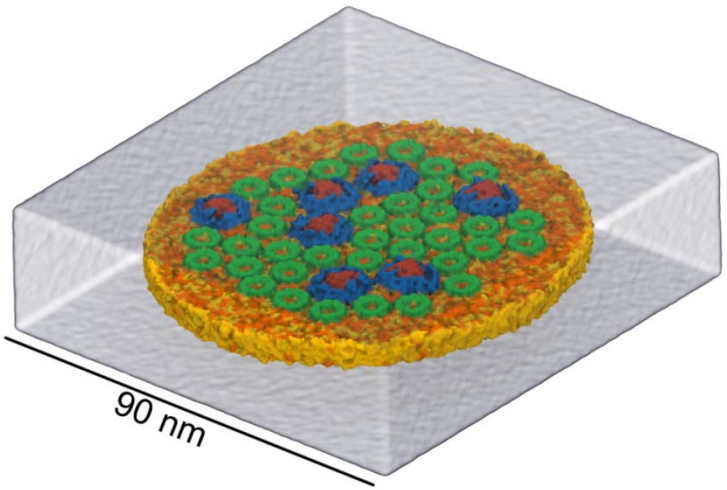
Discretized lattice models derived from continuous model shown in a surface representation

Improved Support for Large Datasets in VMD

- New structure building tools, file formats, and data structures enable VMD to operate efficiently up to 150M atoms
  - Up to 30% more memory efficient
  - Analysis routines optimized for large structures, up to 20x faster for calculations on 100M atom complexes where molecular structure traversal can represent a significant amount of runtime
  - New and revised graphical representations support smooth trajectory animation for multi-million atom complexes; VMD remains interactive even when displaying surface reps for 20M atom membrane patch
- Uses multi-core CPUs and GPUs for the most demanding computations

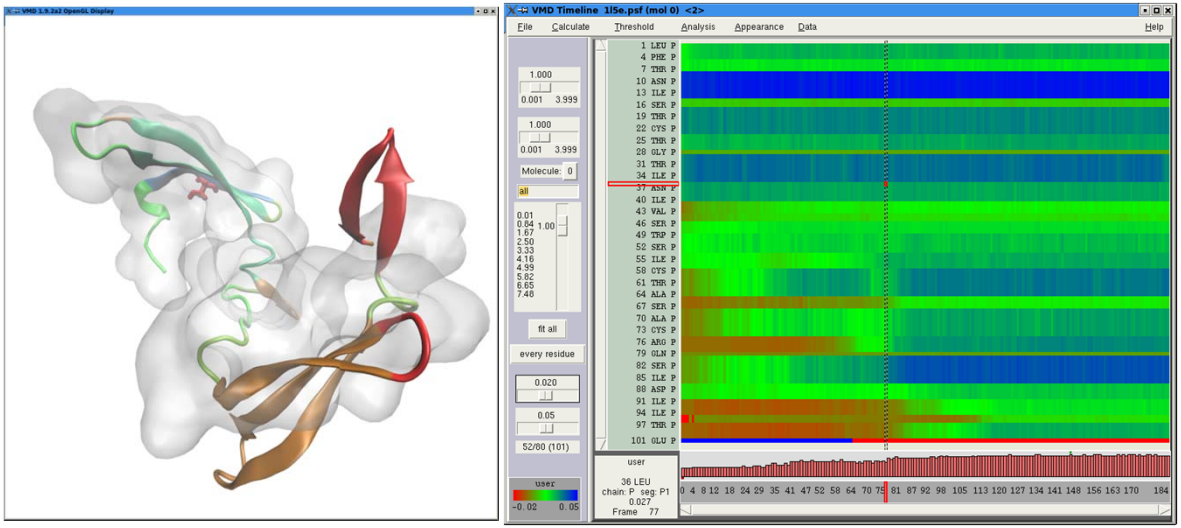
20M atoms:

membrane patch and solvent



Timeline Plugin: Analyze MD Trajectories for Events

MDFF quality-of-fit for cyanovirin-N



VMD Timeline plugin: live 2D plot linked to 3D structure

- Single picture shows changing properties across entire structure+trajectory
- Explore time vs. per-selection attribute, linked to molecular structure
- Many analysis methods available; user-extendable

Recent progress:

- Faster analysis with new VMD SSD trajectory formats, GPU acceleration
- Per-secondary-structure native contact and density correlation graphing

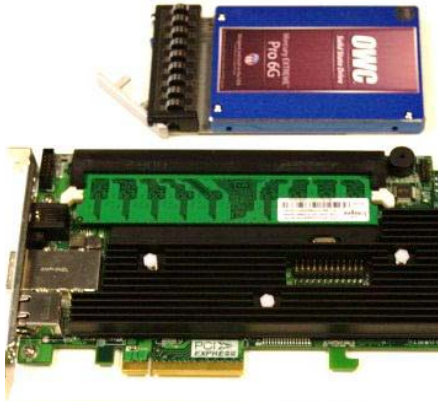
New Interactive Display & Analysis of Terabytes of Data:

Out-of-Core Trajectory I/O w/ Solid State Disks

450MB/sec

to 4GB/sec

A DVD movie per second!

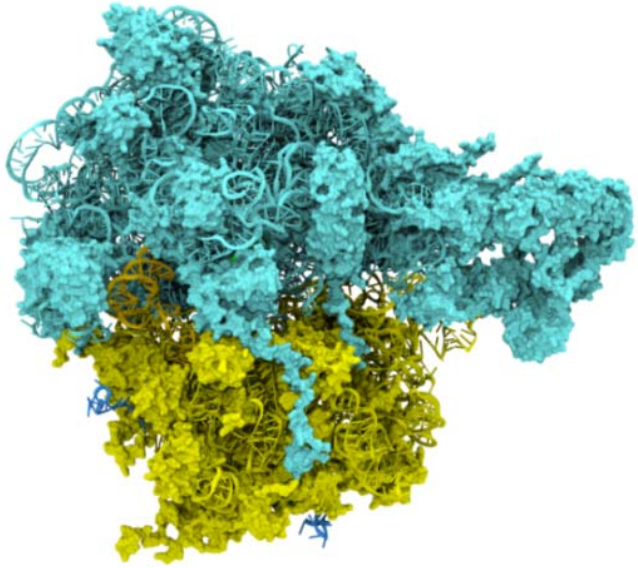


Commodity SSD, SSD RAID

- Timesteps loaded on-the-fly (out-of-core)
  - Eliminates memory capacity limitations, even for multi-terabyte trajectory files
  - High performance achieved by new trajectory file formats, optimized data structures, and efficient I/O
- Analyze long trajectories significantly faster
- New SSD Trajectory File Format 2x Faster vs. Existing Formats

Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories. J. Stone, K. Vandivort, and K. Schulten. *Lecture Notes in Computer Science*, 6939:1-12, 2011.

VMD Out-of-Core Trajectory I/O Performance: SSD-Optimized Trajectory Format, 8-SSD RAID

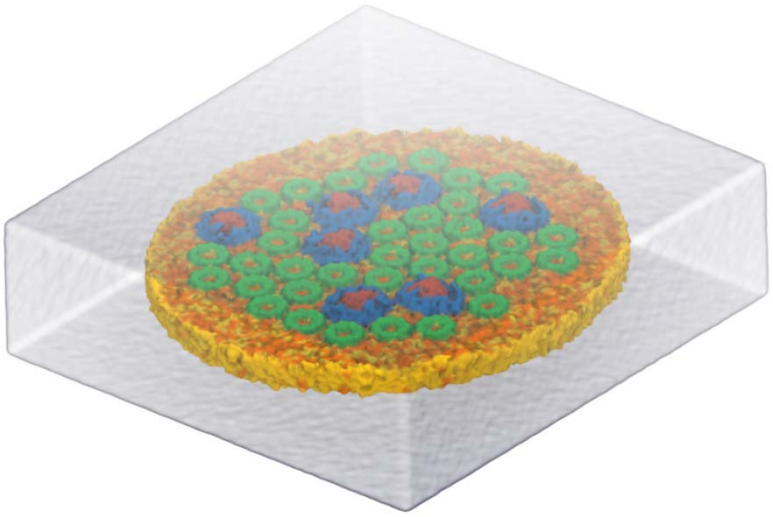


Ribosome w/ solvent

3M atoms

3 frames/sec w/ HD

60 frames/sec w/ SSDs



Membrane patch w/ solvent

20M atoms

0.4 frames/sec w/ HD

8 frames/sec w/ SSDs

New SSD Trajectory File Format 2x Faster vs. Existing Formats

VMD I/O rate ~2.1 GB/sec w/ 8 SSDs

Molecular Visualization and Analysis Challenges for Petascale Simulations

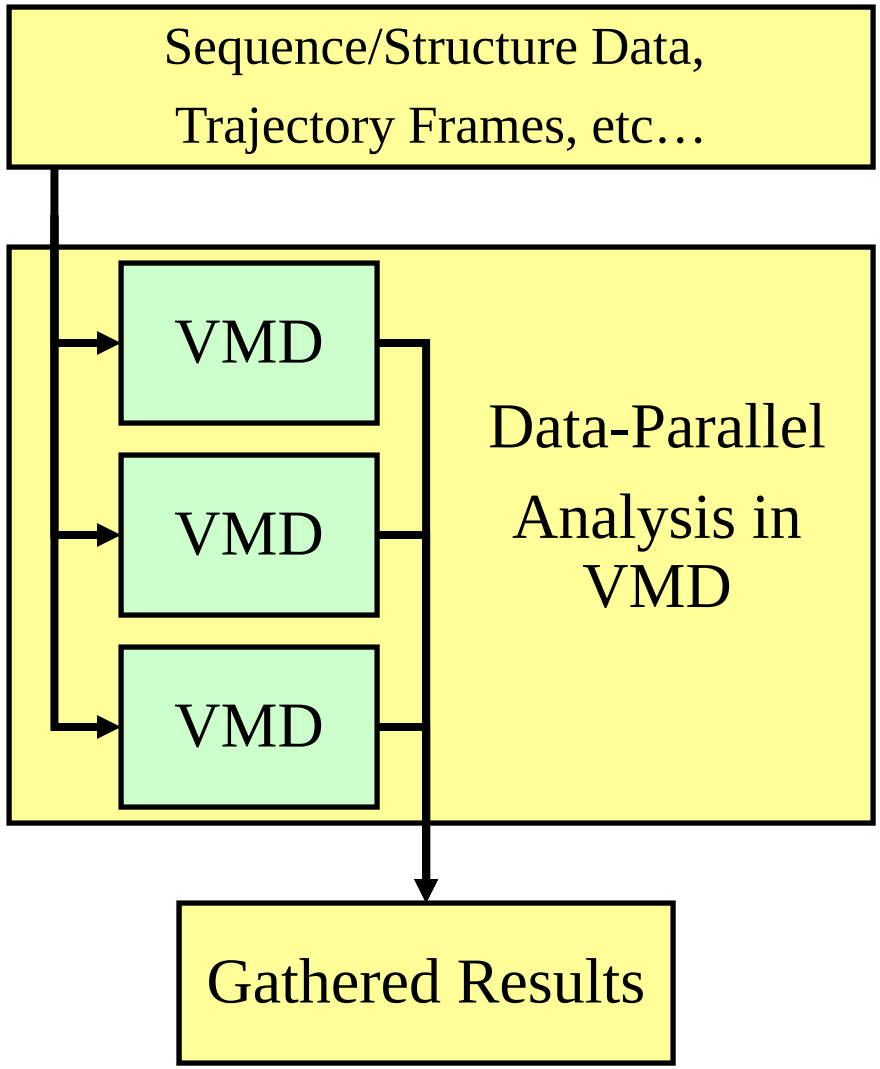
- Very large structures (10M to over 100M atoms)
  - 12-bytes per atom per trajectory frame
  - One 100M atom trajectory frame: 1200MB!
- Long-timescale simulations produce huge trajectories
  - MD integration timesteps are on the femtosecond timescale (10^{-15} sec) but many important biological processes occur on microsecond to millisecond timescales
  - Even storing trajectory frames infrequently, resulting trajectories frequently contain millions of frames
- Terabytes to petabytes of data, far too large to move
- Viz and analysis must be done primarily on the supercomputer where the data already resides

Approaches for Visualization and Analysis of Petascale Molecular Simulations with VMD

- Abandon conventional approaches, e.g. bulk download of trajectory data to remote viz/analysis machines
  - In-place processing of trajectories on the machine running the simulations
  - Use remote visualization techniques: Split-mode VMD with remote front-end instance, and back-end viz/analysis engine running in parallel on supercomputer
- Large-scale parallel analysis and visualization via distributed memory MPI version of VMD
- Exploit GPUs and other accelerators to increase per-node analytical capabilities, e.g. NCSA Blue Waters Cray XK6
- In-situ on-the-fly viz/analysis and event detection through direct communication with running MD simulation

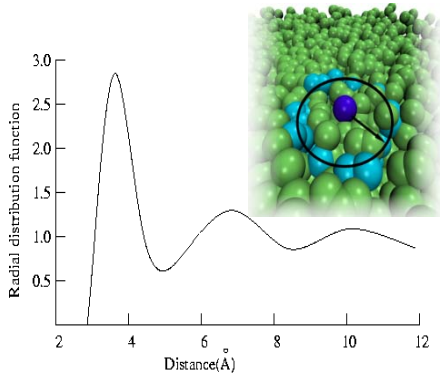
Parallel VMD Analysis w/ MPI

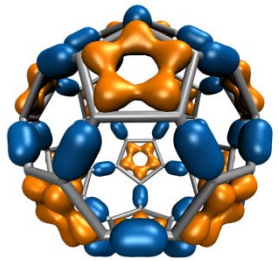
- Analyze trajectory frames, structures, or sequences in parallel supercomputers:
  - Parallelize user-written analysis scripts with minimum difficulty
  - Parallel analysis of independent trajectory frames
  - Parallel structural analysis using custom parallel reductions
  - Parallel rendering, movie making
- Dynamic load balancing:
  - Recently tested with up to 15,360 CPU cores
- **Supports GPU-accelerated clusters and supercomputers**



GPU Accelerated Trajectory Analysis and Visualization in VMD

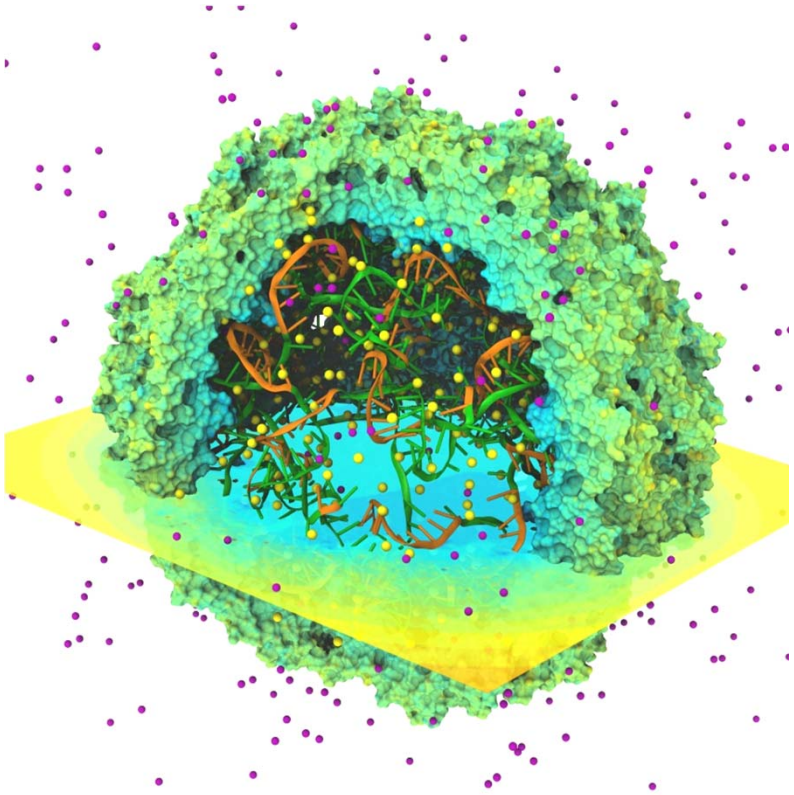
GPU-Accelerated Feature	Speedup vs. single CPU core
Molecular orbital display	120x
Radial distribution function	92x
Electrostatic field calculation	44x
Molecular surface display	40x
Ion placement	26x
MDFF density map synthesis	26x
Implicit ligand sampling	25x
Root mean squared fluctuation	25x
Radius of gyration	21x
Close contact determination	20x
Dipole moment calculation	15x





Time-Averaged Electrostatics Analysis on Energy-Efficient GPU Cluster

- **1.5 hour** job (CPUs) reduced to **3 min** (CPUs+GPU)
- Electrostatics of thousands of trajectory frames averaged
- Per-node power consumption on NCSA “AC” GPU cluster:
  - CPUs-only: 299 watts
  - CPUs+GPUs: 742 watts
- GPU Speedup: **25.5x**
- Power efficiency gain: **10.5x**



Quantifying the Impact of GPUs on Performance and Energy Efficiency in HPC Clusters. J. Enos, C. Steffen, J. Fullop, M. Showerman, G. Shi, K. Esler, V. Kindratenko, J. Stone, J. Phillips. *The Work in Progress in Green Computing*, pp. 317-324, 2010.

NCSA Blue Waters Early Science System
Cray XK6 nodes w/ NVIDIA Tesla X2090 GPUs

Time-Averaged Electrostatics Analysis on NCSA Blue Waters Early Science System

NCSA Blue Waters Node Type	**Seconds per trajectory frame for one compute node**
Cray XE6 Compute Node: 32 CPU cores (2xAMD 6200 CPUs)	9.33
Cray XK6 GPU-accelerated Compute Node: 16 CPU cores + **NVIDIA X2090 (Fermi) GPU**	2.25
Speedup for GPU XK6 nodes vs. CPU XE6 nodes	**GPU nodes are 4.15x faster overall**

Preliminary performance for VMD time-averaged electrostatics w/ Multilevel Summation Method on the NCSA Blue Waters Early Science System

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- NCSA Blue Waters Team
- NCSA Innovative Systems Lab
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