VMD: Preparation and Analysis of Molecular and Cellular Simulations

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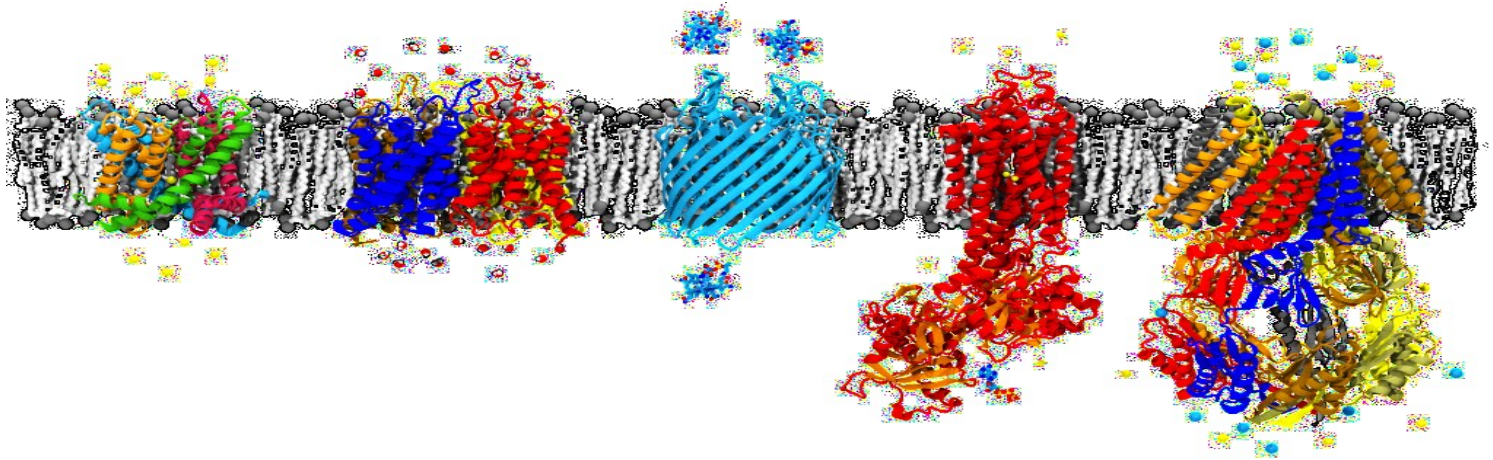


VMD Tutorial Materials on PDC ‘beskow’

- All of the VMD tutorial materials are locally available on the PDC Cray XC40 ‘beskow’ in case downloads from USA are too slow
- Copy VMD tutorials and scripts to your own directory on ‘beskow’ so you can modify them as you like:

  cd $SNIC_NOBACKUP

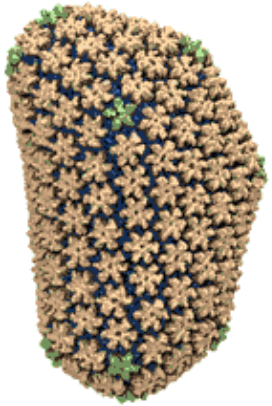
  rsync -av /cfs/klemming/nobackup/j/johnst/tutorials .
- You can then copy them to your laptop / workstation to work through the interactive tutorials there
- Use the example scripts on ‘beskow’ if you manage to get to the MPI-based VMD examples this week
- I may provide a GPU-enabled MPI build of VMD on ‘tegner’ later in the week if people want to try it out there as well

VMD Tutorial Home Page

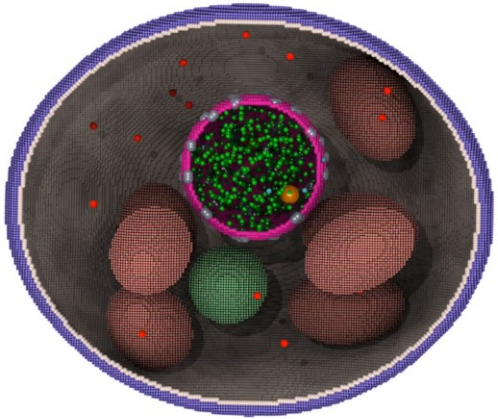
- http://www.ks.uiuc.edu/Training/Tutorials/
  - Main VMD tutorial
  - QwikMD simulation preparation and analysis plugin
  - VMD images and movies tutorial
  - Structure check
  - VMD quantum chemistry visualization tutorial
  - Visualization and analysis of CPMD data with VMD
  - Parameterizing small molecules using ffTK

VMD – “Visual Molecular Dynamics”

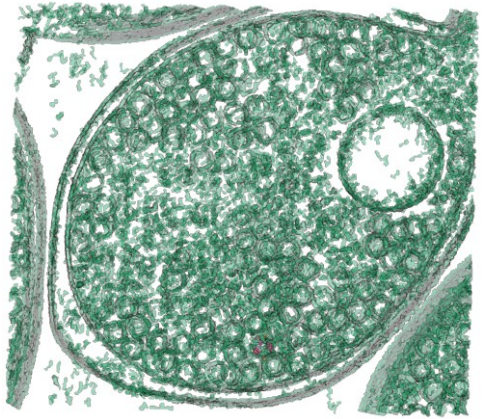
- Unique capabilities:
  - Trajectories are fundamental to VMD
  - Support for very large systems, now reaching billions of particles
  - Extensive GPU acceleration
  - Parallel analysis/visualization with MPI
- Visualization and analysis of:
  - Molecular dynamics simulations
  - “Particle” systems and whole cells
  - Cryo-EM densities, volumetric data
  - Quantum chemistry calculations
  - Sequence information



MD Simulations



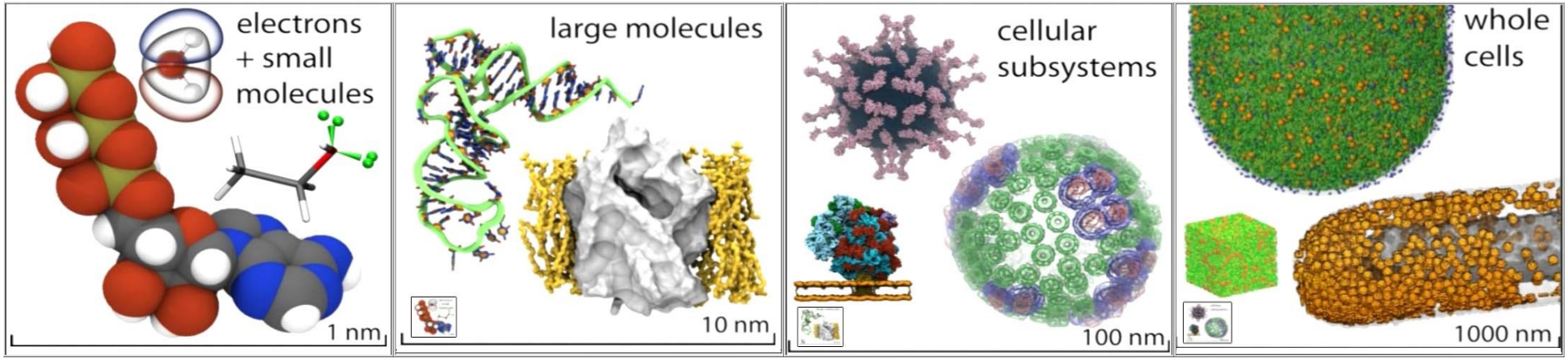
Cell-Scale Simulation



Integrate w/ Cryo-EM/ET

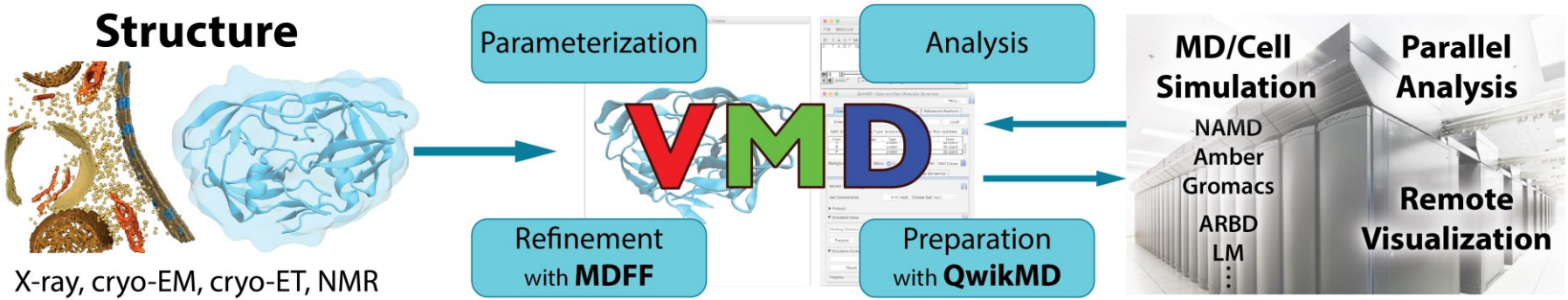
VMD Serves Many Communities

- VMD user statistics:
  - 103,000 unique registered users; 17,000 (16%) are NIH funded researchers
  - 20,000 citations, over 2,800 citations per year
- Supports key data types, file formats, and databases
- User extensible to support new tools, data types, custom analyses



VMD Interoperates with Mainstream Research Tools

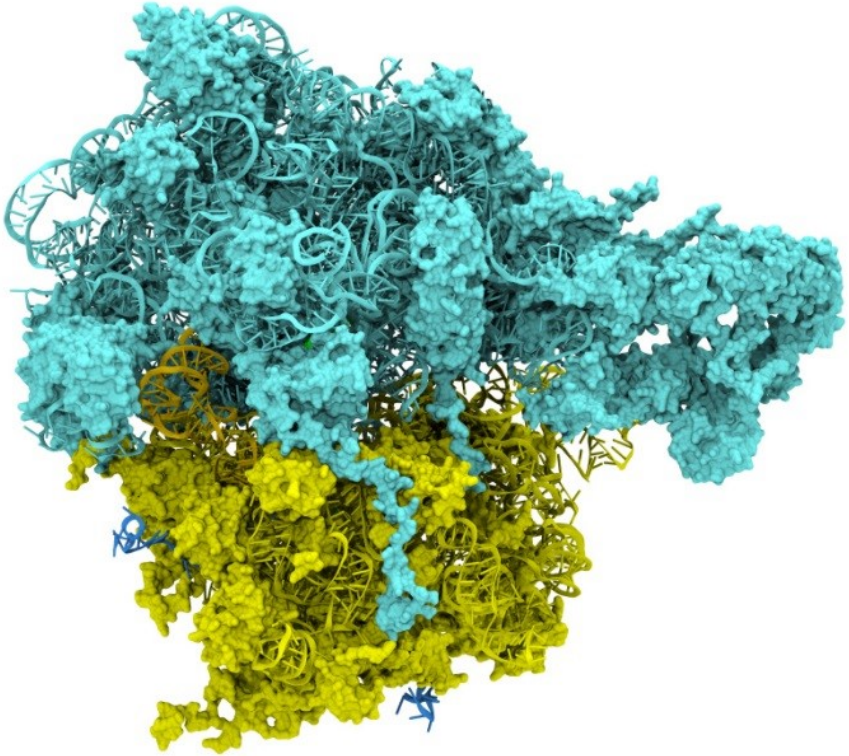
- Provides tools for simulation preparation, visualization, and analysis
- Interpret and process multi-modal structural information
- Connects with key software tools to enable state-of-the-art simulations
- Openness, extensibility, and interoperability are VMD hallmarks
- Uses advanced algorithms and hardware technologies to address data size challenges posed by cutting-edge experimental imaging and simulation



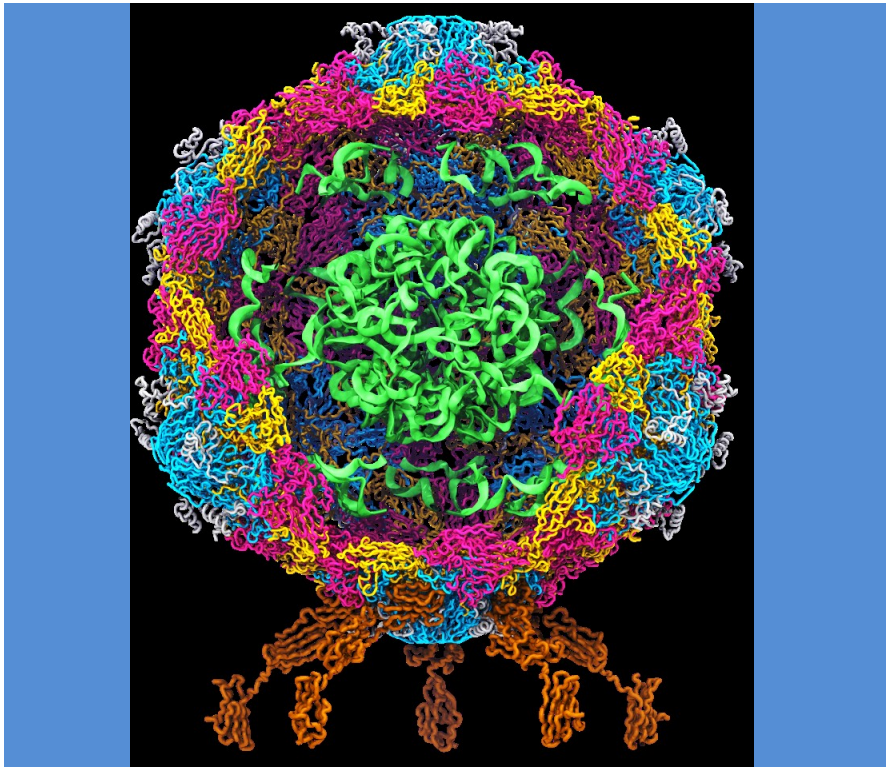
Goal: A Computational Microscope

Study the molecular machines in living cells

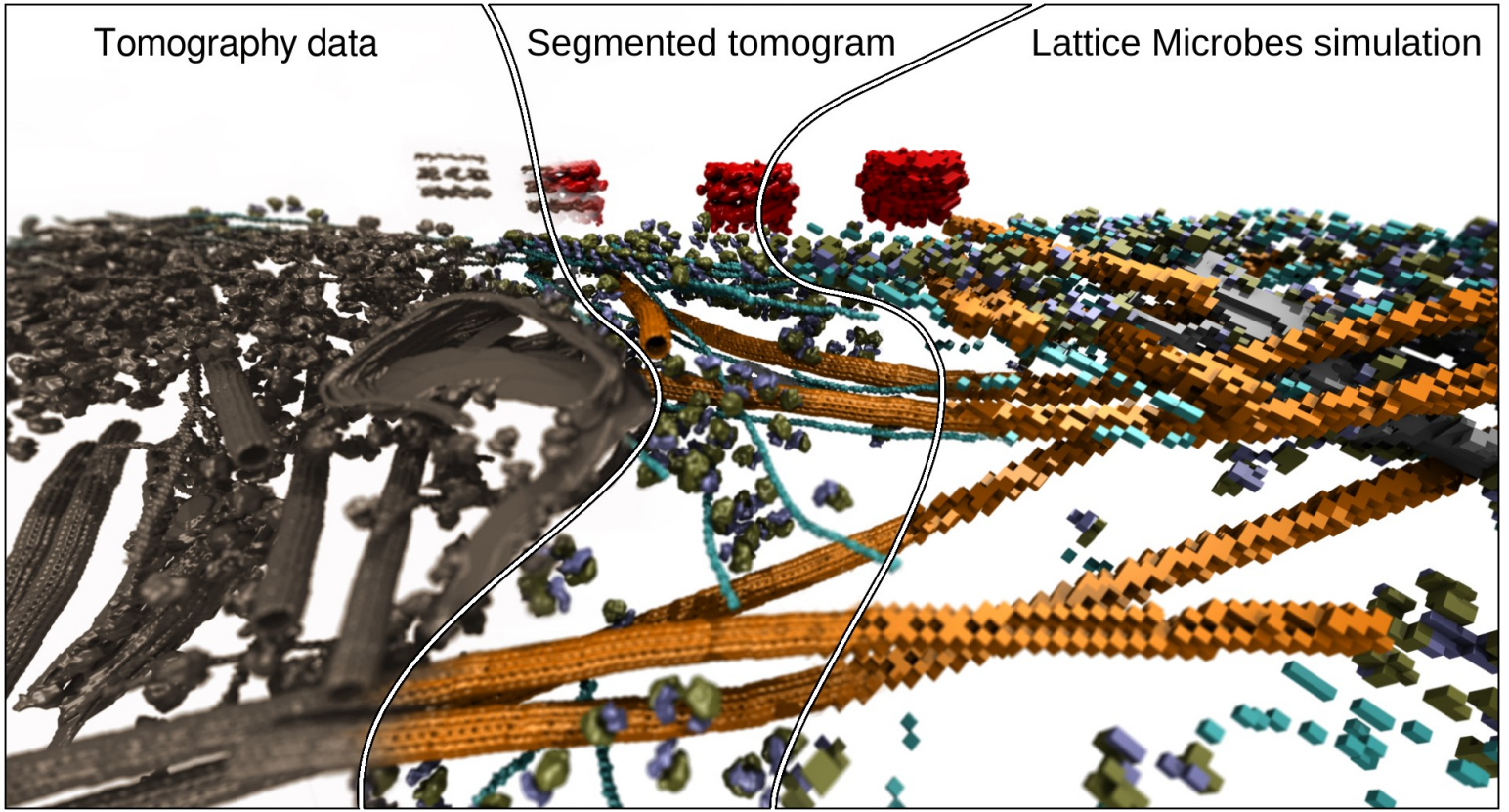
Ribosome: target for antibiotics



Poliovirus



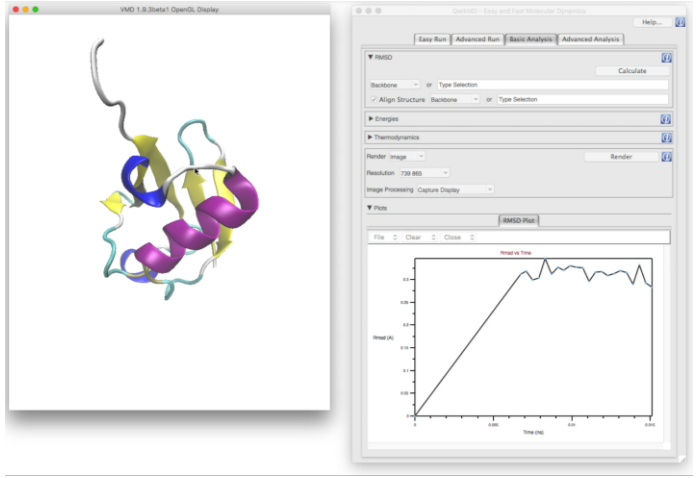
VMD is a Tool for Accessing Information about the Cell



VMD Achievements, Foundation for the Future

VMD 1.9.3 Released Nov 30, 2016

- Over 20,000 users so far
- Many visualization/analysis advances:
  - **Major GPU+CPU ray tracing advances**
  - Cryo-ET, vector-field volumetric maps …
  - NanoShaper: molecular surfaces, cavity calc.
  - Parallel analysis, visualization on HPC systems
- New, updated, and user-contributed plugins:
  - **QwikMD simulation prep/analysis**
  - **ffTK force field parameterization**
  - Plumed – free energy + collective variable analysis
  - Multiseq – improved MAFFT alignment support
- New platform support:
  - Amazon AWS EC2 Cloud
  - Cray XC50 w/ NVIDIA Tesla P100
  - IBM Power8, OpenPOWER w/ GPUs
  - Intel MIC Xeon Phi, AVX-512
  - NVIDIA Pascal GPUs: CUDA 8, OptiX 4, EGL



New QwikMD simulation preparation plugin

Recent Publications:

- eLife, 2016
- Scientific Reports, 2016
- J. Parallel Comp. 2016.
- IEEE HPDAV, 2016.
- IEEE HCW, 2016.

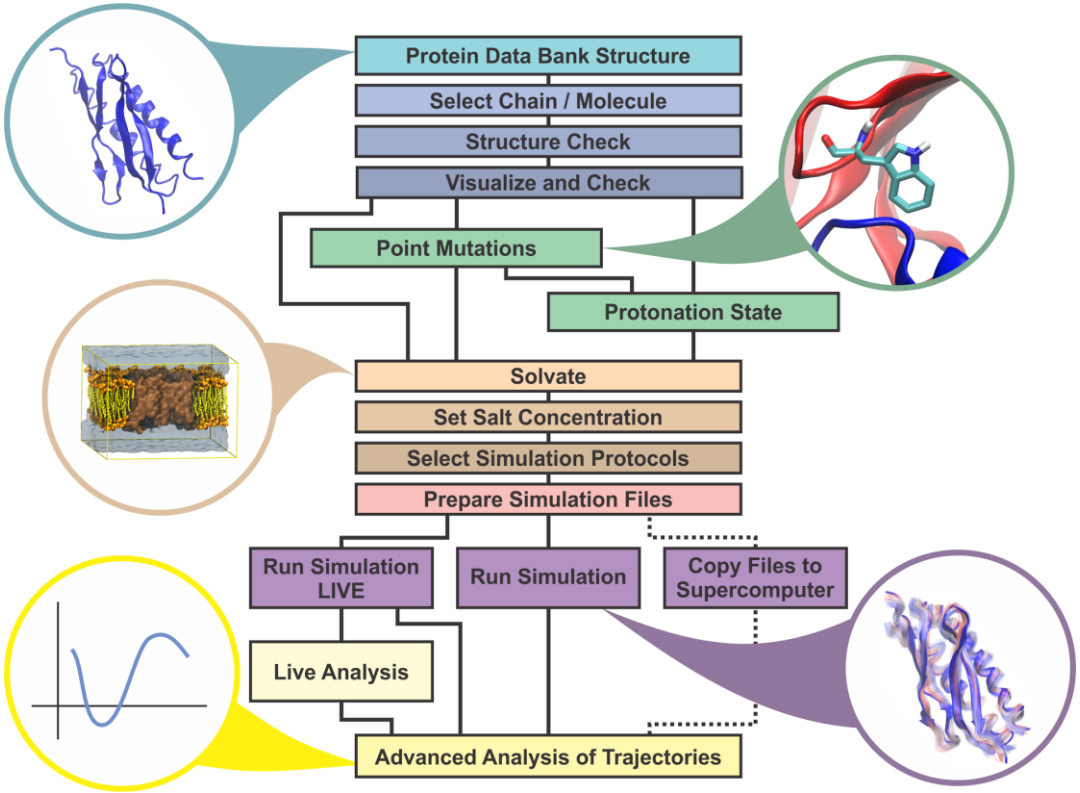
QwikMD: Guided MD Simulation and Training

Smooths initial learning curve (non-expert users)

Speed up tedious simulation preparation tasks (expert users)

Reproducibility: detailed log of all steps

Interactive preparation, simulation, and analysis



Ribeiro, et al. QwikMD - Integrative Molecular Dynamics Toolkit for Novices and Experts. ***Sci. Rep***. 6, 26536, 2016

Parametrization with the Force Field Toolkit (FFTK)

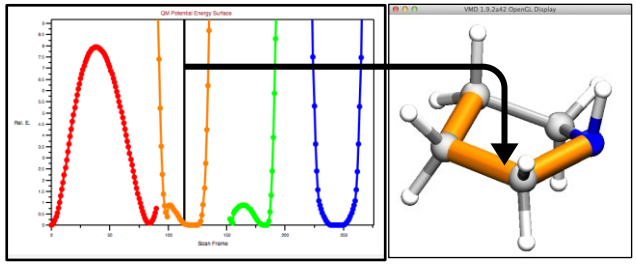
A plugin enabling the simulation of drug-like small molecules by lowering force field development barriers

A graphical interface organized to follow the standardized CGenFF workflow

**** NEW in VMD 1.9.3 ****

Import data from the CGenFF Program webserver to assign initial parameters by analogy

Leverages VMD's powerful graphics capabilities to visualize parameter-related data within the context of molecular structure

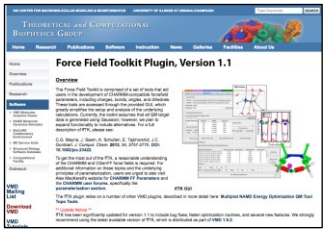


Interactively explore energy profiles

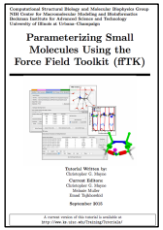
Future Plans:

- Support free-for-academics QM software, ORCA (Neese, Max Planck)
- Parametrization tools for additional MM force fields
  - AMBER force field (Gumbart, Georgia Tech.)
  - Drude polarizable force fields (Roux, U. Chicago; MacKerell, U. Maryland)

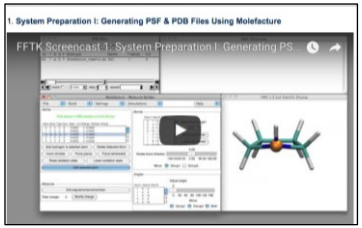
Extensive training material available from the Center's website



Documentation Website



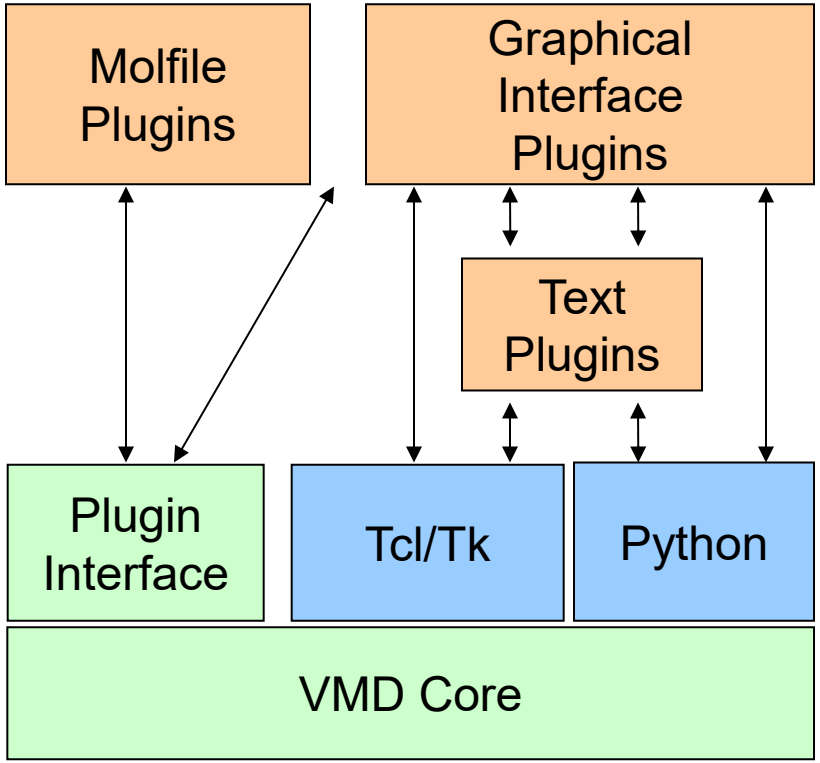
Workshop Tutorial



Screencast Demos

VMD is a Platform for Developing Research Tools
Over 110 VMD Plugins, Half Developed by Users

- VMD user-extensible scripting w/ Tcl/Tk, Python
- User-developed plugins:
  - Alanine Scanning
  - Collective Variable Analyzer
  - Clustering Tool
  - Carbon Nanostructure Builder
  - TorsionPlot
  - RMSD Trajectory Tool
  - Many others…



Selected VMD Plugins: Center Developed, and User Developed

Analysis

- APBSRun
- CatDCD
- Contact Map
- GofRGUI
- HeatMapper
- ILSTools
- IRSpecGUI
- MultiSeq
- NAMD Energy
- NAMD Plot
- NetworkView
- NMWiz
- ParseFEP
- PBCTools
- PMEpot
- PropKa GUI
- RamaPlot
- RMSD Tool
- RMSD Trajectory Tool
- RMSD Visualizer Tool
- Salt Bridges
- Sequence Viewer
- Symmetry Tool
- Timeline
- TorsionPlot
- VolMap

Modeling

- AutoIonize
- AutoPSF
- Chirality
- Cionize
- Cispeptide
- CGTools
- Dowser
- ffTK
- Inorganic Builder
- MDFF
- Membrane
- Merge Structs
- Molefacture
- Mutator
- Nanotube
- Psfgen
- RESPTool
- RNAView
- Solvate
- SSRestraints
- Topotools

Visualization

- Clipping Plane Tool
- Clone Rep
- DemoMaster
- Dipole Watcher
- Intersurf
- Navigate
- NavFly
- MultiMolAnim
- Color Scale Bar
- Remote
- Palette Tool
- ViewChangeRender
- ViewMaster
- Virtual DNA Viewer
- VMD Movie Maker

Simulation

- AlaScan
- AutoIMD
- IMDMenu
- NAMD GUI
- NAMD Server
- QMTool

Collaboration

- Remote Control

Data Import and Plotting

- Data Import
- Multiplot
- PDBTool
- MultiText

Externally Hosted Plugins and Extensions

- Check sidechains
- MultiMSMS
- Interactive Essential Dynamics
- Mead Ionize
- Clustering Tool
- iTrajComp
- Swap RMSD
- Intervor
- SurfVol
- vmdICE

75 MolFile I/O Plugins:
structure, trajectory, sequence, and density map

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

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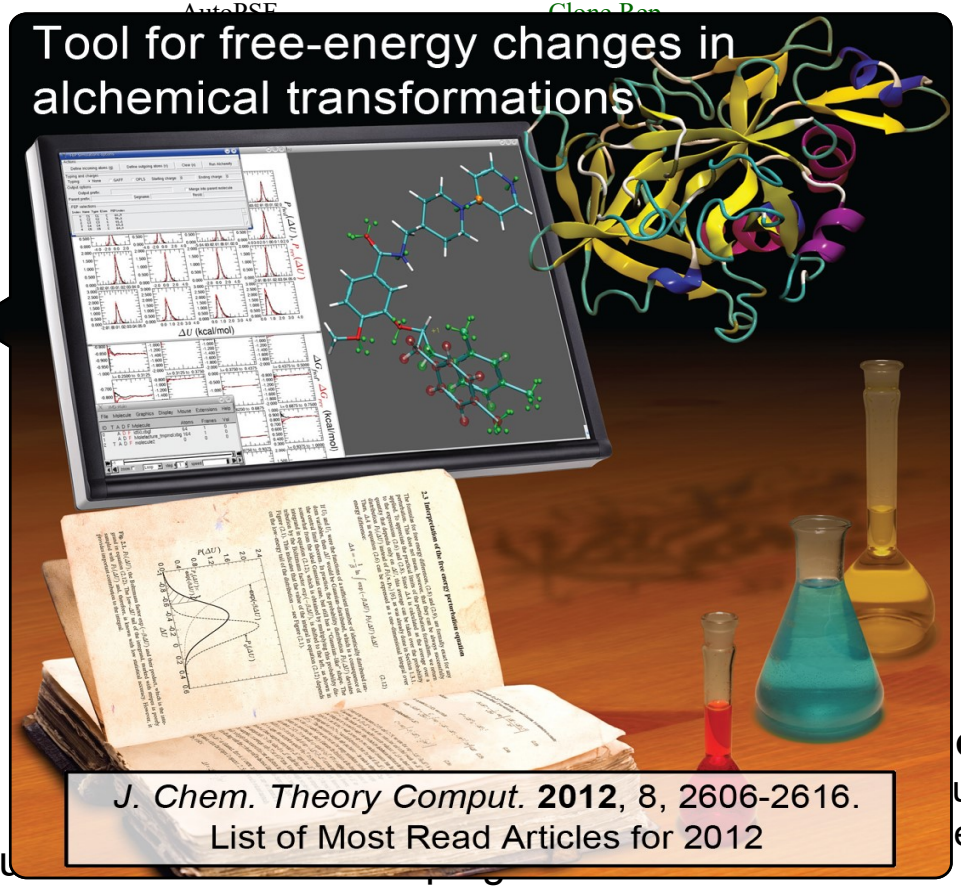

olFile I/O Plugins:

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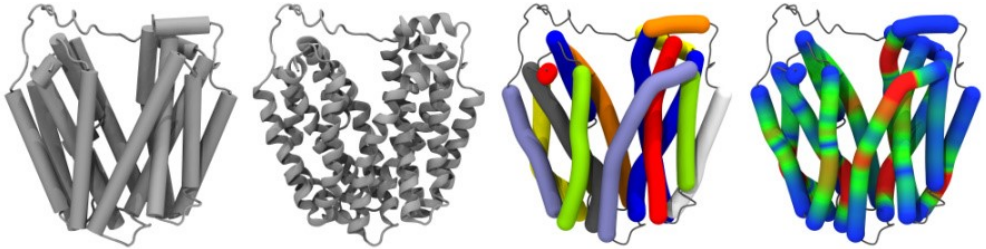
http://www.ks.uiu

Example VMD Visualization and Analysis Plugins



Bendix

Dahl ACE, Chavent M and Sansom MSP Bendix: intuitive helix geometry analysis and abstraction. *Bioinformatics* 2012 28(16): 2193-2194.

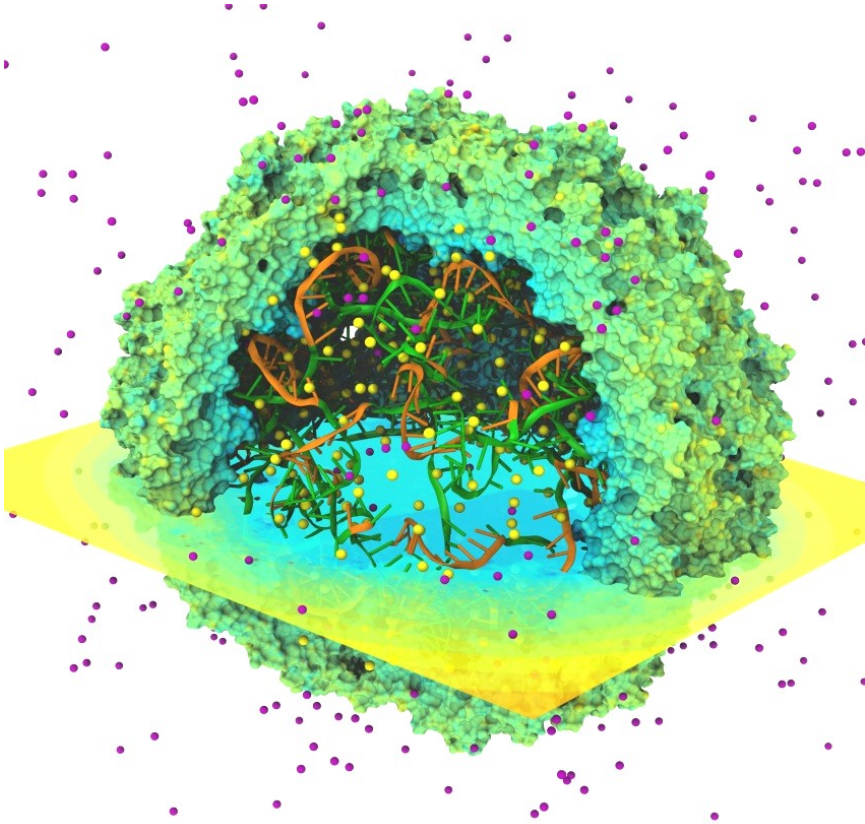
Normal Mode Wizard

Bakan A, Meireles LM, Bahar I ProDy: Protein Dynamics Inferred from Theory and Experiments. *Bioinformatics* 2011 27(11):1575-1577.

VMD Visualization Concepts

Biomolecular Visualization Challenges

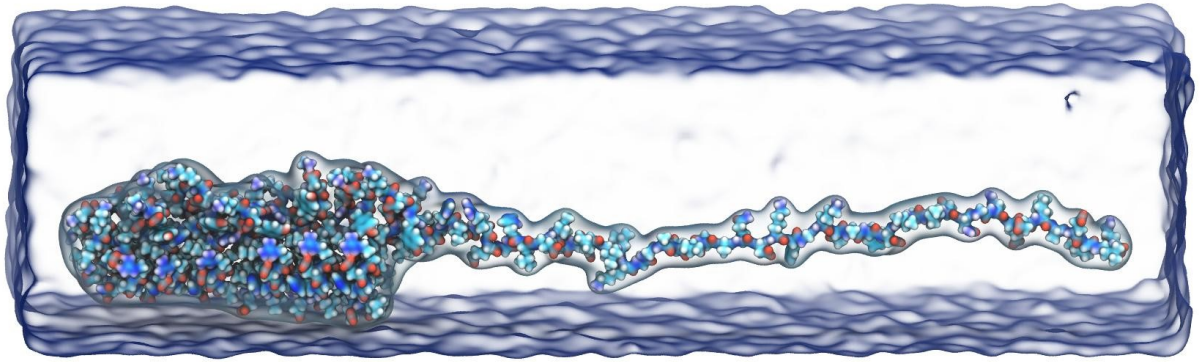
- Geometrically complex scenes
- Spatial relationships important to see clearly: fog, shadows, AO helpful
- Often show a mix of structural and spatial properties
- Time varying!



Structure Visualization

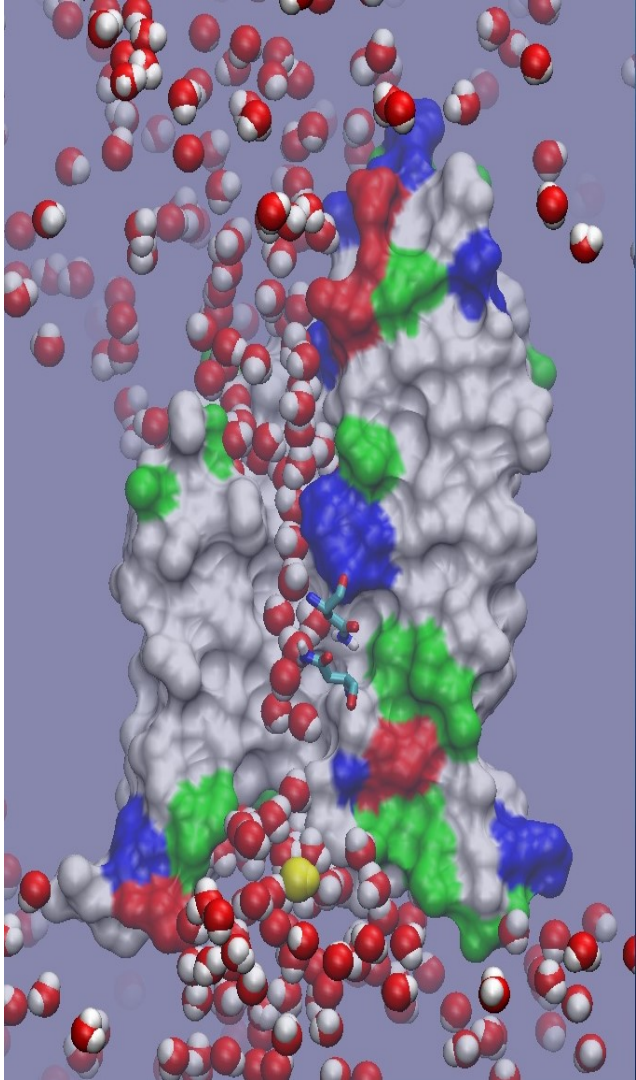
Molecular representations provide different levels of abstraction, atomic detail vs. higher level organizational information

- Atoms, VdW spheres, bonds, ball-stick, …
- Molecular orbitals (quantum chemistry)
- Molecular surfaces
- Coarse-grained “beads”
- Ribbons, secondary structure, “cartoon” reps, RNA/DNA



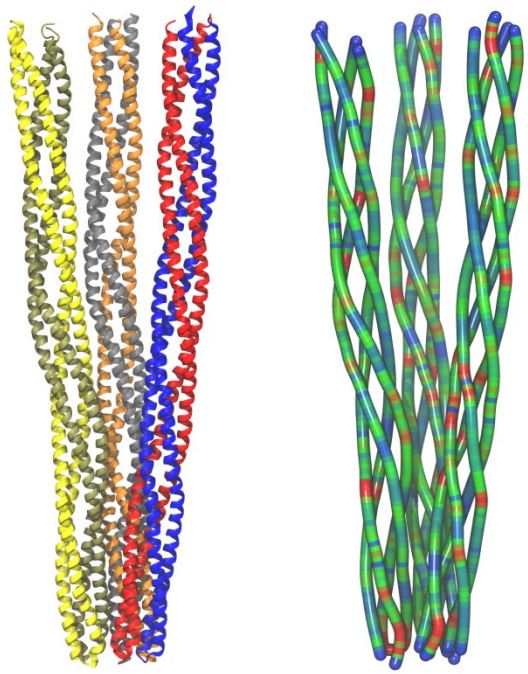
Selection, Filtering

- Most viz tools allow interactive visual picking, menu-driven selections of structure components to display or operate on
- VMD also extensively uses a text-based selection language (think google):
  - “water within 10 of protein and z > 0”
  - Allows selection on user-defined fields
  - ***Promotes synergy between interactive and scripting interfaces***
  - Works very well when dealing with huge time-varying structures



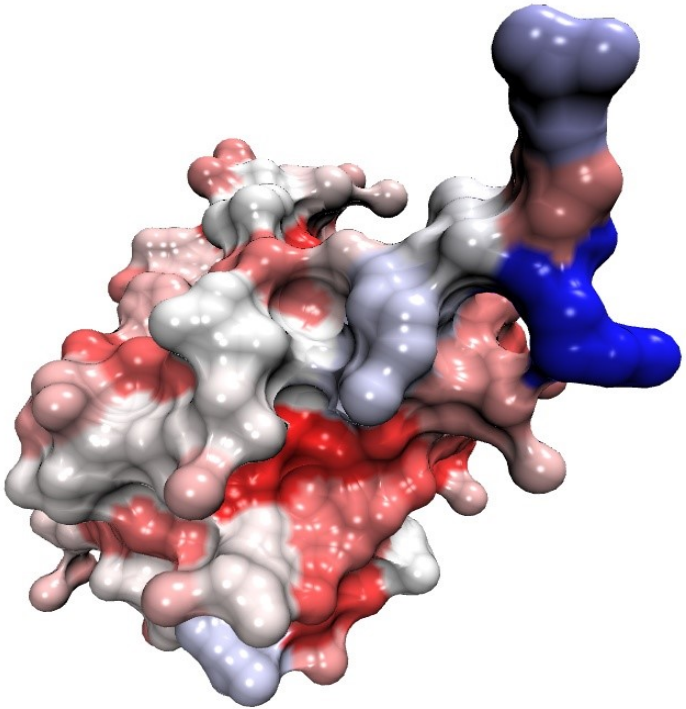
Computed Properties

- Smoothing of thermal noise
- Secondary structure
- Hydrogen bonds, salt bridges
- Forces, energies, stress, strain
- Time averaging of electrostatic fields, occupancy maps
- Quality-of-fit cross correlation with cryo-EM density maps
- Normal modes, principal component analysis, essential dynamics
- Cluster simulation trajectory timesteps by structural similarity

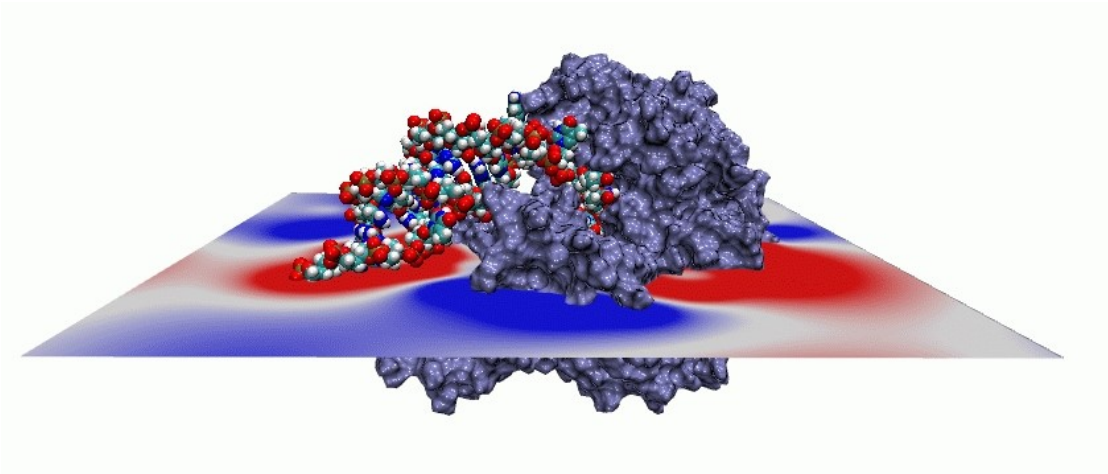


Chemoreceptor trimer-of-dimers analysis with Bendix plugin in VMD

Display of Computed Properties on Structures

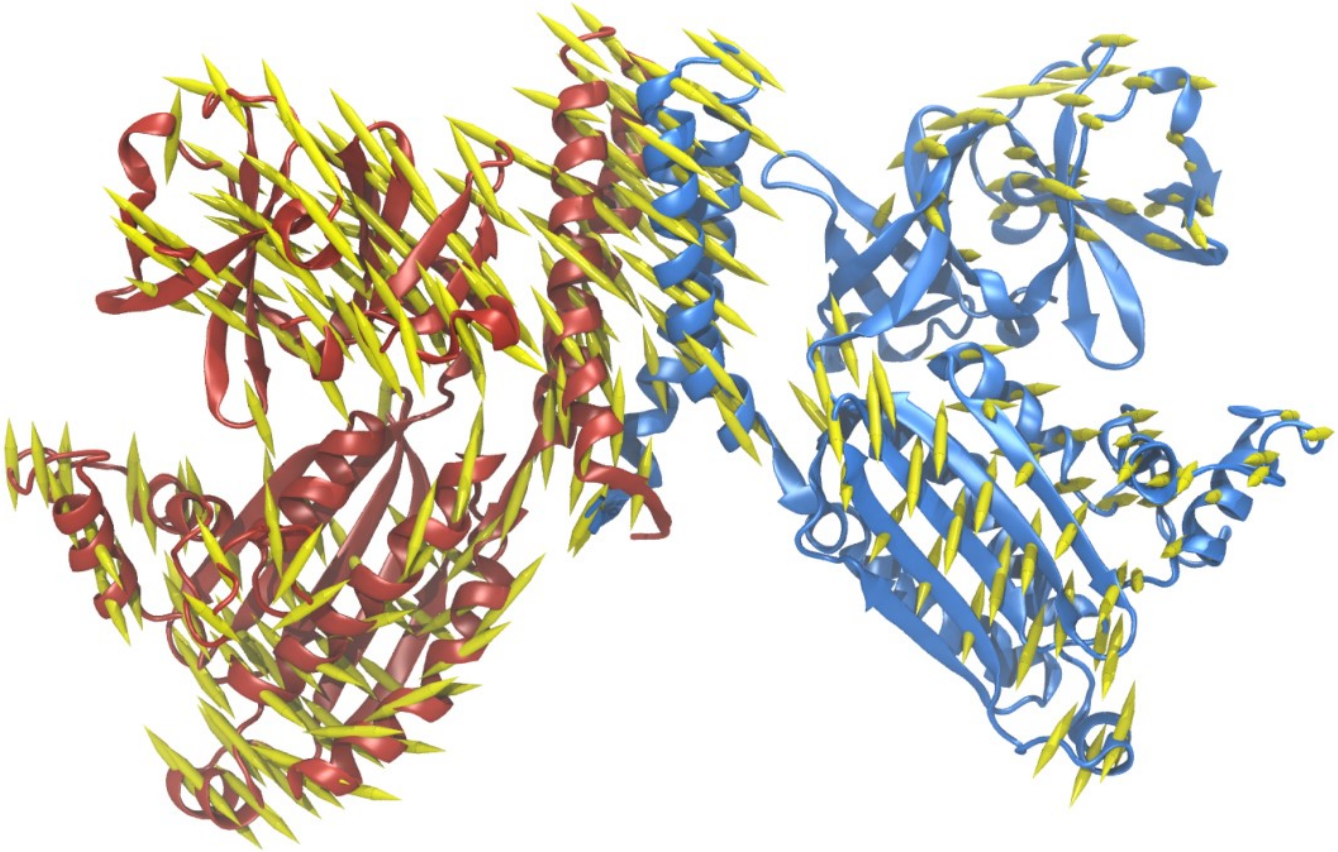


Per-residue solvent-accessible surface area of Ubiquitin



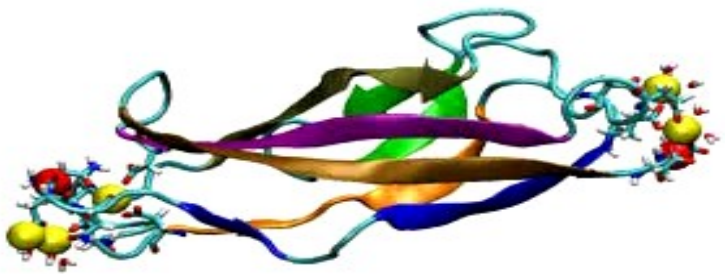
PME electrostatic potential contour for a helicase on a volumetric slice plane

CheA kinase PCA: first principal component porcupine plot



Visualization of Molecular Dynamics

- Molecular dynamics simulations save trajectories of atomic coordinates as simulated time progresses
- Researchers study trajectories by analyzing force profiles, energies, structural changes, etc.
- **Visualization selections, graphics, structure properties recomputed for each trajectory timestep!**

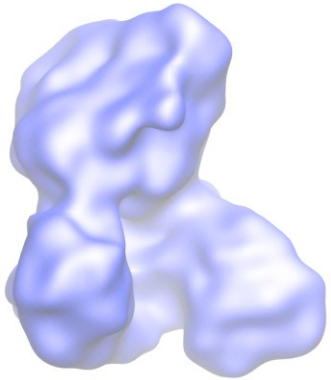


Petascale Computing - A Key Instrument for Life Science

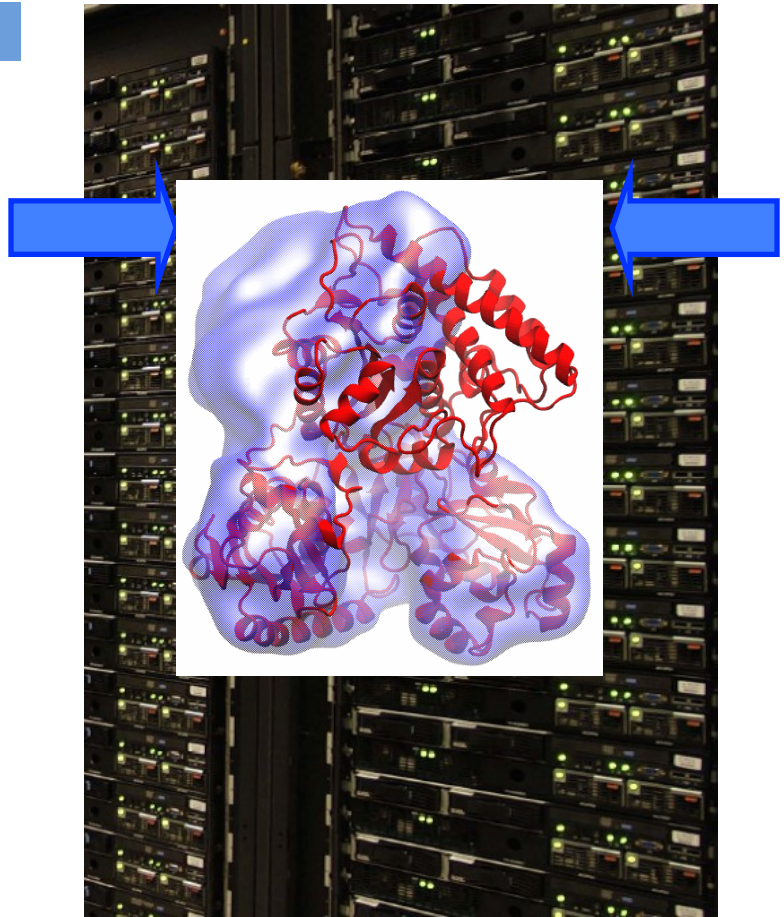
MDFF Solves Structures from X-ray Crystallography and Cryo-EM

Electron microscopy

FEI microscope

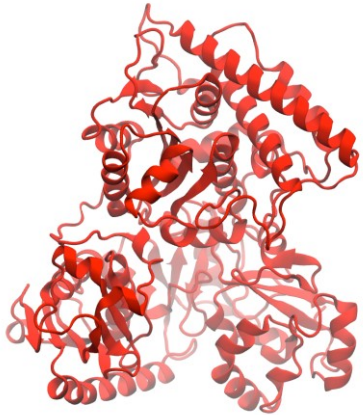


Electron density of protein in action at low resolution



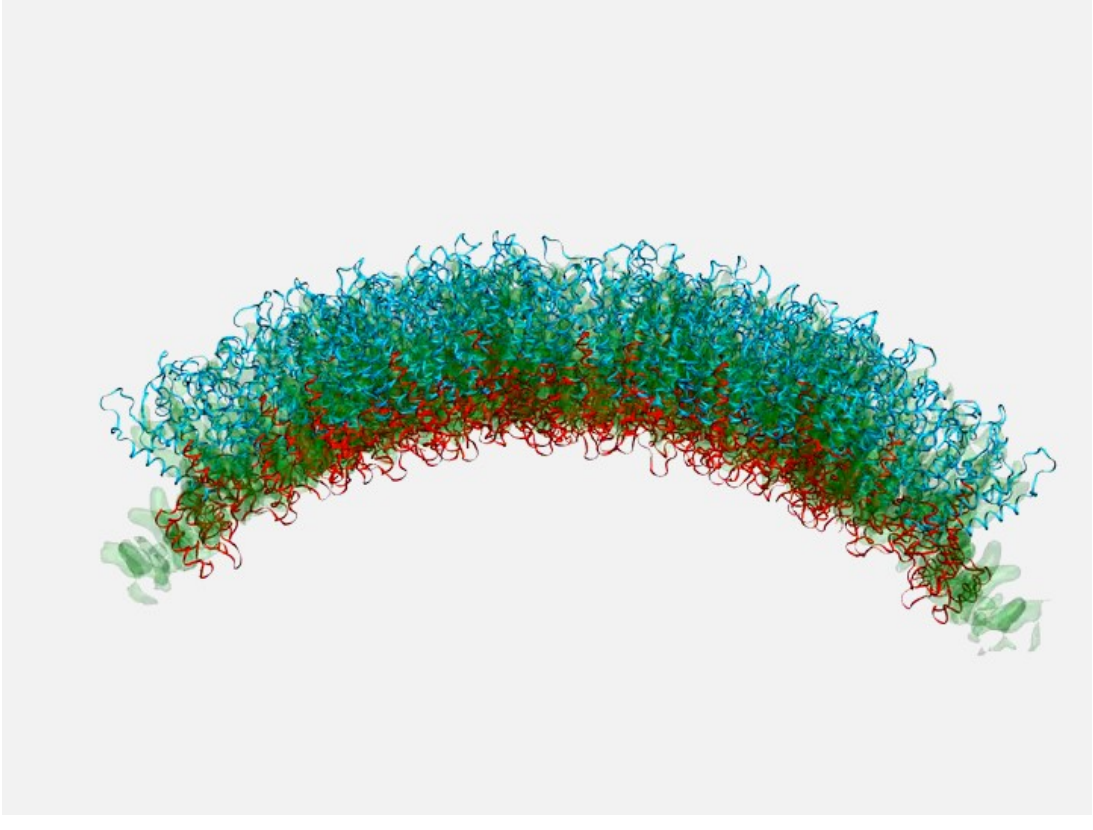
X-ray crystallography

APS at Argonne



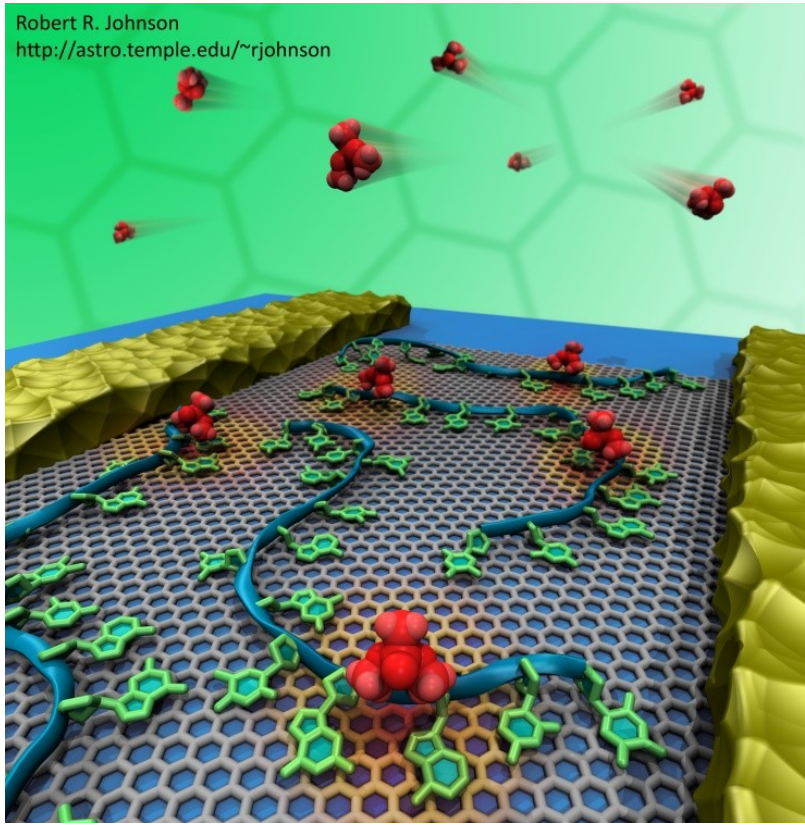
Ideal protein structure at high resolution
Acetyl – CoA Synthase

Hexamer of hexamers HIV capsid substructure Molecular Dynamics Flexible Fitting (MDFF) simulation. All-atom structure fitting into cryo-EM density map.



Ray Tracing in VMD

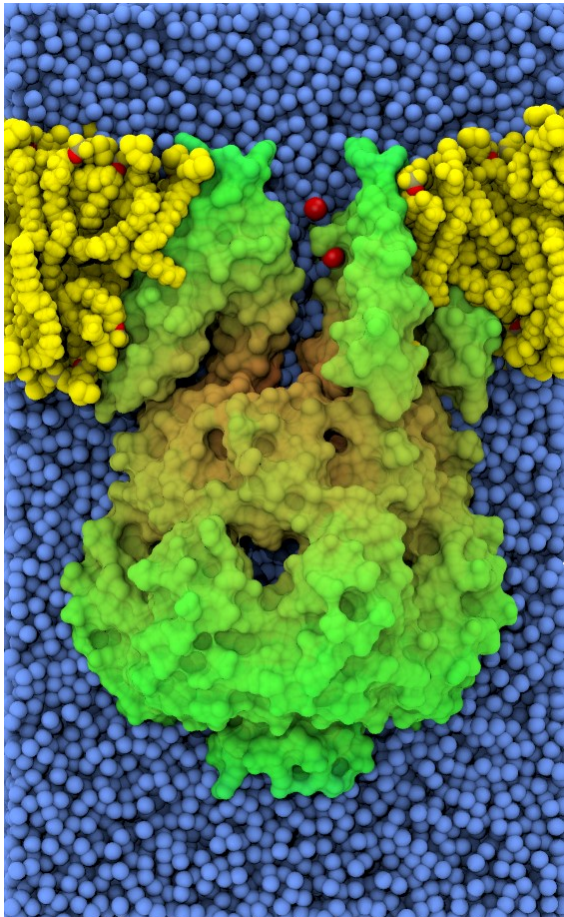
- Support for ray tracing of VMD molecular scenes began in 1995
- Tachyon parallel RT engine interfaced with VMD (1999)
- Tachyon embedded as an internal VMD rendering engine (2002)
- Built-in support for large scale parallel rendering (2012)
- Refactoring of VMD to allow fully interactive ray tracing as an alternative to OpenGL (2014)



Geometrically Complex Scenes

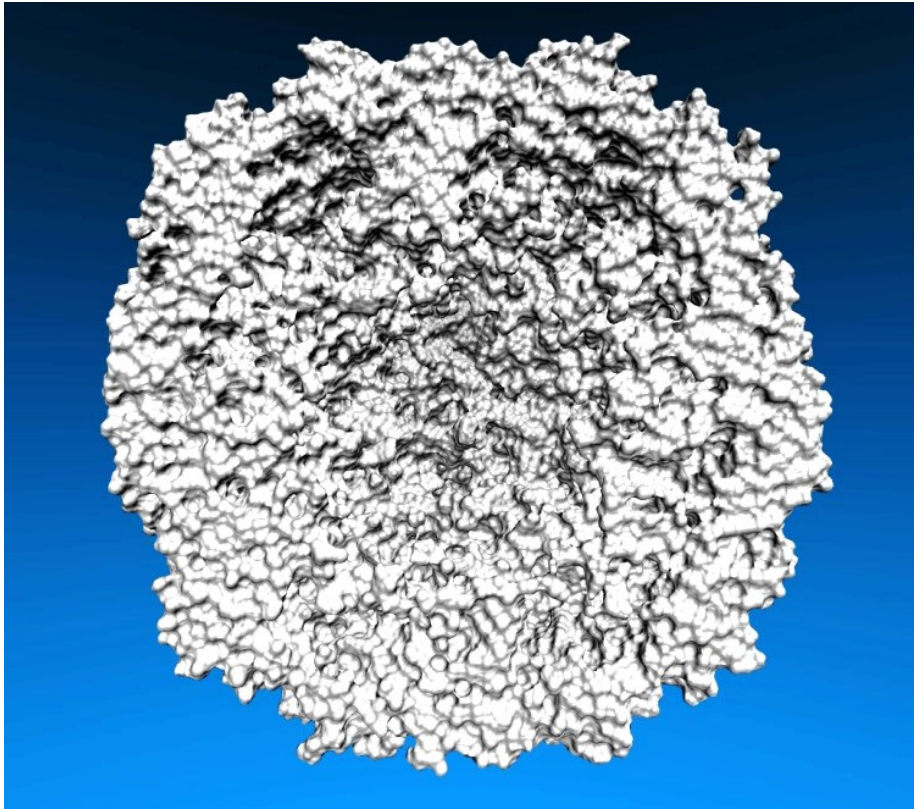
Ray tracing techniques well matched to molecular viz. needs:

- Curved geometry, e.g. spheres, cylinders, toroidal patches, easily supported
- Greatly reduced memory footprint vs. polygonalization
- Runtime scales only moderately with increasing geometric complexity
- Occlusion culling is “free”, RT acceleration algorithms do this and much more

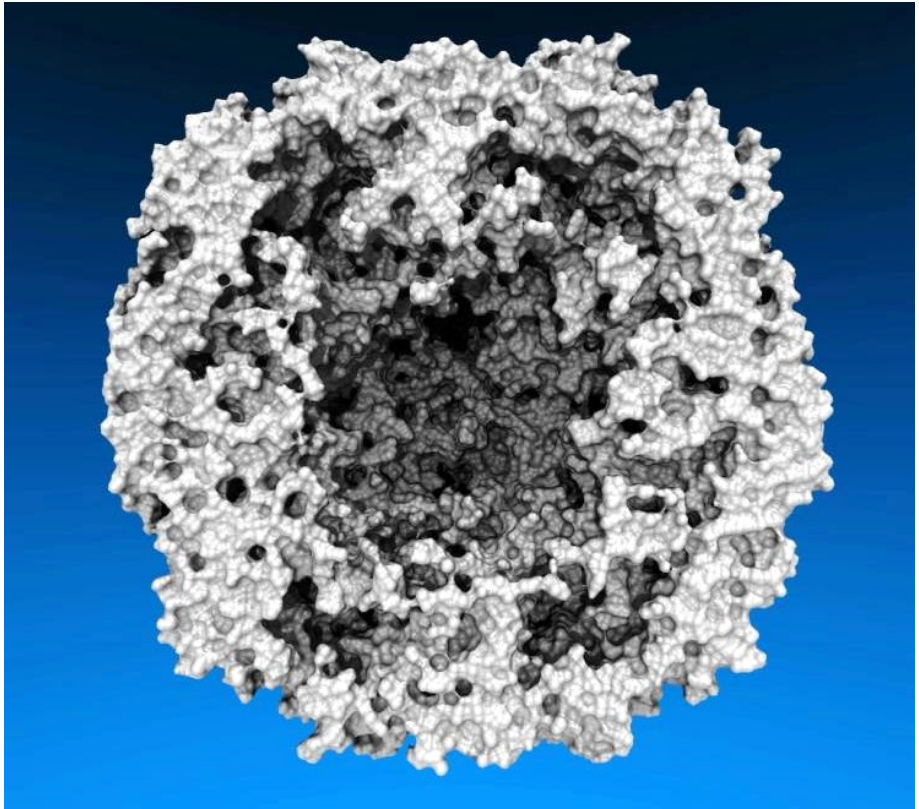


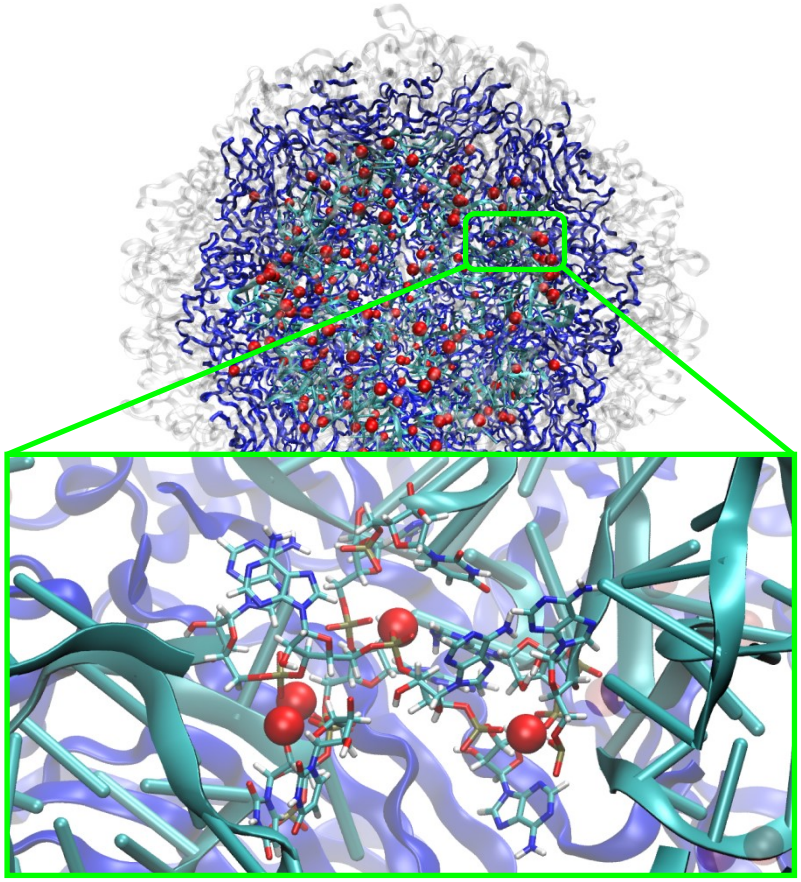
Interactive Ray Tracing, Lighting Comparison: STMV Capsid

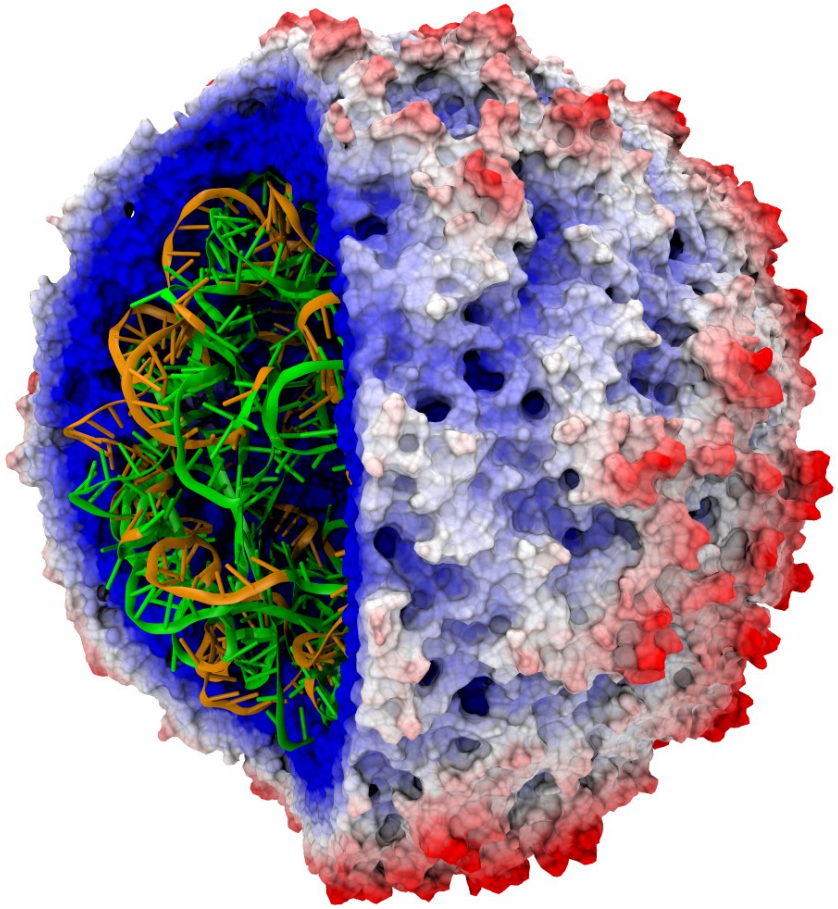
Two lights, no shadows (e.g. as used by OpenGL)



Ambient occlusion lighting and shadows w/ RT



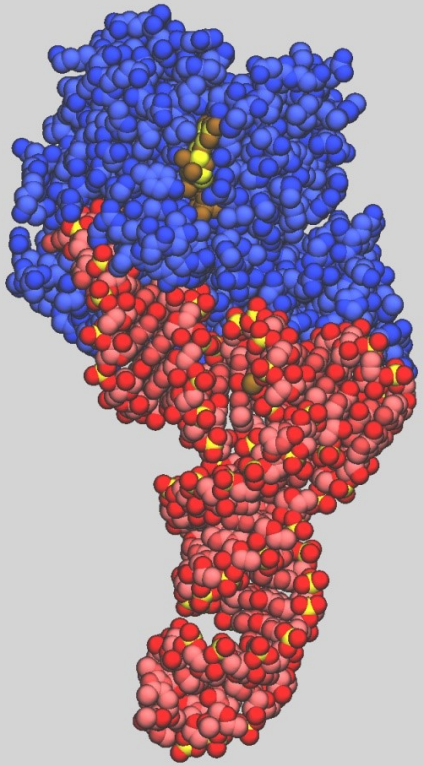




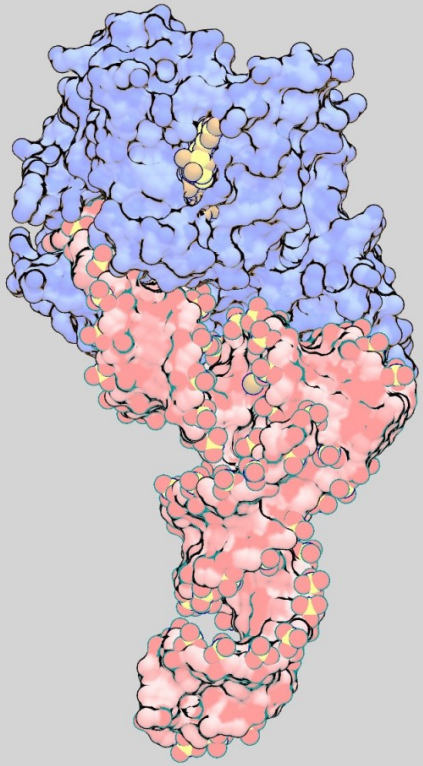
Satellite Tobacco Mosaic Virus

VMD Shading Comparison: EF-Tu

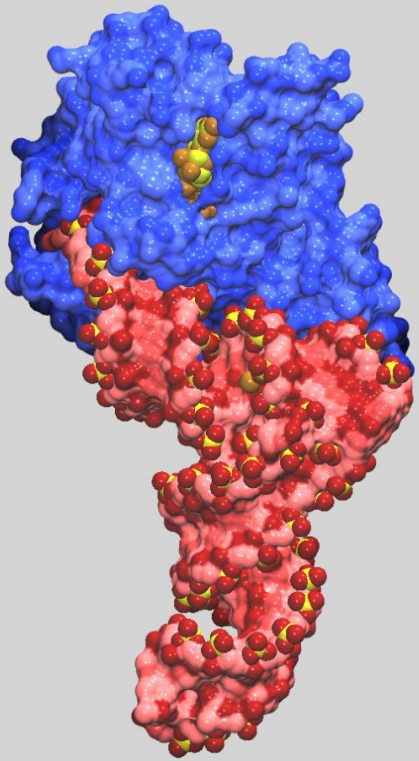
Outline Shader



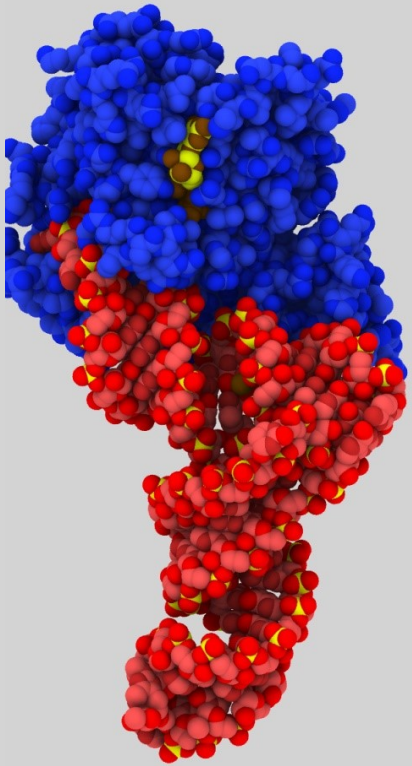
“Goodsell” Shader

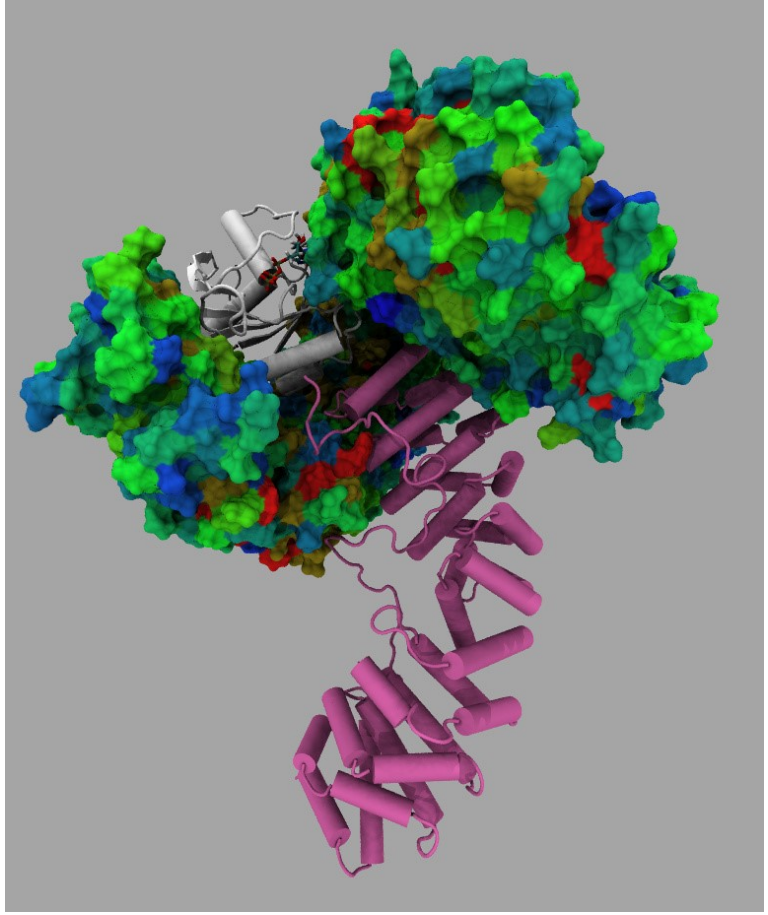


Glossy Shader

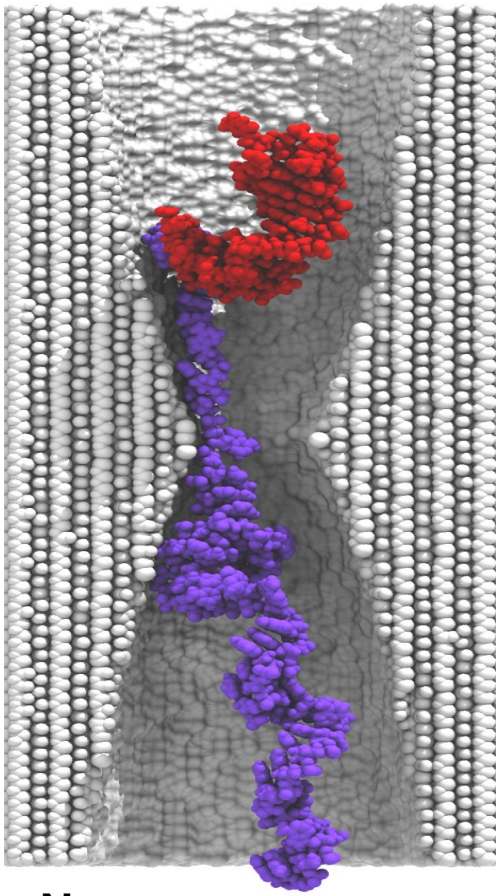


Ambient Occlusion, Shadowing





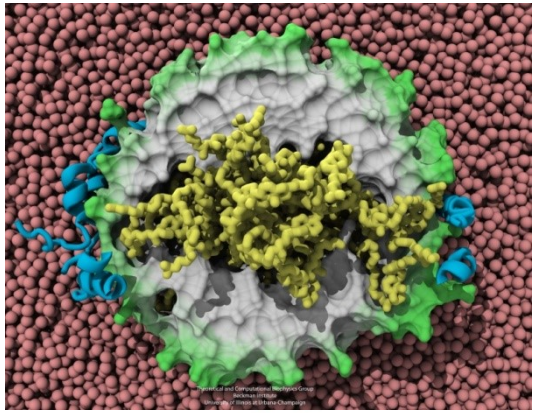
Exportin Cse1p

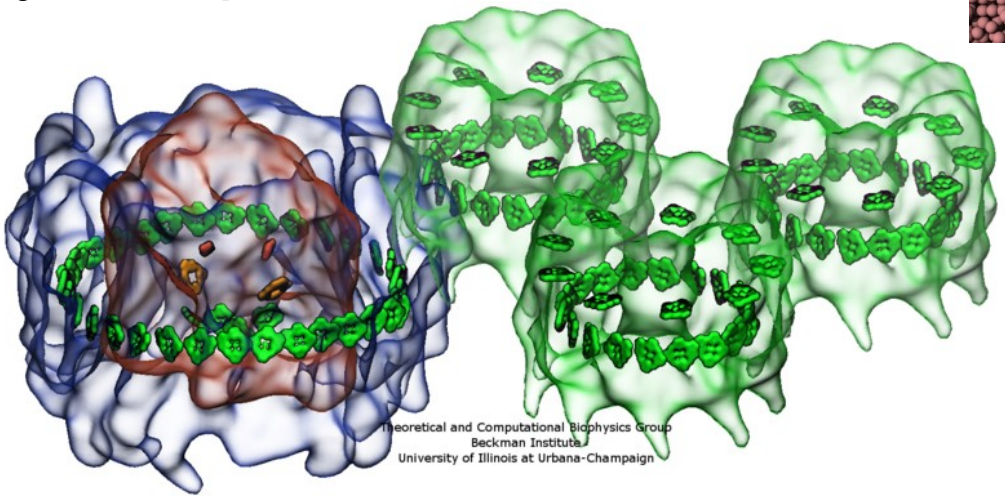


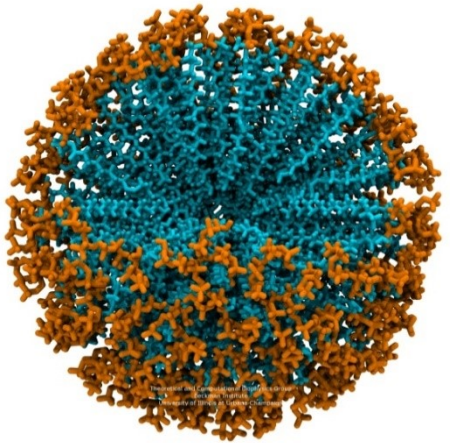
Nanopore

Benefits of Advanced Lighting and Shading Techniques

- Exploit visual intuition
- Spend computer time in exchange for scientists' time, make images that are more easily interpreted

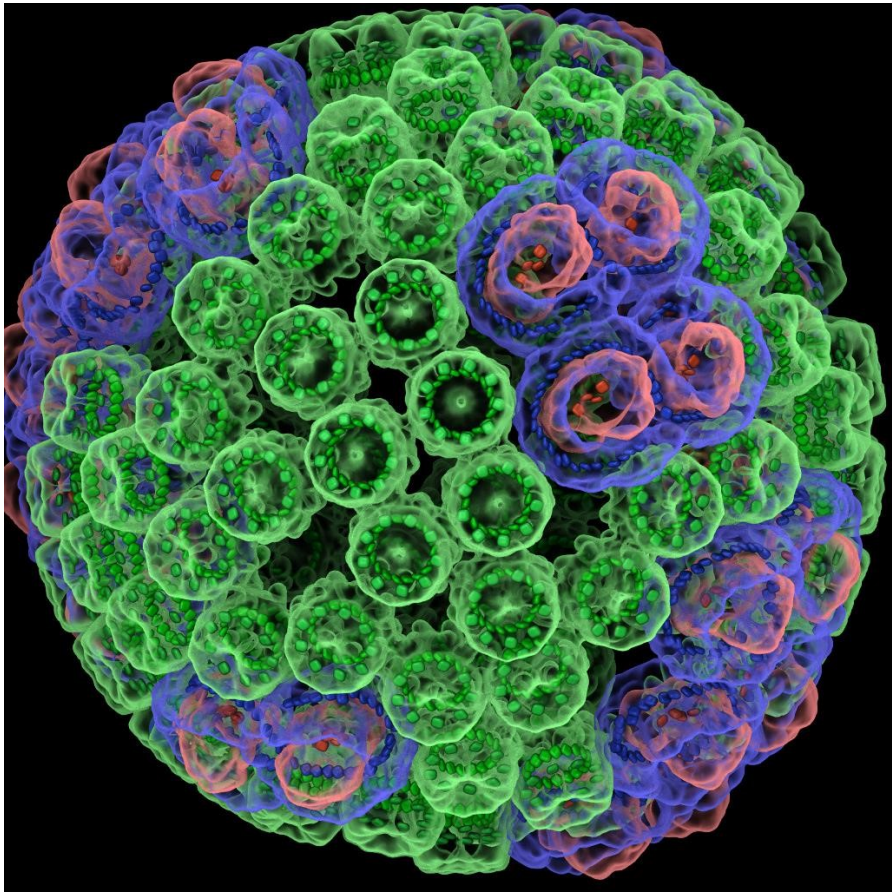


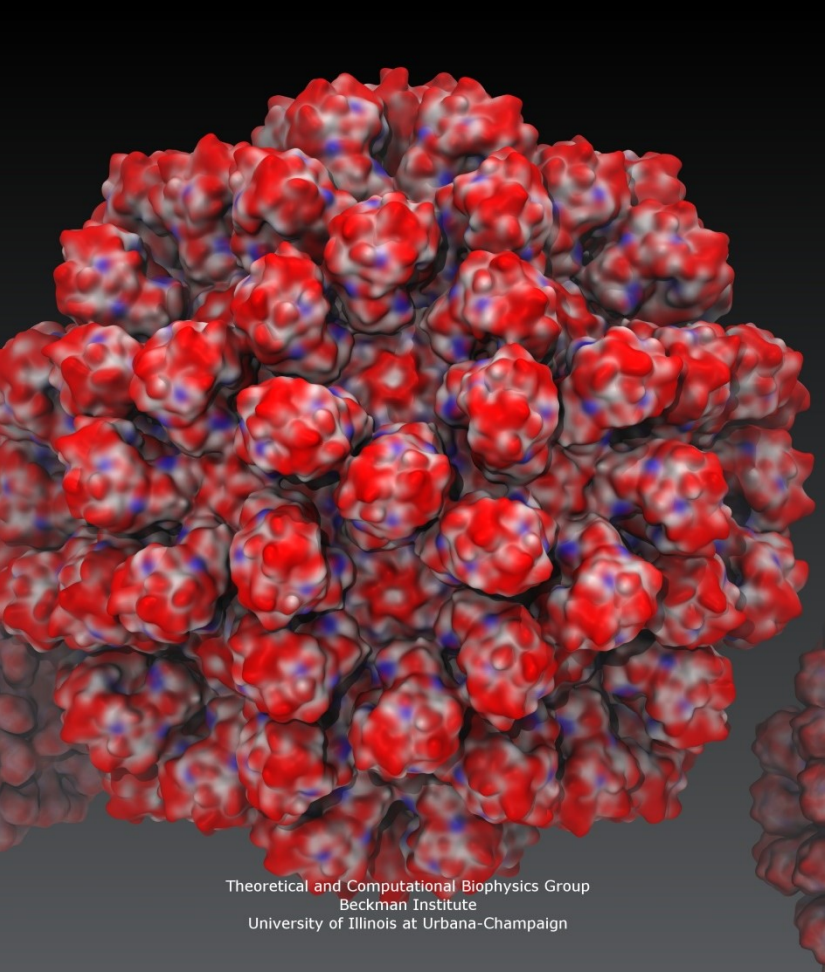


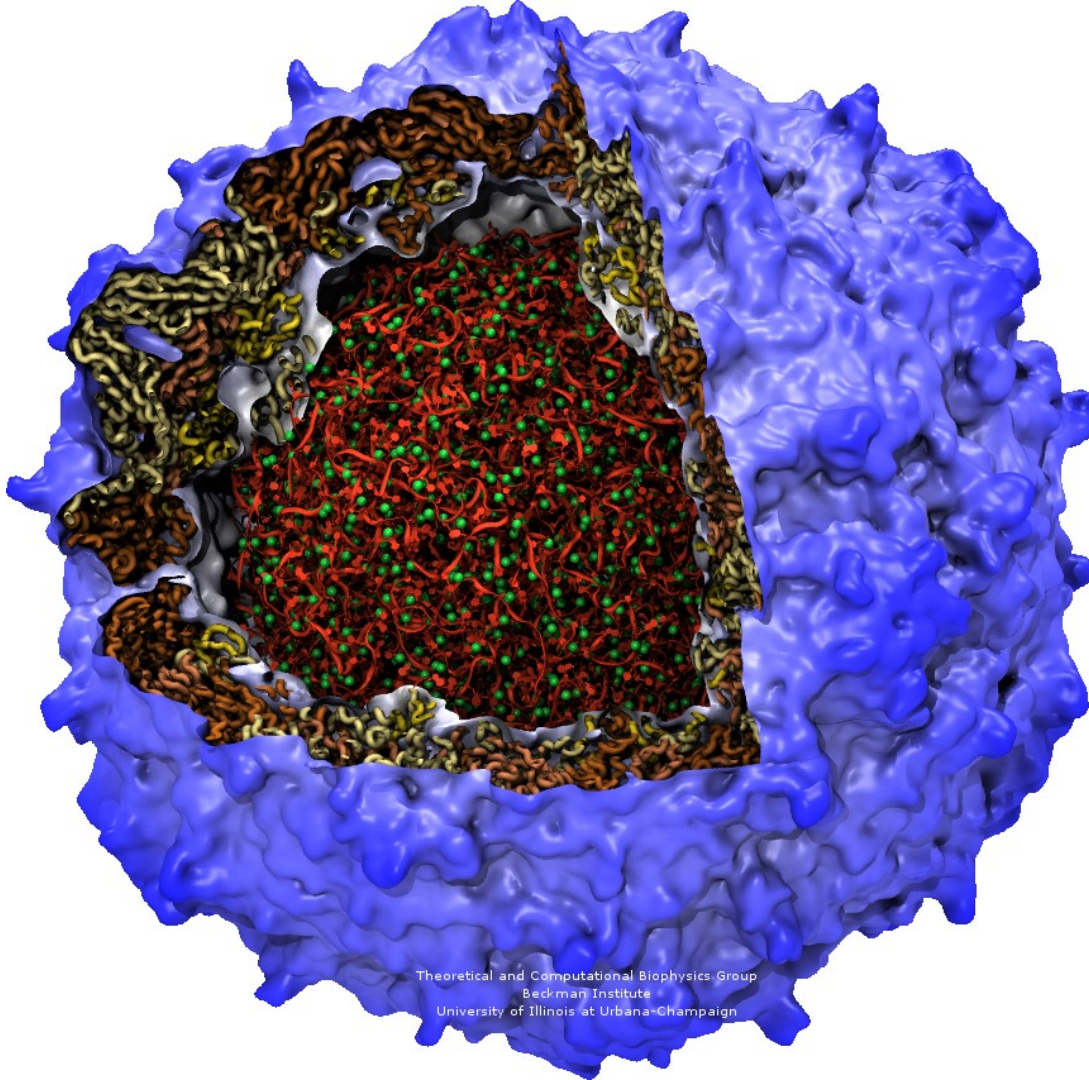


High Fidelity Interactive Visualization

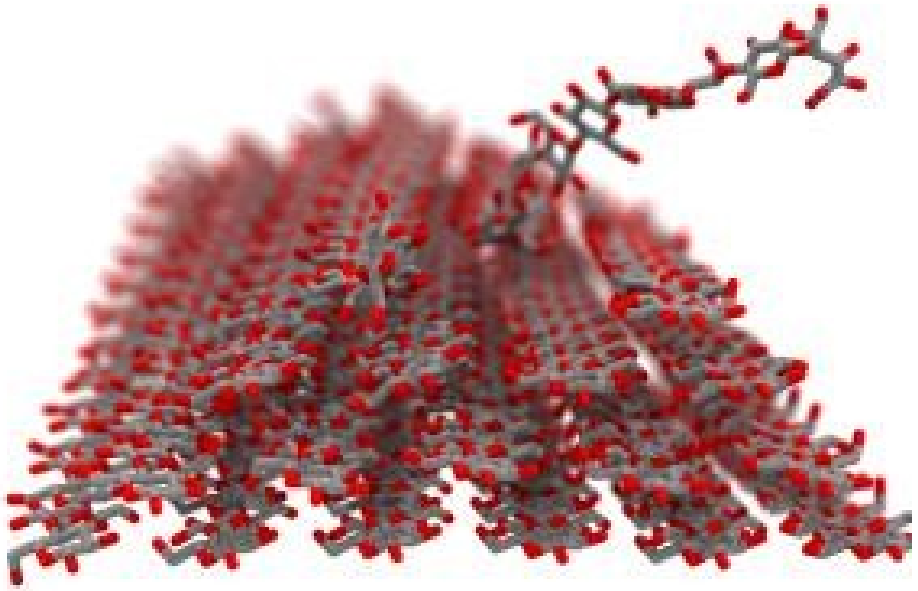
- VMD interactive ray tracing
  - Interactive ray tracing on GPUs with progressive refinement of image and lighting quality
  - Fully interactive rendering of large structures with advanced lighting features, and WYSIWYG “What you see is what you get” final image output



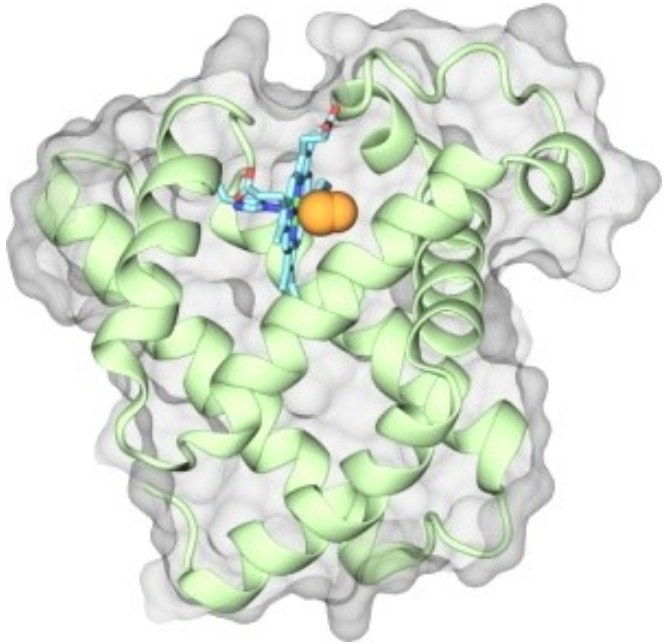

Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign


Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

Diverse Shading and Lighting Approaches

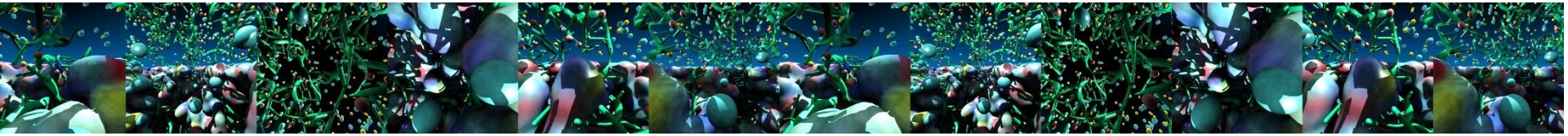


Decrystallization: Interactive Ray Tracing w/ Ambient Occlusion Lighting, Depth of Field Focal Blur

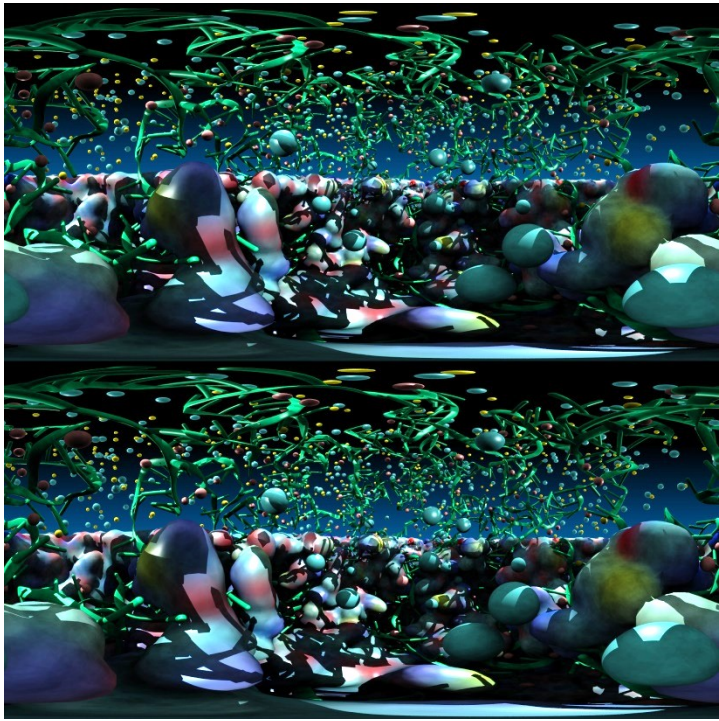


Myoglobin

Stereoscopic Panorama Ray Tracing

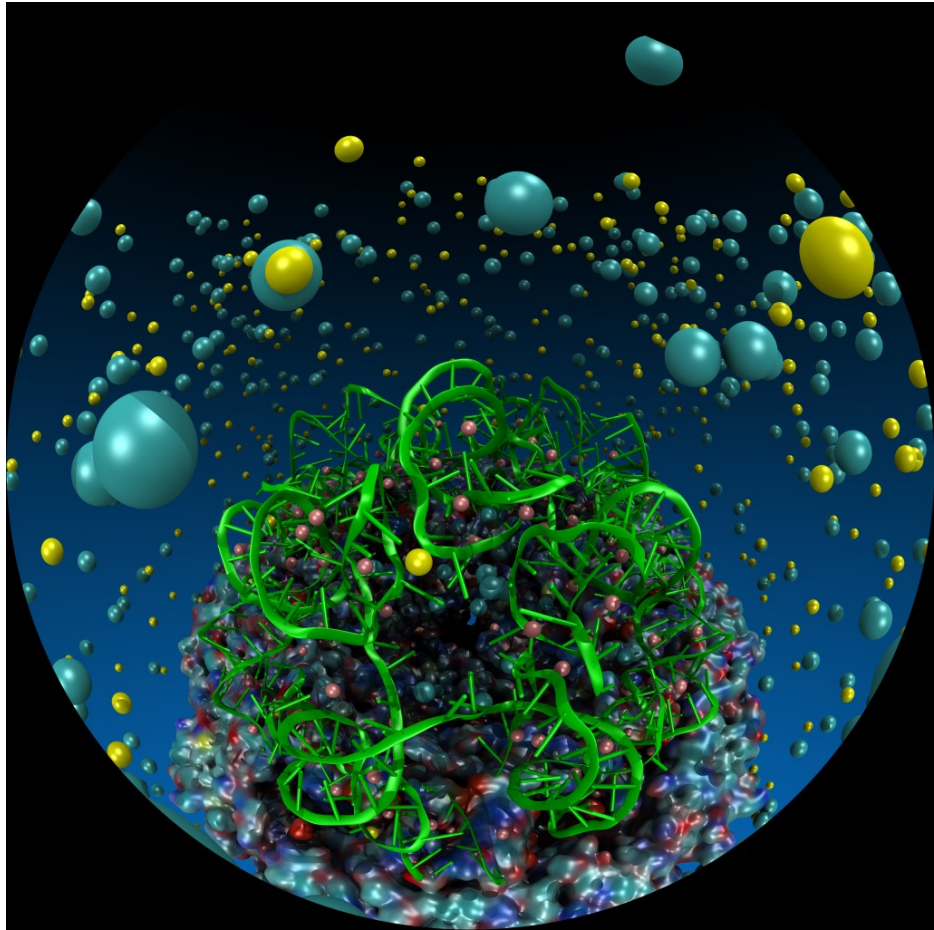


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard, YouTube VR**
- Ray trace omnidirectional stereo spheremaps or cubemaps for very high-frame-rate reprojection and display via OpenGL texturing
- Stereo requires spherical camera projections **poorly suited to rasterization**
- Benefits from OptiX multi-GPU rendering and load balancing, **remote visualization**



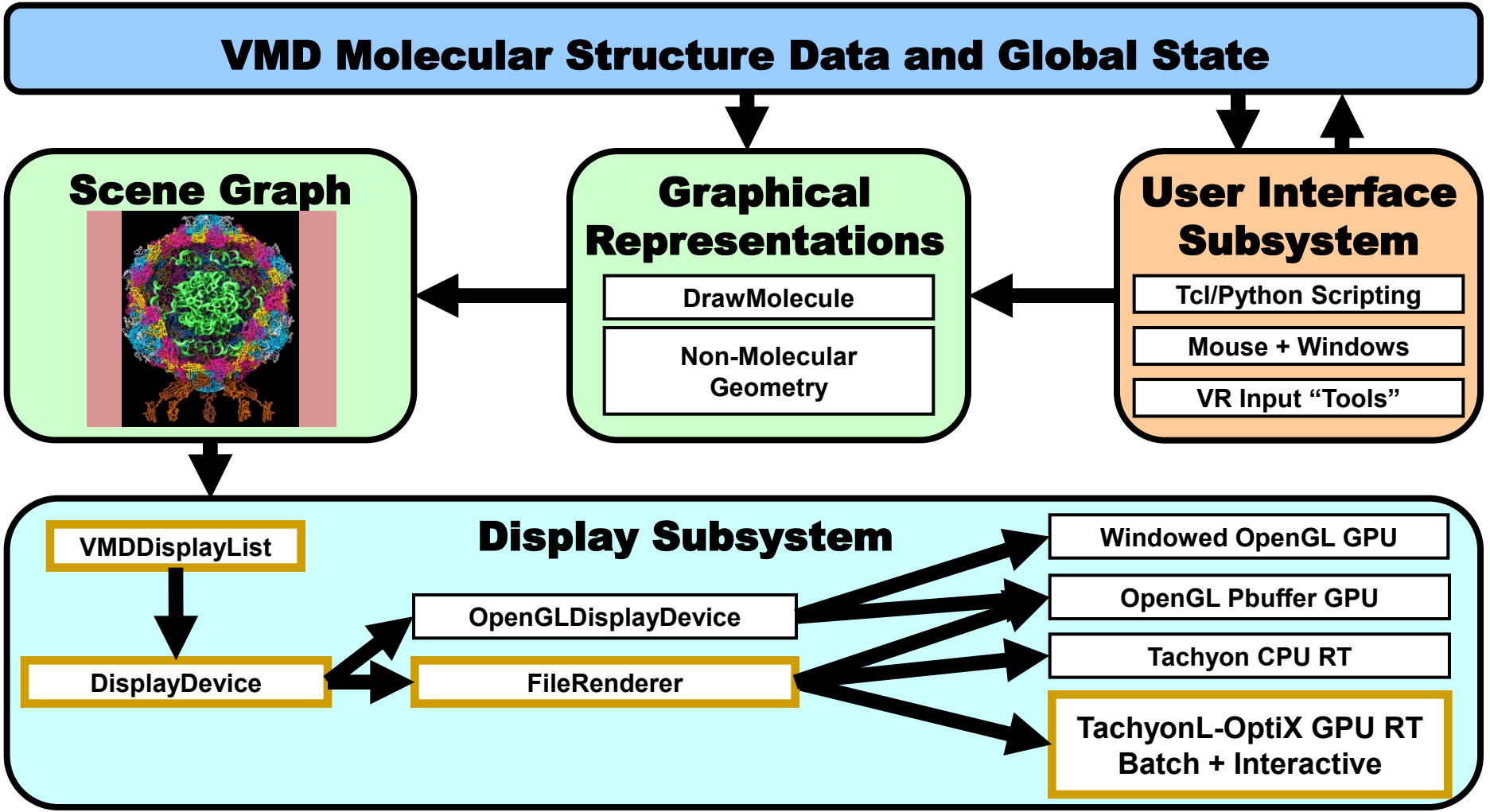
VMD Planetarium Dome Master Camera

- RT-based dome projection -- rasterization poorly suited to non-planar projections
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required

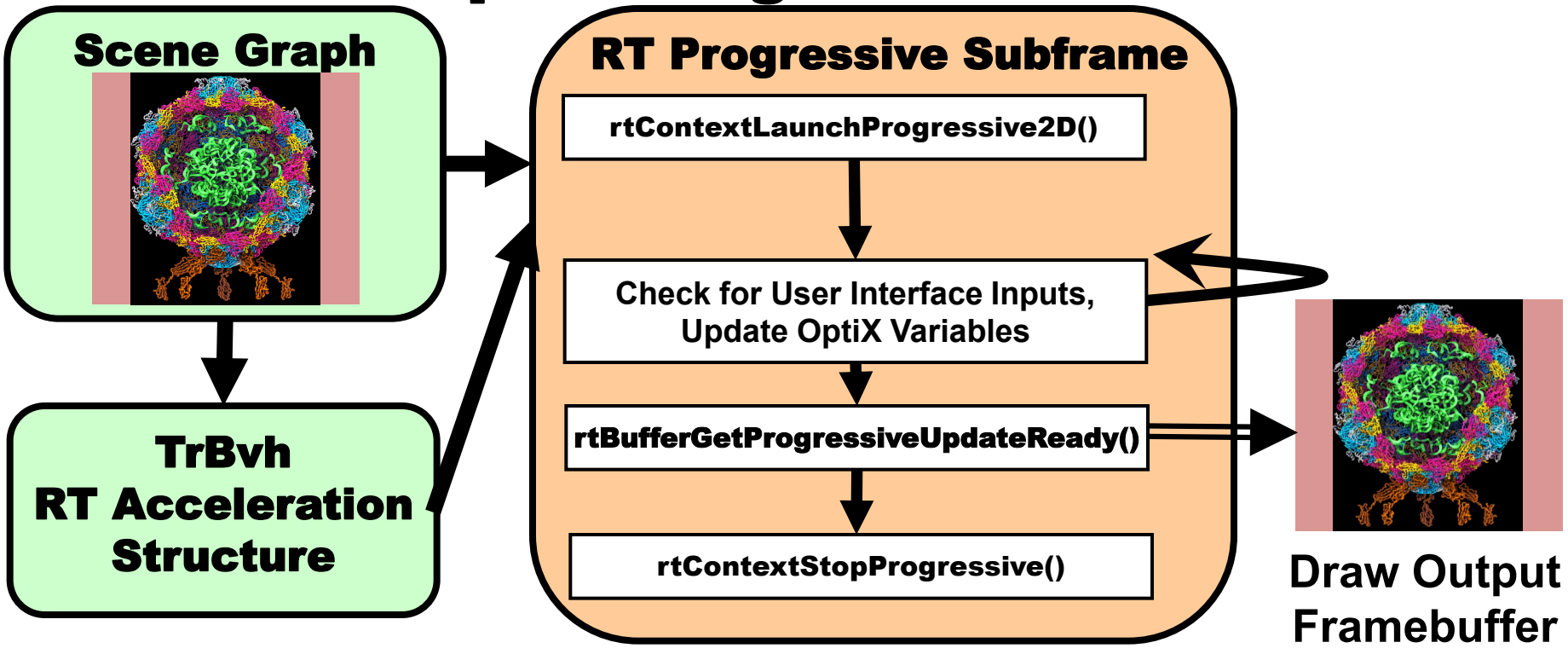


Ray Tracing Performance

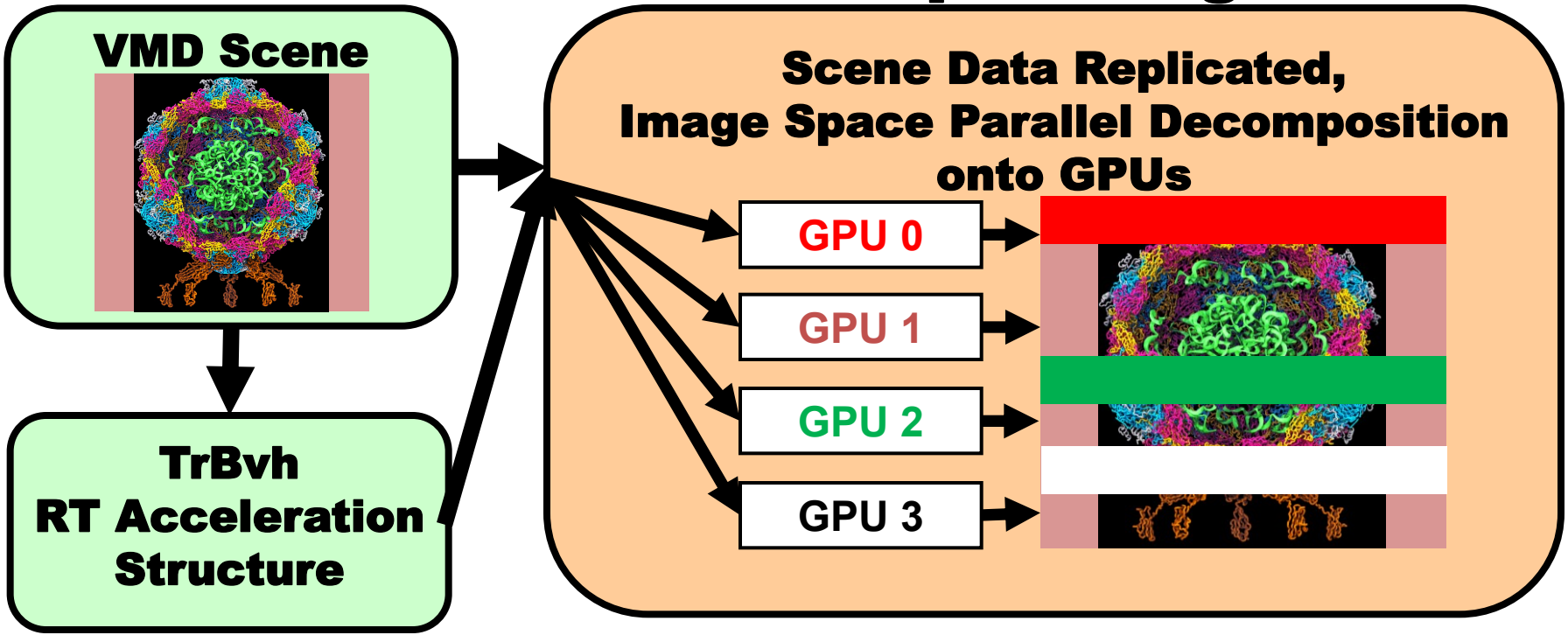
- Well suited to massively parallel hardware
- Peak performance requires full exploitation of SIMD/vectorization, multithreading, efficient use of memory bandwidth
- Traditional languages+compilers not yet up to the taskParallel SPMD-oriented languages and compilers address the shortcomings of traditional tools
- RT frameworks provide performance-critical algorithms:
  - NVIDIA OptiX/CUDA: general RT framework for writing high performance GPU ray tracing engines
  - Intel OSPRay/ISPC: general RT framework and library, includes not only basic kernels but also complete renderer implementations


VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input "Tools"
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL Pbuffer GPU
Tachyon CPU RT
TachyonL-OptiX GPU RT
Batch + Interactive

VMD TachyonL-OptiX Interactive RT w/ OptiX Progressive API

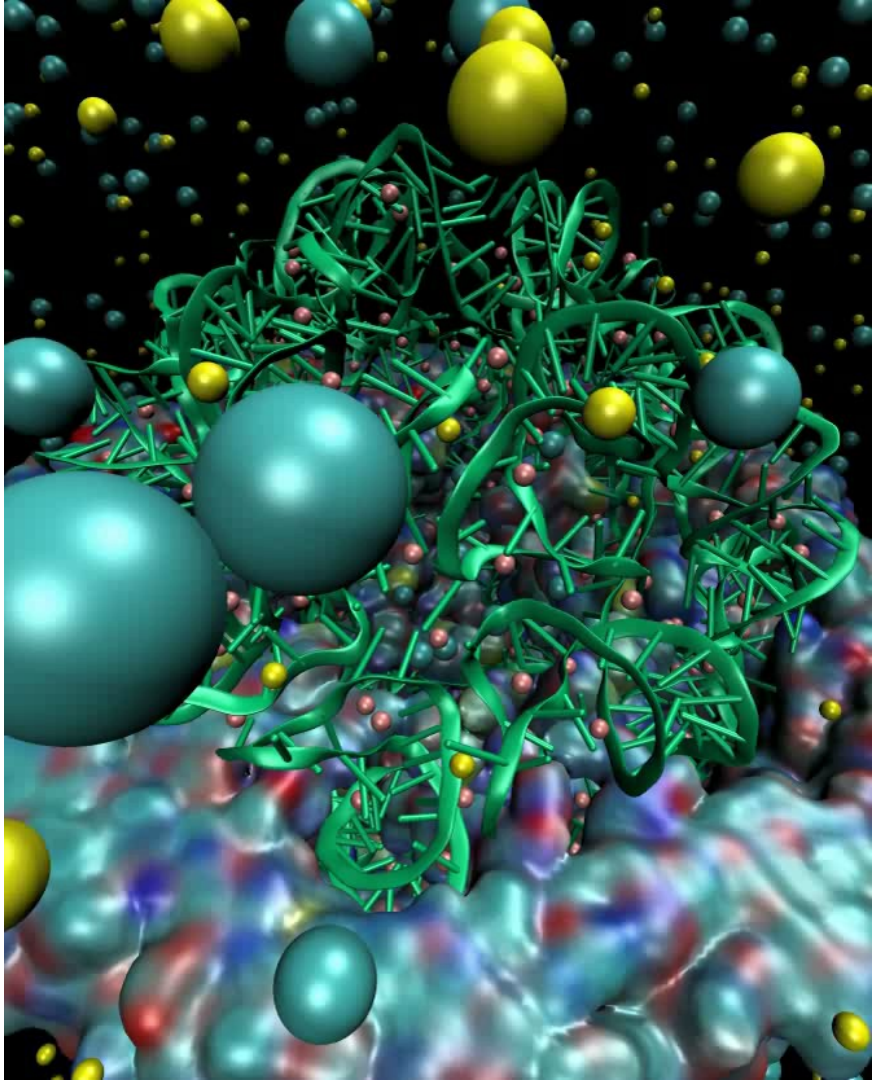


VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node



VMD Interactive GPU Ray Tracing

- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides – ***interactive*** – ray tracing on laptops, desktops, and ***remote*** visual supercomputers
- **Movie was recorded live while using remote visualization**

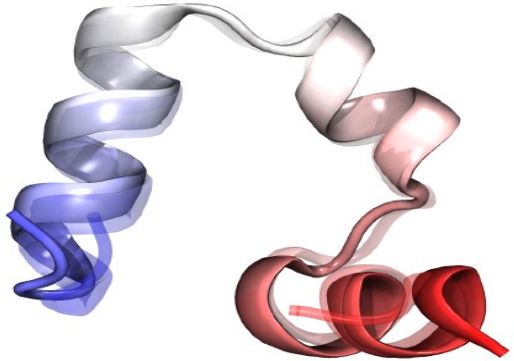


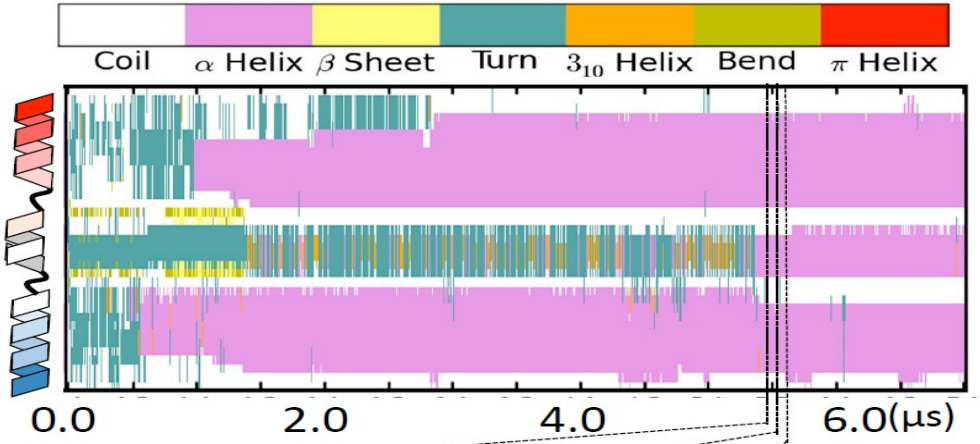
Trajectory and Large System Analysis and Visualization on GPUs, Clusters, and Supercomputers

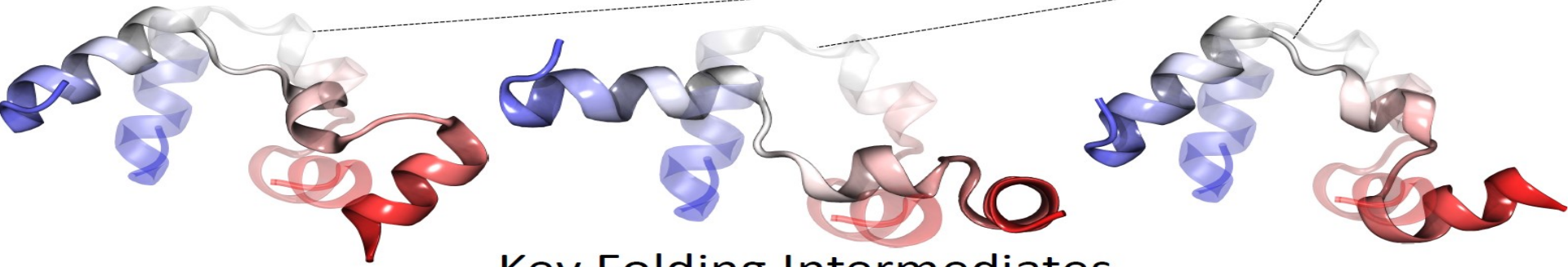
Folding Dynamics of Villin Headpiece Unveiled

6.9μs folding simulation of 30K atoms: 380GB trajectory

Schulten et al. *Biophys J* **94**:L75, 2008, **97**: 2009



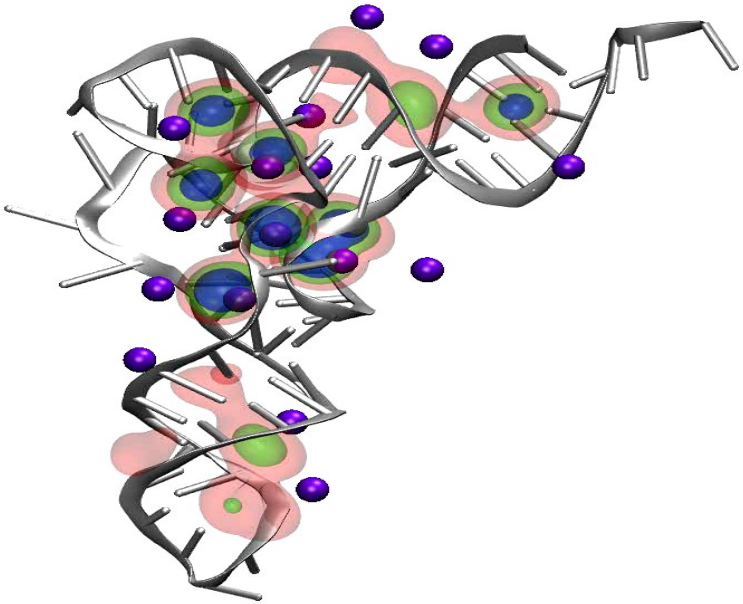




Key Folding Intermediates

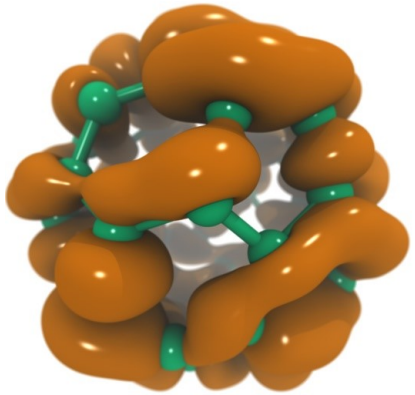
Time-Averaged Volumetric Properties

- Compute density, distance, occupancy, potential maps for a frame or averaged over a trajectory
- Example: display binding sites for diffusively bound ions as probability density isosurfaces



tRNA magnesium ion occupancy: VMD volmap plugin

VMD Tesla P100 Performance for C_{60} Molecular Orbitals, 516x519x507 grid



Hardware platform	Runtime,	Speedup
IBM Power8 (2 socket) (ORNL 'crest') [1]	8.03s,	0.4x
Intel Xeon E5-2660v3 (2 socket) [1]	7.14s,	0.5x
IBM Power8 (ORNL 'crest') + 1x Tesla K40 [1]	3.49s,	**1.0x**
Intel Xeon E5-2698v3 + 1x Tesla P100	**1.35s,**	**2.5x**
IBM Power8 "Minsky" + 1x Tesla P100	**1.09s,**	**3.3x**
IBM Power8 (ORNL 'crest') + 4x Tesla K40 [1]	0.91s,	3.8x
Intel Xeon E5-2698v3 + 4x Tesla P100	**0.37s,**	**9.4x**
IBM Power8 "Minsky" + 4x Tesla P100	**0.30s,**	**11.6x**

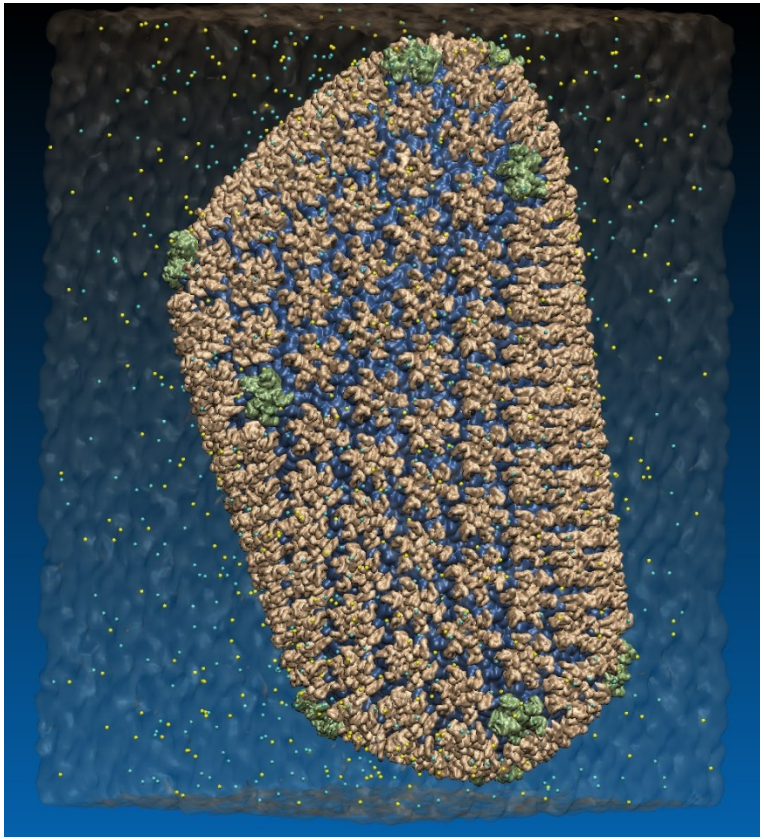
NVLink perf. boost w/ no code tuning

[1] Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software to GPU-Accelerated OpenPOWER Platforms. J. E. Stone, A.-P. Hynninen, J. C. Phillips, K. Schulten. International Workshop on OpenPOWER for HPC (IWOPH'16), LNCS 9945, pp. 188-206, 2016.

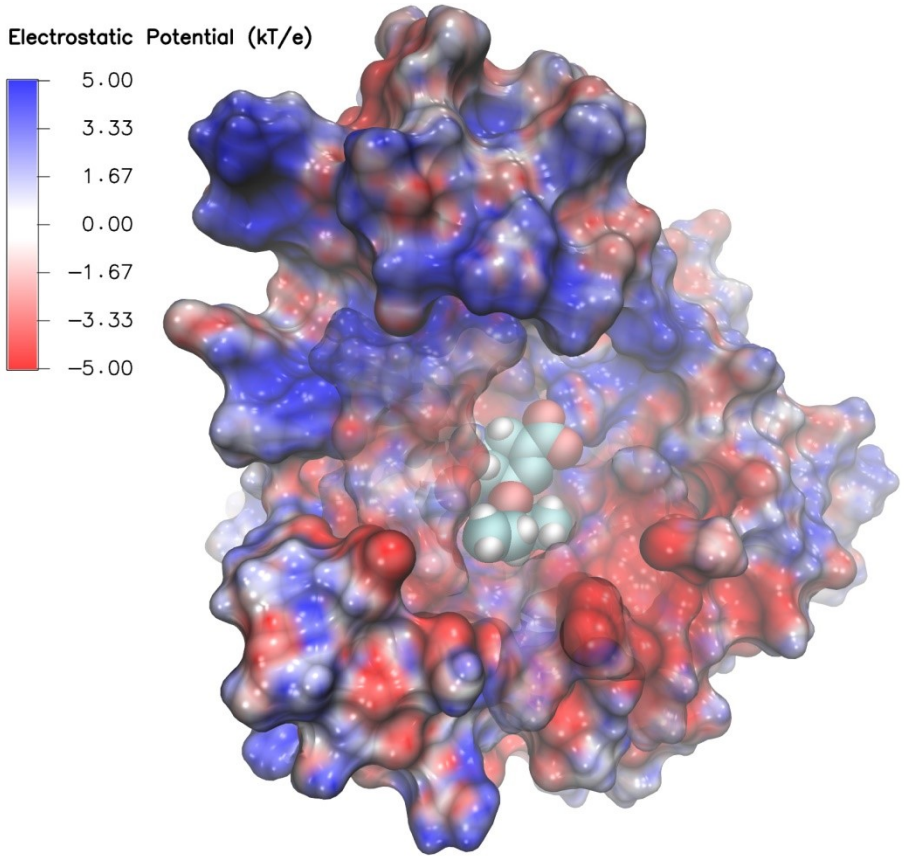
VMD EGL Performance on Amazon EC2 Cloud

MPI Ranks	EC2 "G2.8xlarge" GPU Instances	HIV-1 movie rendering time (sec), (I/O %) 3840x2160 resolution
1	1	626s (10% I/O)
2	1	347s (19% I/O)
4	1	221s (31% I/O)
8	2	141s (46% I/O)
16	4	107s (64% I/O)
32	8	90s (76% I/O)

Performance at 32 nodes reaches ~48 FPS



64M atom HIV-1 capsid simulation rendered via EGL



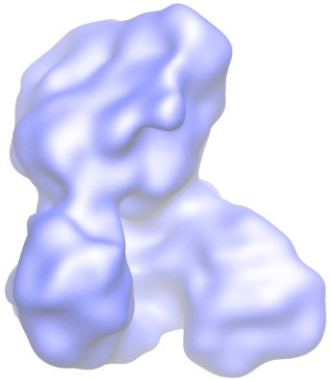
Swine Flu A/H1N1 neuraminidase bound to Tamiflu: VMD EGL rendering demonstrating full support for all VMD shaders and OpenGL features, multisample antialiasing, ray cast spheres, 3-D texture mapping, ...

Petascale Computing - A Key Instrument for Life Science

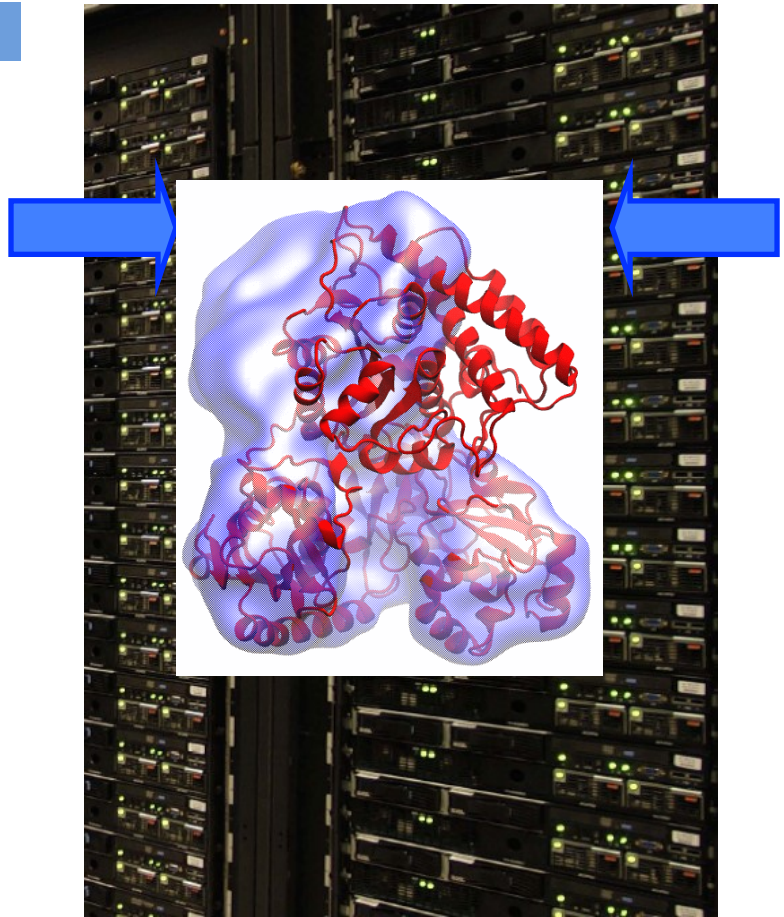
MDFF Solves Structures from X-ray Crystallography and Cryo-EM

Electron microscopy

FEI microscope

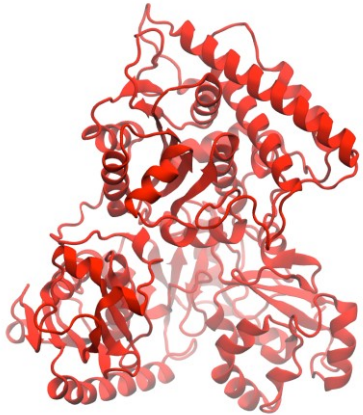


Electron density of protein in action at low resolution



X-ray crystallography

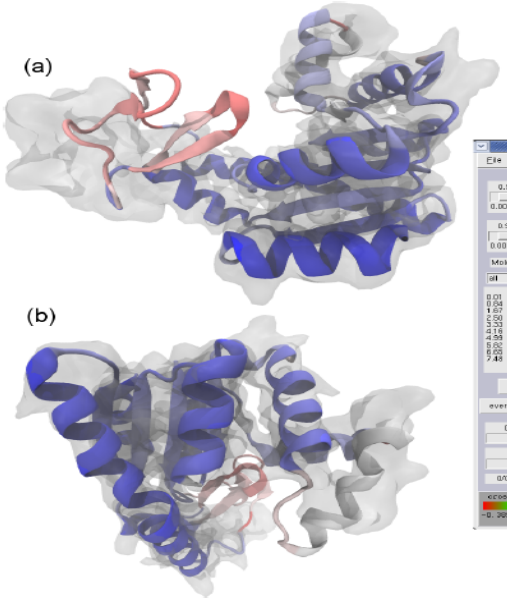
APS at Argonne

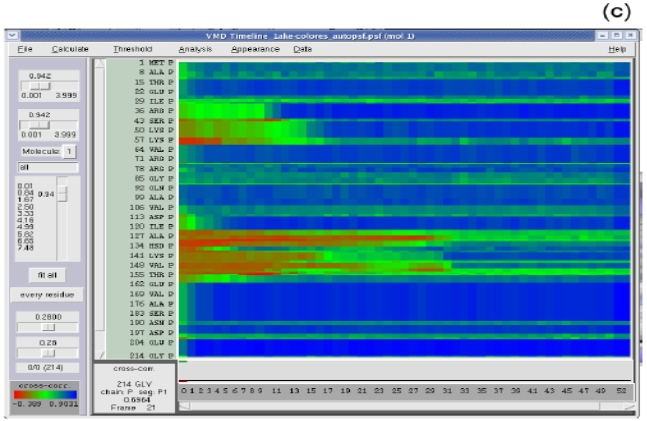


Ideal protein structure at high resolution
Acetyl – CoA Synthase

VMD Timeline Plugin: Analyze MD Traiectories for Events

GPU-accelerated MDFF
Cross Correlation Timeline
Regions with poor fit
Regions with good fit



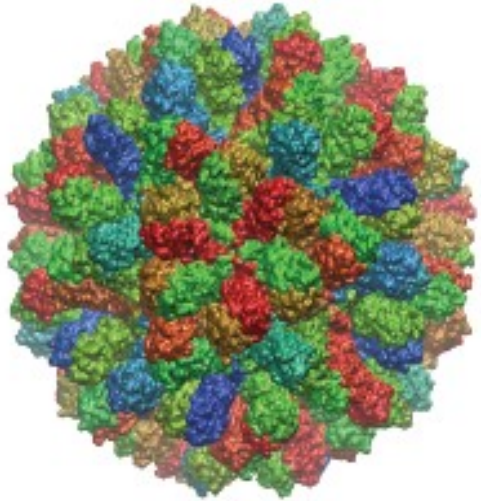


- **Interactive** 2-D heatmap plot linked to 3-D structure
- Single picture shows changing properties across structure+trajectory
- Explore time vs. per-selection attribute, linked to molecular structure
- Many analysis methods available; user-extendable

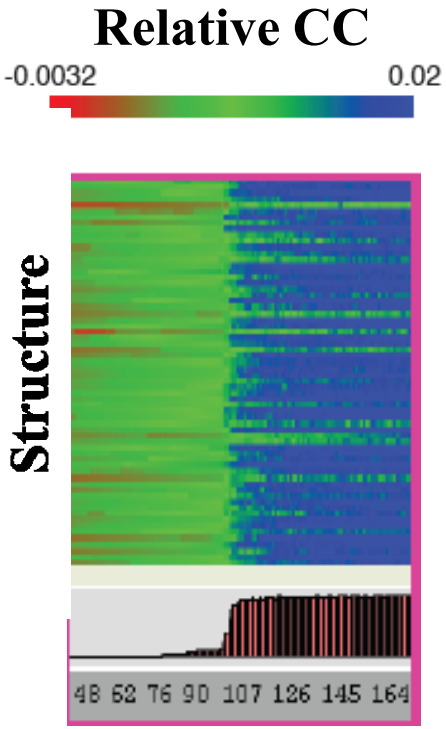
Parallel MDFF Cross Correlation Analysis on Cray XK7

Rabbit Hemorrhagic Disease Virus (RHDV)	
Traj. frames	10,000
Structure component selections	720
Single-node XK7 (projected)	336 hours (14 days)
128-node XK7	3.2 hours 105x speedup
2048-node XK7	19.5 minutes 1035x speedup

Calculation of 7M CCs would take **5 years** using serial CPU algorithm!



RHDV colored by relative CC



Stone et al., Faraday Discuss., 169:265-283, 2014.

VMD MDFF Cross Correlation

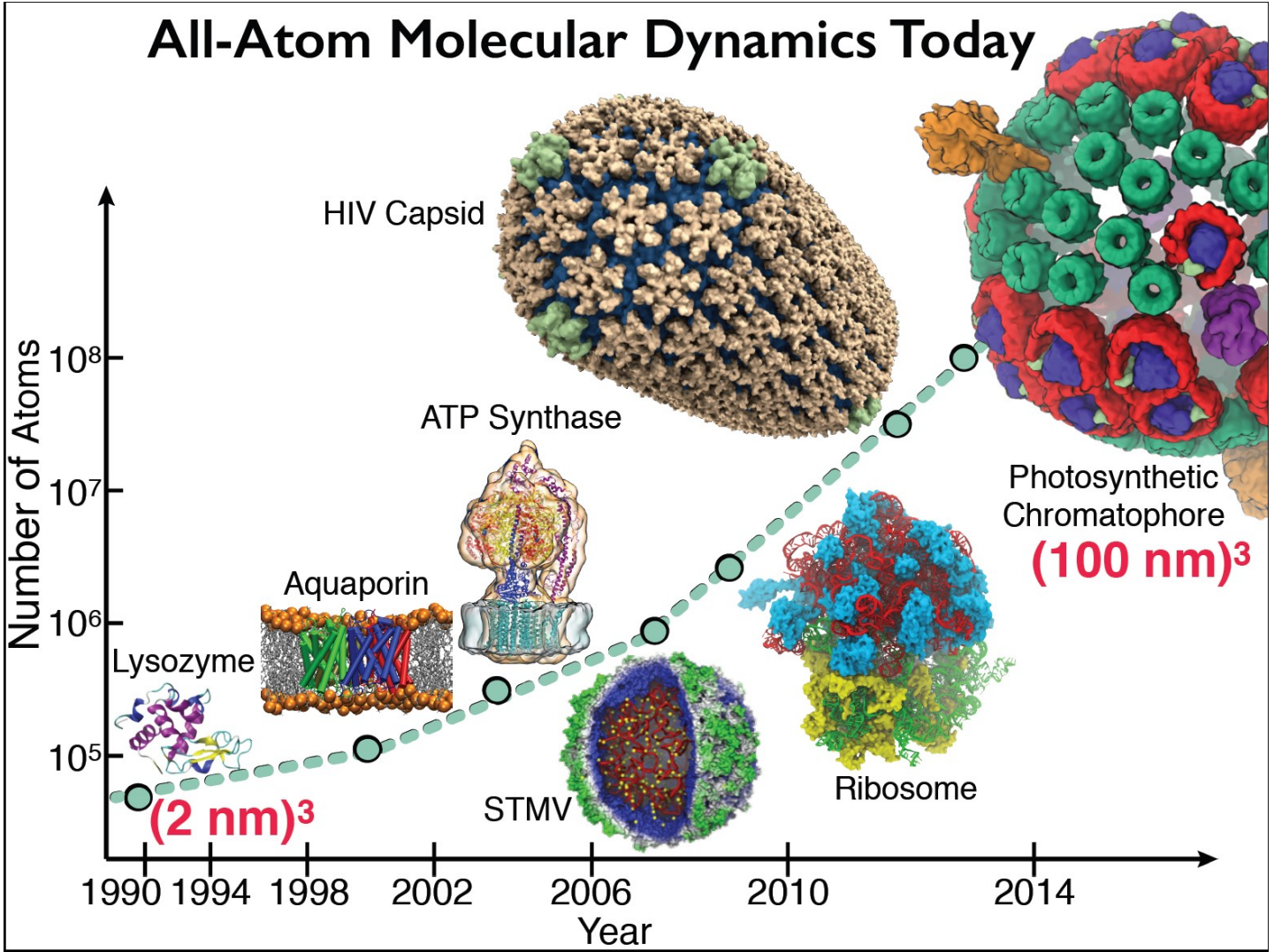
Rabbit Hemorrhagic Disease Virus: 702K atoms, 6.5Å resolution

Software, Hardware platform	Runtime, Speedup vs. Chimera,	VMD+GPU
Chimera, Intel Xeon E5-2687W (2 socket) [1]	15.860s, 1x	
VMD, Intel Xeon E5-2687W (2 socket) [1]	0.779s, 20x	
VMD-CUDA, Intel Xeon E5-2687W + Quadro K6000 [1,2]	0.458s, 35x	**1.0x**
VMD-CUDA, Intel Xeon E5-2698v3 + Tesla P100 [3]	**0.090s,** 176x	**5.1x**
VMD-CUDA, IBM Power8 "Minsky" + Tesla P100 [3]	**0.080s,** 198x	**5.7x**

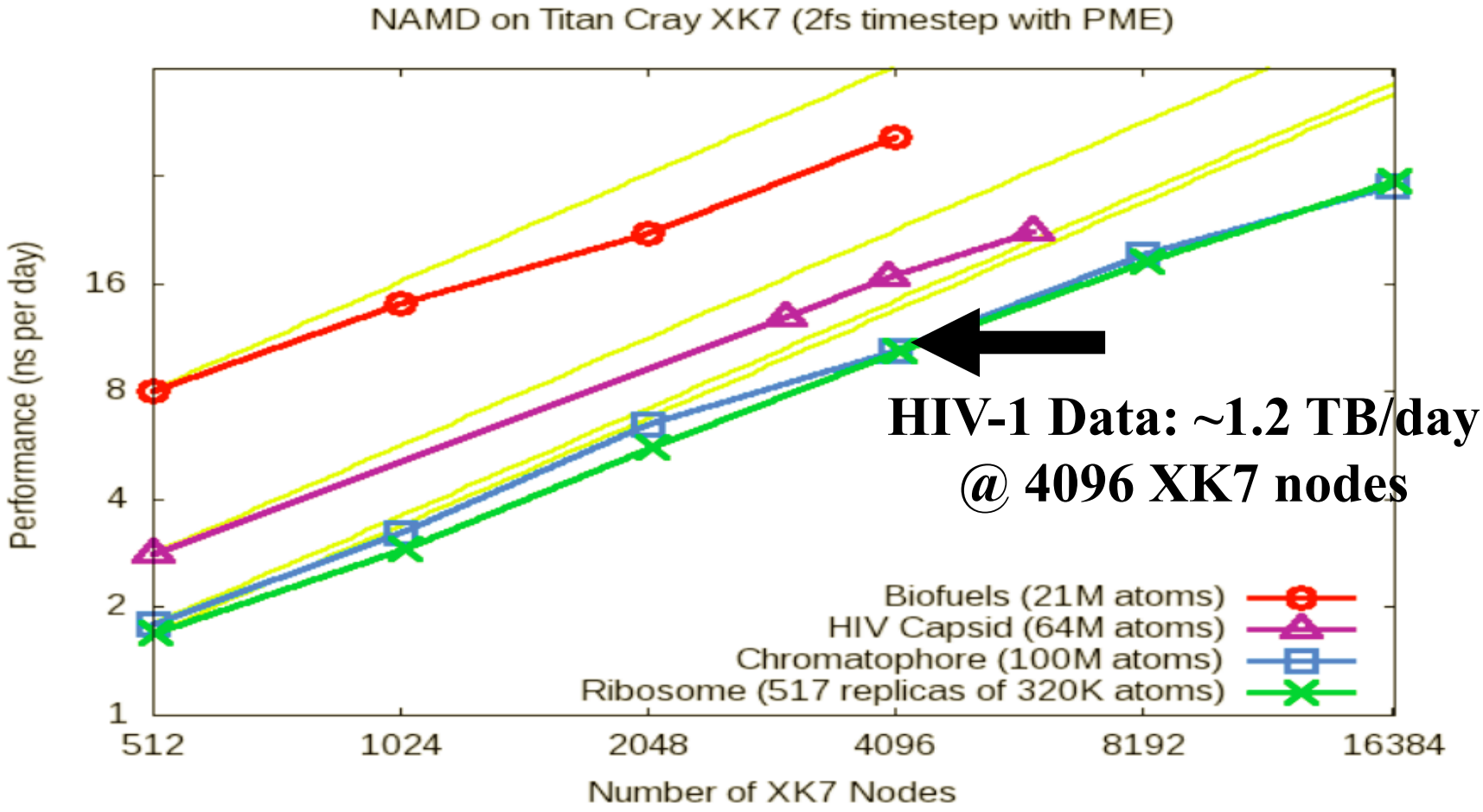
[1] GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting. J.E. Stone, R. McGreevy, B. Isralewitz, and K. Schulten. Faraday Discussions 169:265-283, 2014.

[2] Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software to GPU-Accelerated OpenPOWER Platforms. J. E. Stone, A.-P. Hynninen, J.C. Phillips, K. Schulten. IIWOPH'16, LNCS 9945, pp. 188-206, 2016.

[3] Latest results, VMD 1.9.3 November 2016


All-Atom Molecular Dynamics Today
HIV Capsid
ATP Synthase
Aquaporin
Lysozyme
STMV
Ribosome
Photosynthetic Chromatophore
(100 nm)3
(2 nm)3
Number of Atoms
10^8
10^7
10^6
10^5
1990
1994
1998
2002
2006
2010
2014
Year

NAMD Titan XK7 Performance August 2013

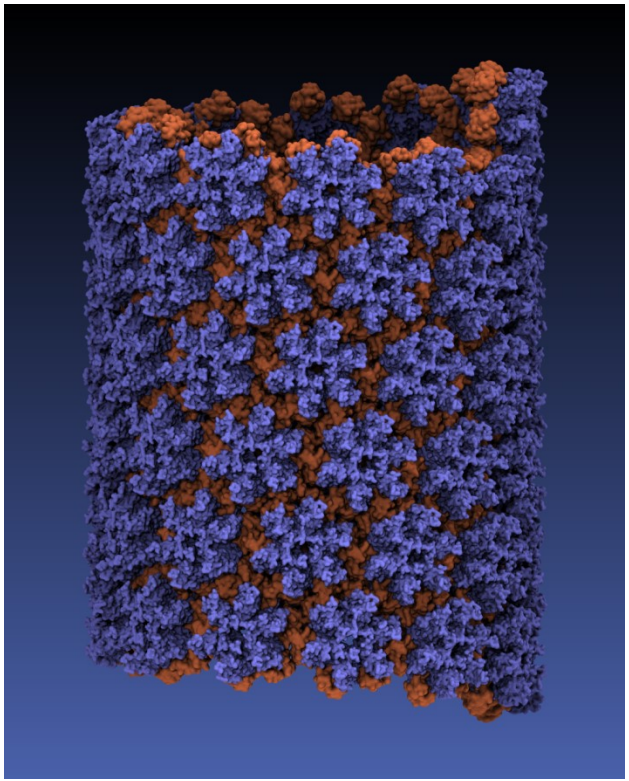


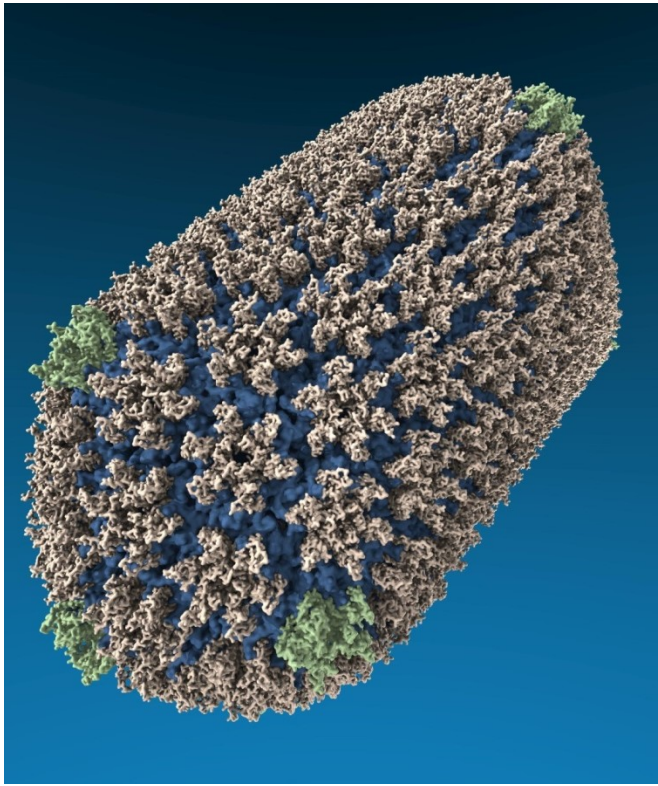
VMD Petascale Visualization and Analysis

- Analyze/visualize large trajectories too large to transfer:
  - Time-averaged electrostatic fields, MDFF quality-of-fit, etc.
  - User-defined parallel analysis operations, data types
  - Parallel rendering, movie making
- Parallel I/O up to **275 GB/sec** on 8192 nodes – read **231 TB in 15 minutes!**
- VMD uses GPU-accelerated Cray XK7 nodes for both visualization and analysis
  - **OpenGL, Ray Tracing**
  - **Future: Remote Interactive Viz!**

NCSA Blue Waters Hybrid
Cray XE6 / XK7 Supercomputer
22,640 XE6 CPU nodes
4,224 XK7 nodes w/ GPUs

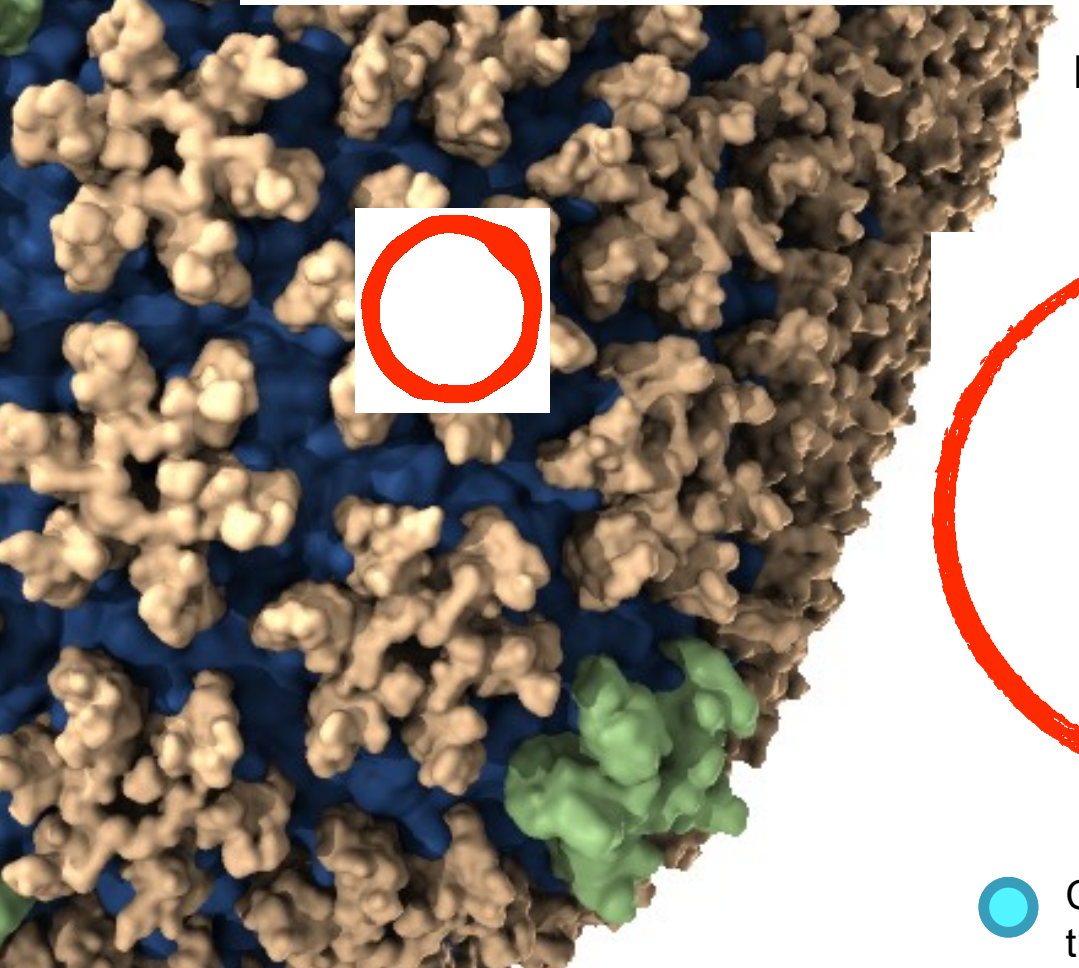
VMD “QuickSurf” Representation, Ray Tracing



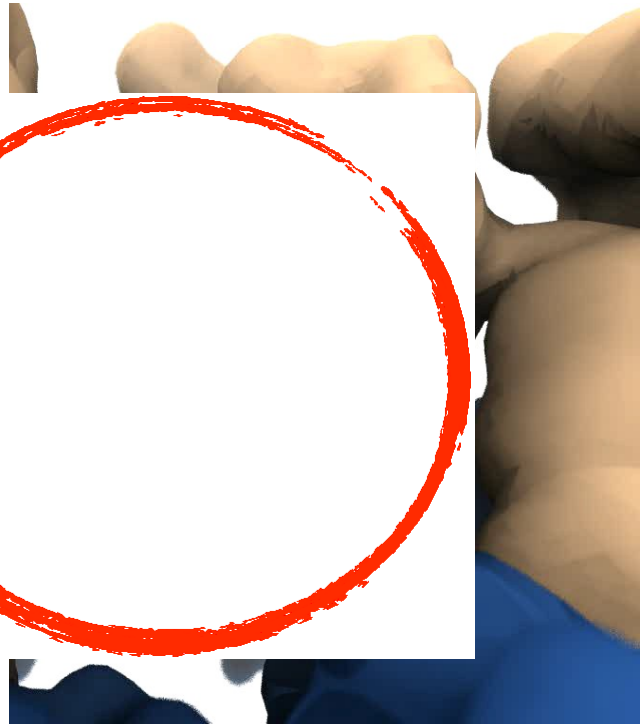


All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

Capsid acts as an osmotic regulator

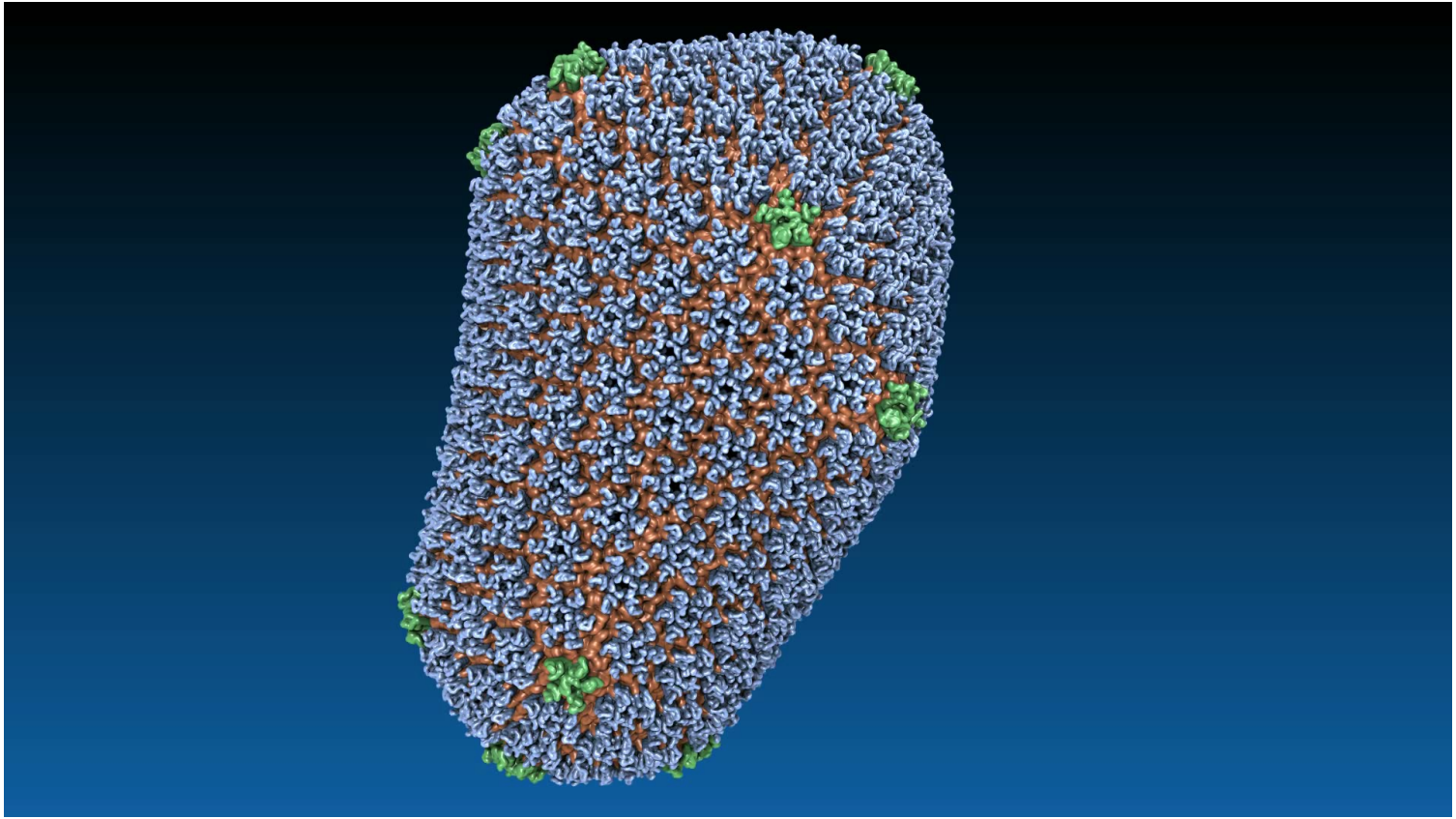


Results from 64 M atom, 1 μs sim

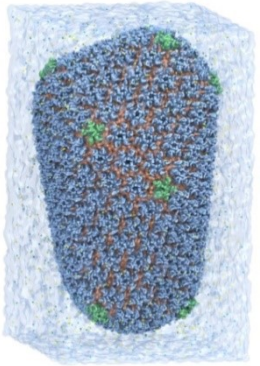


Chloride ions permeate through the hexameric center

HIV-1 Capsid



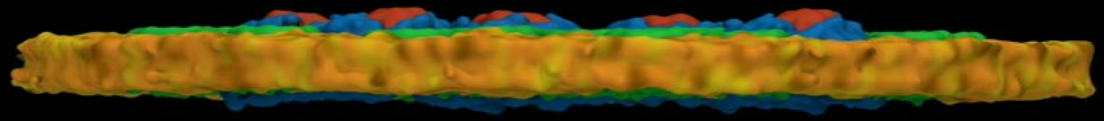
HIV-1 Parallel HD Movie Rendering on Blue Waters Cray XE6/XK7



New VMD TachyonL-OptiX on XK7 vs. Tachyon on XE6:
K20X GPUs yield **up to twelve times** geom+ray tracing speedup

Ray Tracer Version	Node Type and Count	Script Load	State Load	Geometry + Ray Tracing	Total Time
New TachyonL-OptiX	64 XK7 Tesla K20X GPUs	2 s	39 s	435 s	476 s
New TachyonL-OptiX	**128 XK7 Tesla K20X GPUs**	**3 s**	**62 s**	**230 s**	**295 s**
TachyonL-OptiX [1]	64 XK7 Tesla K20X GPUs	2 s	38 s	655 s	695 s
TachyonL-OptiX [1]	128 XK7 Tesla K20X GPUs	4 s	74 s	331 s	410 s
TachyonL-OptiX [1]	**256 XK7 Tesla K20X GPUs**	**7 s**	**110 s**	**171 s**	**288 s**
Tachyon [1]	**256 XE6 CPUs**	7 s	160 s	**1,374 s**	**1,541 s**
Tachyon [1]	512 XE6 CPUs	13 s	211 s	808 s	1,032 s

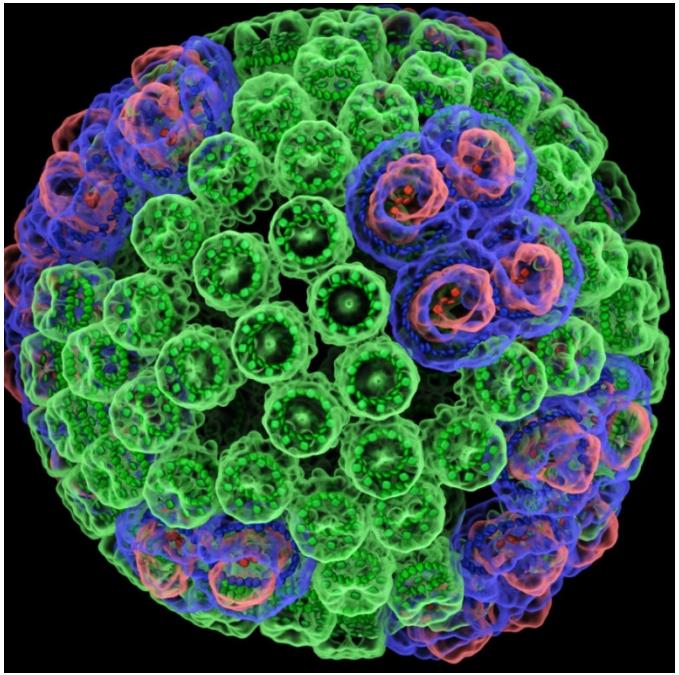
[1] GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13: Proceedings of the 8th International Workshop on Ultrascale Visualization, pp. 6:1-6:8, 2013.



20 M atom chromatophore patch

VMD Chromatophore Rendering on Blue Waters

- New representations, GPU-accelerated molecular surface calculations, memory-efficient algorithms for huge complexes
- VMD GPU-accelerated ray tracing engine w/ OptiX+CUDA+MPI+Pthreads
- ***Each revision:*** 7,500 frames render on ~96 Cray XK7 nodes in 290 node-hours, 45GB of images prior to editing

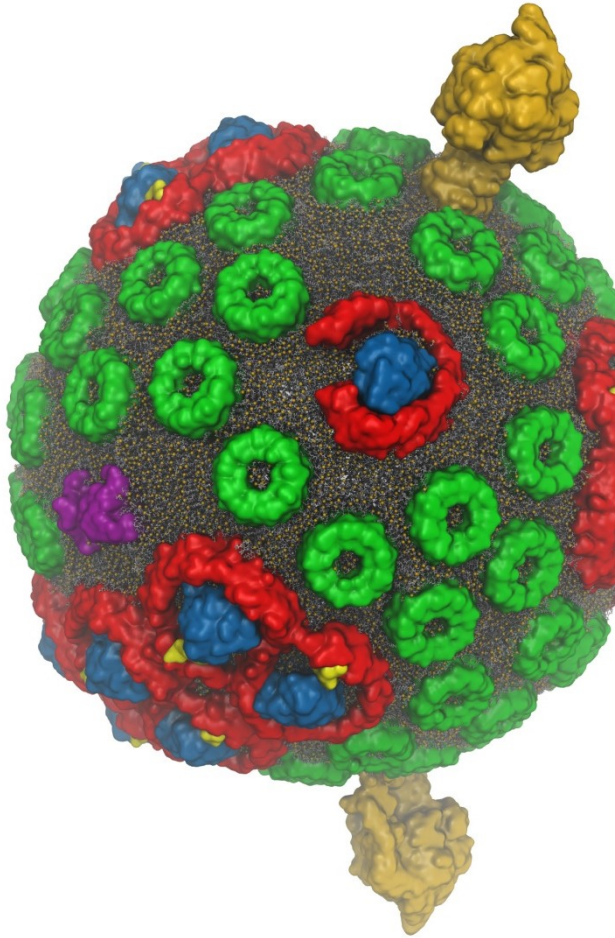


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.
M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.
Winner of the SC'14 Visualization and Data Analytics Showcase

VMD 1.9.3+OptiX 4 – ~1.5x Performance Increase on Blue Waters Supercomputer

- OptiX GPU-native **“Trbvh” acceleration structure builder** yields substantial perf increase vs. CPU builders running on Opteron 6276 CPUs
- New optimizations in VMD TachyonL-OptiX RT engine:
  - **CUDA C++ Template specialization of RT kernels**
    - **Combinatorial expansion of ray-gen and shading kernels at compile-time: stereo on/off, AO on/off, depth-of-field on/off, reflections on/off, etc…**
    - **Optimal kernels selected from expansions at runtime**
  - **Streamlined OptiX context and state management**
  - **Optimization of GPU-specific RT intersection routines, memory layout**

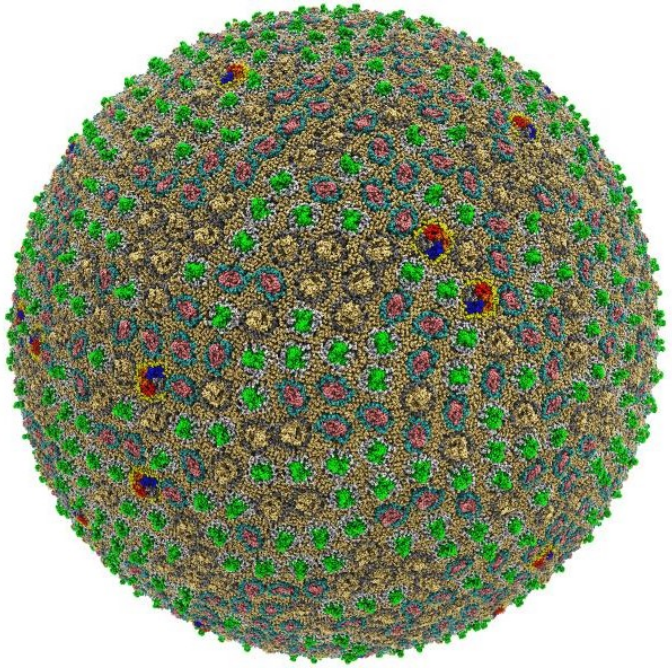


VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.

Preparation, Visualization, Analysis of All-Atom Cell-Scale Simulations

- Support for large memory (TB), up to **2 billion atoms per "molecule" now**
- Interactive rasterization w/ Vulkan, EGL
- **Interactive ray tracing on CPUs and GPUs**
- Parallel analysis, visualization w/ MPI

- 200 nm spherical envelope
- Membrane with ~50% occupancy by proteins
- 63M atoms in envelope model

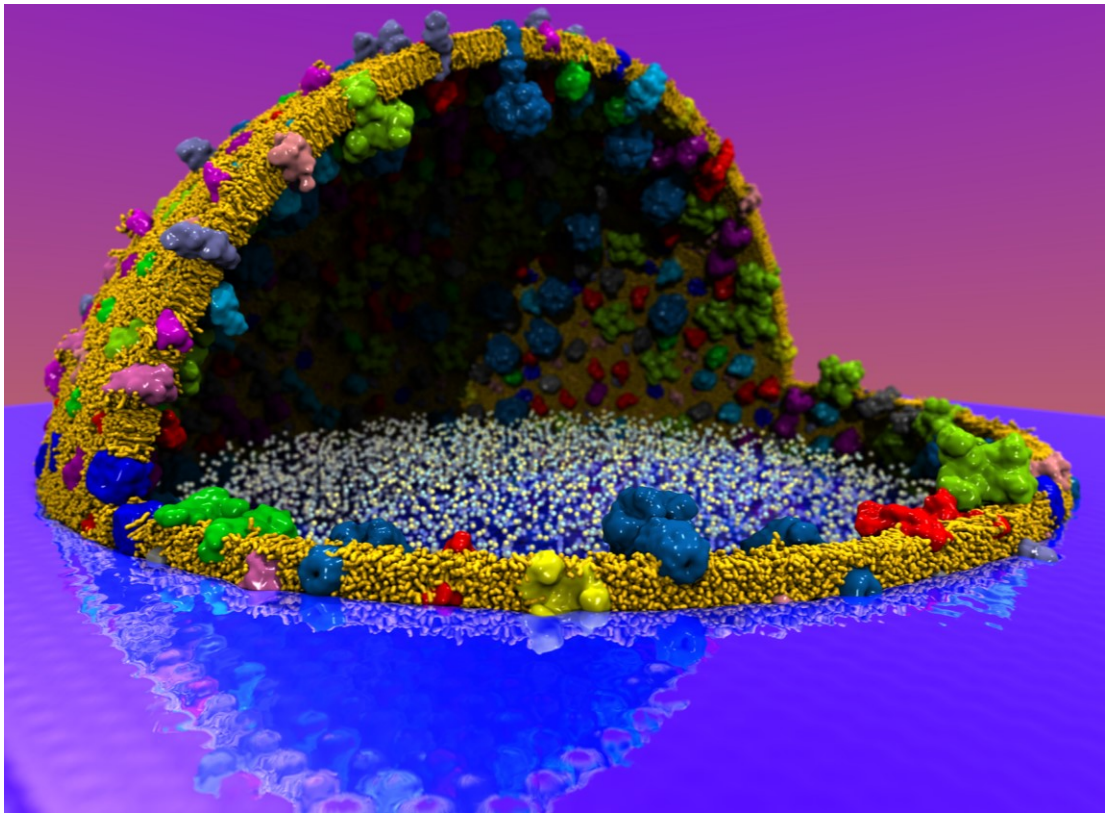


Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J.E. Stone, …, K. Schulten, J. Parallel Computing, 55:17-27, 2016.

High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. J.E. Stone, ..., K. Schulten. IEEE High Performance Data Analysis and Visualization, IPDPSW, pp. 1014-1023, 2016.

Modeling, Visualization, Analysis of Cell-Scale Systems

- Build interactive tools for density map manipulation, segmentation, data-guided modeling
- Cell-scale placement of macromolecules
- Fast graphics “instancing”, LoD
- New and improved structure file formats, data compression, …
- Use non-volatile memory technologies to facilitate cell-scale modeling with high performance

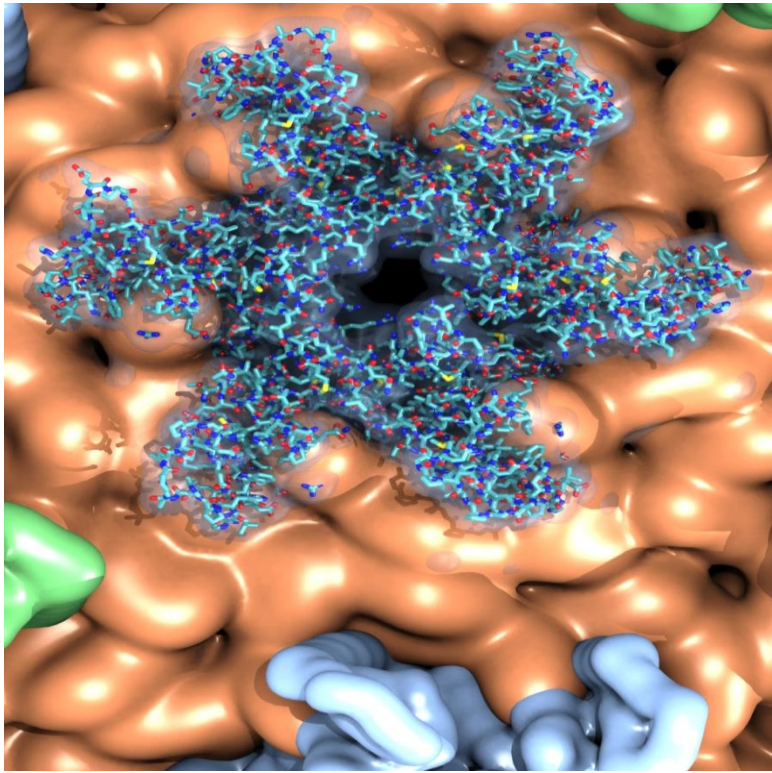


VMD “Coming Soon”: Built-in Remote Visualization Virtual Reality HMDs

VMD Coming Soon

- Improved structure building and analysis tools
- Many new and updated user-contributed plugins:
- Further integration of interactive ray tracing
  - Seamless interactive RT in main VMD display window
  - Support trajectory playback in interactive RT
  - Enable multi-node interactive RT on HPC systems

- Built-in (basic) interactive remote visualization on HPC clusters and supercomputers



GPU Ray Tracing of
HIV-1 Capsid Detail

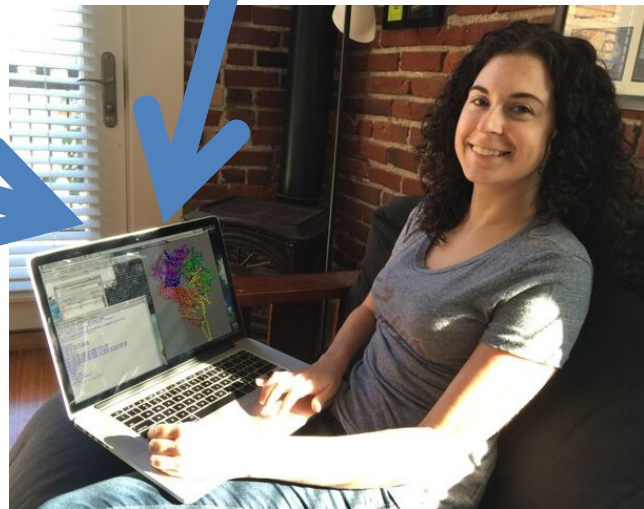
Remote Visualization and Analysis

VMD w/ built-in remote visualization:

- Access **large data** located anywhere in the world
- Enable capabilities not possible with conventional laptops or workstations
- VMD session available to any device, browser

Clusters, Supercomputers

Workstations,
Servers,
Cloud



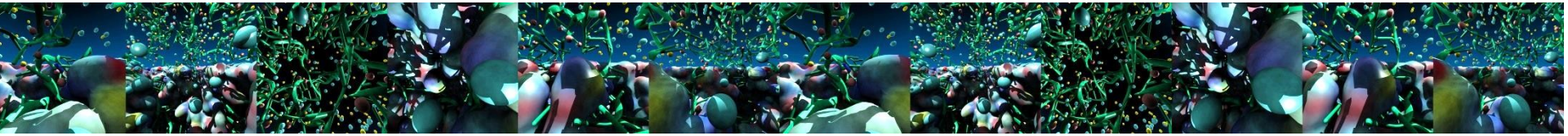
Chemical Visualization of Human Pathogens: the Retroviral Capsids.
J.R. Perilla, B.-C. Goh, J.E. Stone, K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.
Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.
J.E. Stone, …, K. Schulten, J. Parallel Computing, 55:17-27, 2016.
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J.E. Stone, W.R. Sherman, K. Schulten. IEEE HPDAV (IPDPSW), pp. 1048-1057, 2016.

Immersive Viz. w/ VMD

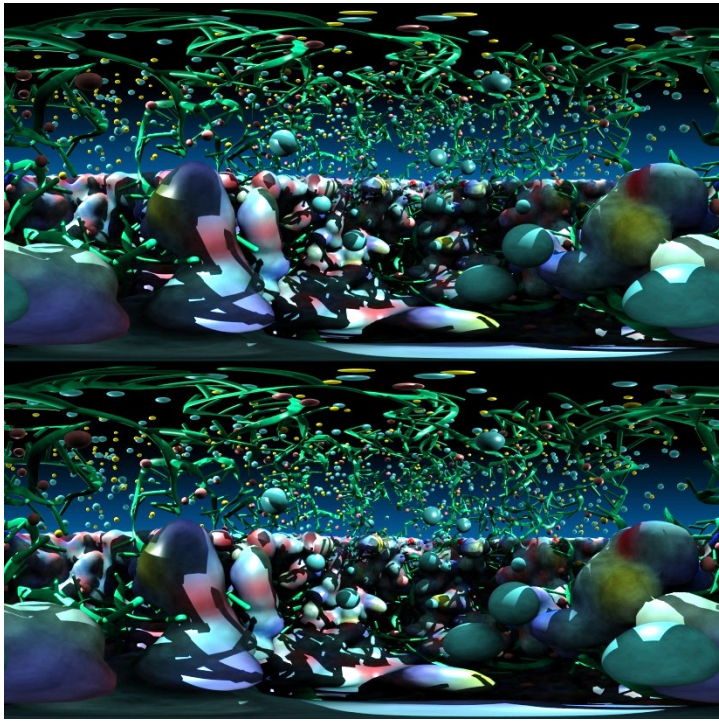
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support for remote visualization
  - UIs, multi-user collaboration/interaction
  - Rendering perf for large molecular systems
  - Accomodating limitations idiosynchracies of commercial HMDs

VMD running in a CAVE

Stereoscopic Panorama Ray Tracing



- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard, YouTube VR**
- Ray trace omnidirectional stereo spheremaps or cubemaps for very high-frame-rate reprojection and display via OpenGL texturing
- Stereo requires spherical camera projections **poorly suited to rasterization**
- Benefits from OptiX multi-GPU rendering and load balancing, **remote visualization**



Progressive Ray Tracing Engine

Ray tracing loop runs continuously in new thread

Decodes H.264 video stream from remote VCA GPU cluster

Omnistereo Image Stream

Camera + Scene

HMD Display Loop

HMD loop runs in main VMD application thread at max OpenGL draw rate

View-dependent stereo reprojection for current HMD head pose

HMD distortion correction

RT Code + Camera + Scene

Omnistereo H.264 Video

HMD Video

HMD Pose

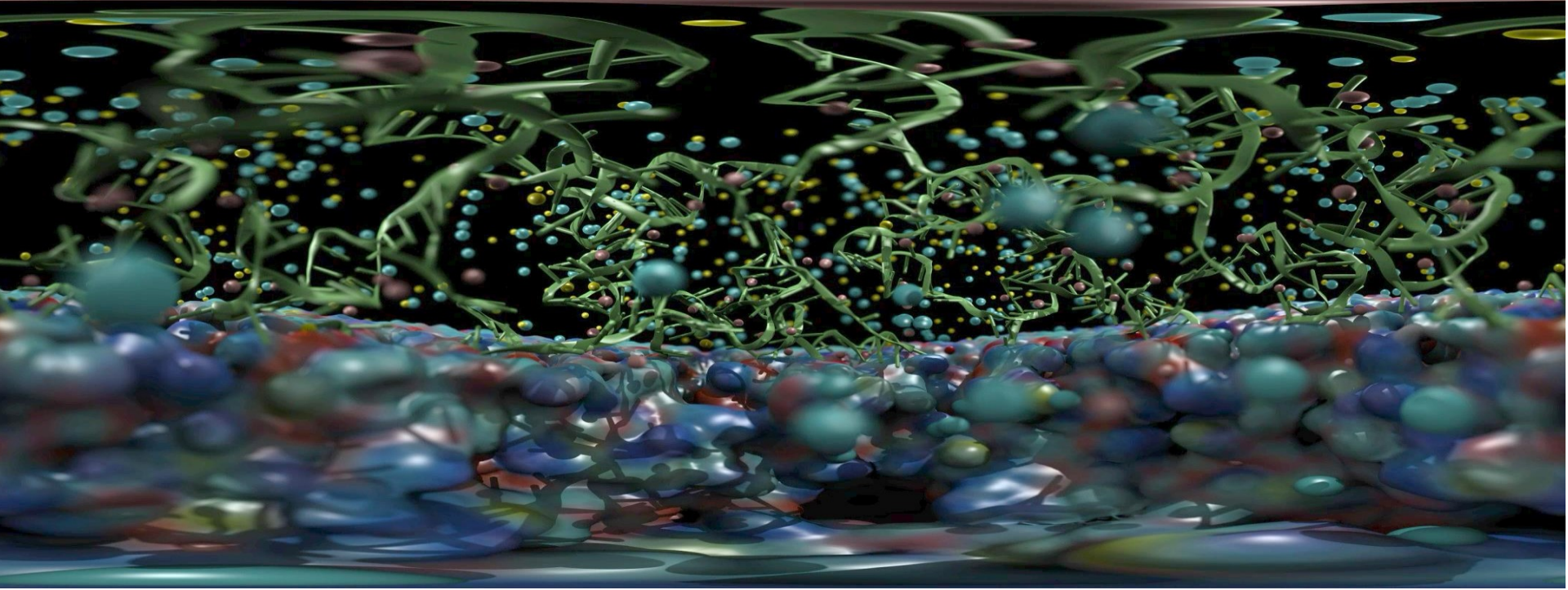
VMD

15Mbps Internet Link

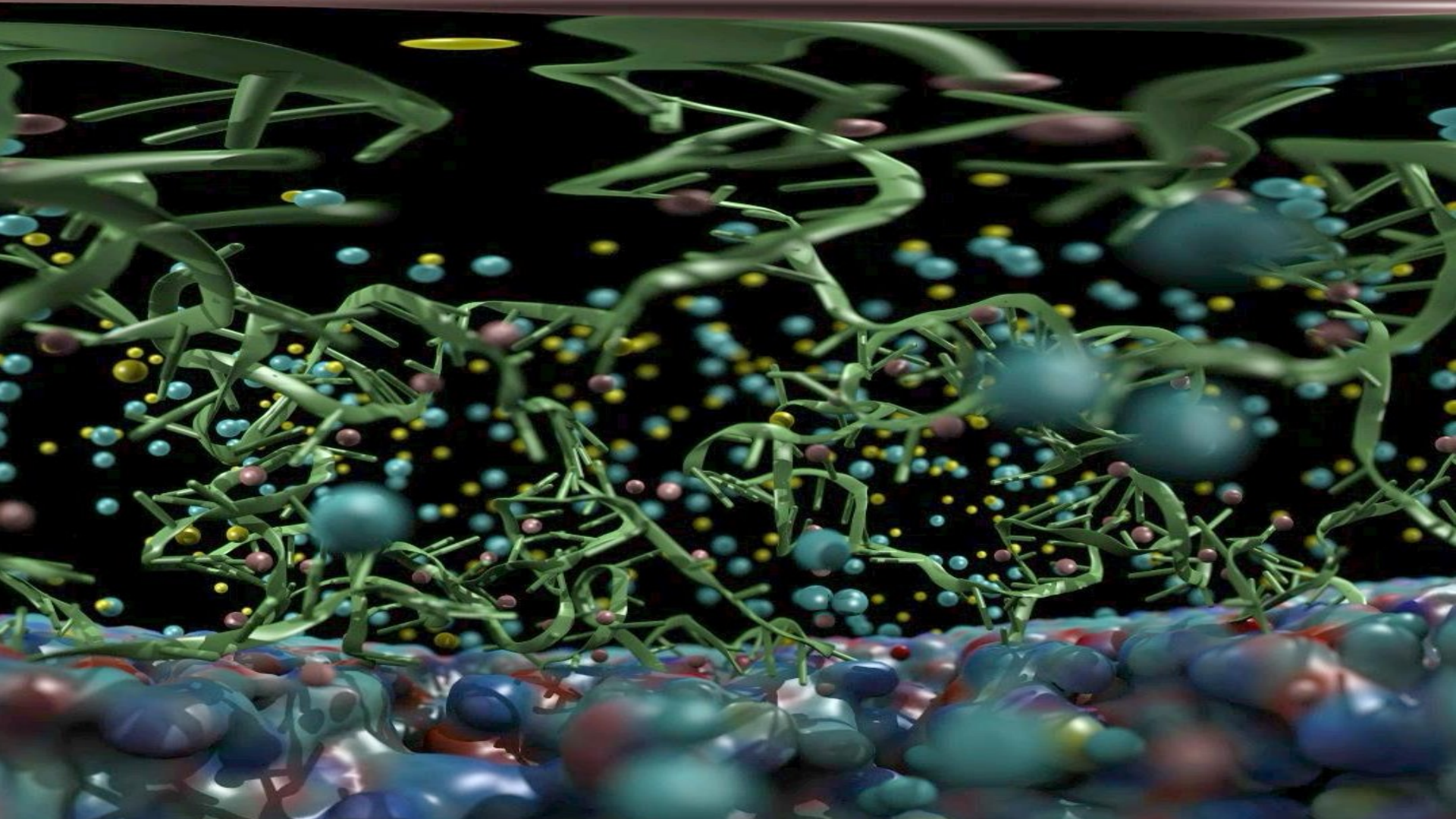
Remote VCA GPU Cluster

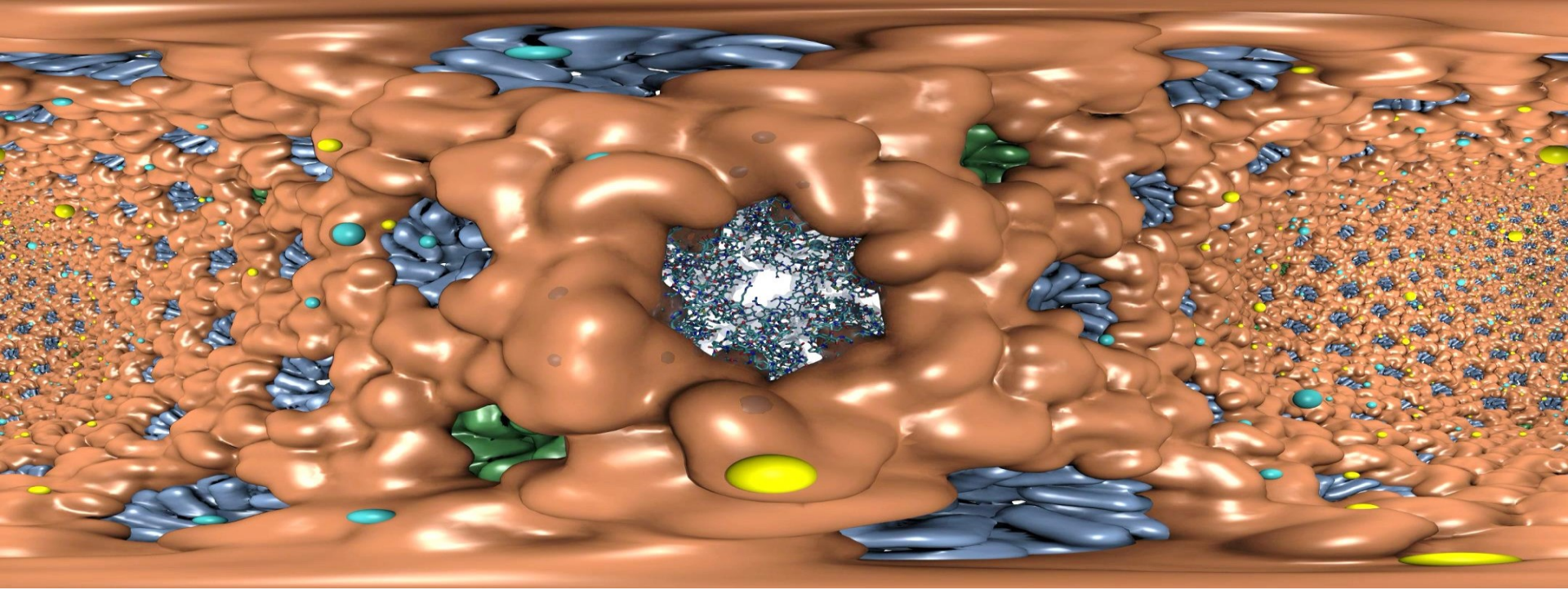
Ray tracing runs continuously, streams H.264 video to VMD client

HMD



Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …





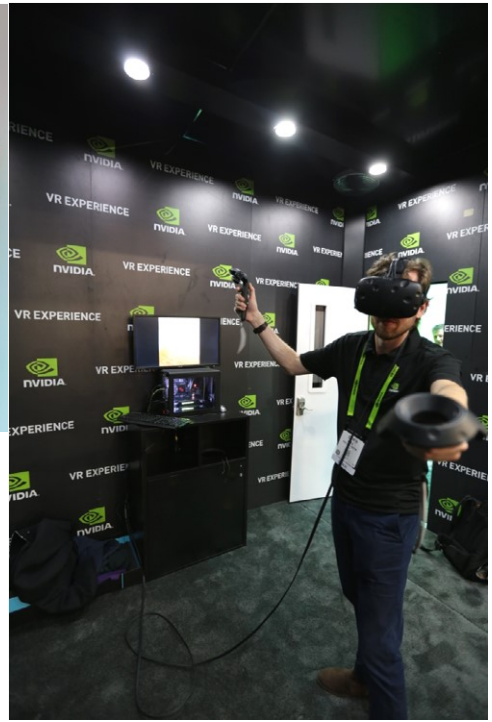
HIV-1 Capsid, Capsid Hexamer Detail, and Ions
Range-Limited Ambient Occlusion Lighting, VR “Headlight”, …


DO NOT SHAKE!
ZEISS
FISHER LENS PAPER

VMD VR Demos

VMD VR ray tracing:
- Google Cardboard [1]
- Demo w/ Indiana U., SC'15 [2]

Prototype of VR user interaction with VMD models in **room-scale VR** with NVIDIA @ SC'16



VMD Chromatophore Demo, NVIDIA VR Room at SC'16

[1] Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. Stone et al., J. Parallel Computing, 55:17-27, 2016.

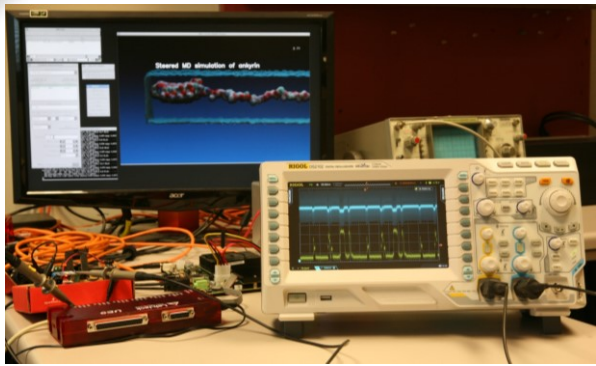
[2] Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J.E. Stone, W.R. Sherman, K. Schulten. IEEE HPDAV (IPDPSW), pp. 1048-1057, 2016.

Technology Opportunities and Collaborations

- Supercomputer Centers, Cray, IBM
  - Remote visualization
  - Performance, power profiling and optimization
- NVIDIA
  - **GPU computing**
  - **Ray tracing**
  - **Remote visualization**
  - ARM, Tablets, power profiling and optimization
- Intel
  - **x86, Xeon Phi optimization, ray tracing**
- Amazon
  - Cloud deployment of VMD/NAMD, related tools
  - Remote visualization
- Universities:
  - **T. Ertl, U. Stuttgart: visualization algorithms**
  - M. Kuttel, U. Cape Town: visualization and analysis
  - G. Fiorin, J. Henin, Toni Giorgino, collective variables
  - W. Sherman, Indiana U.: VR HMDs, visualization
- Touchpress
  - Tablet interfaces, interactive simulation, E-books

VR HMDs, 6DoF input devices

GPU computing,
Ray tracing,
Remote viz.



Energy efficiency: ARM+GPU

Acknowledgements

- NIH Center for Macromolecular Modeling and Bioinformatics, and Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
  - Science images created by many current and former group members
- NVIDIA CUDA Center of Excellence, University of Illinois
- NVIDIA CUDA and OptiX teams
- Intel software defined visualization team
- IBM Power team
- NCSA Blue Waters, ORNL Titan, CSCS Piz Daint, KTH PDC
- Funding:
  - DOE INCITE, ORNL Titan: DE-AC05-00OR22725
  - NSF Blue Waters:
    NSF OCI 07-25070, PRAC “The Computational Microscope”,
    ACI-1238993, ACI-1440026
  - NIH support: 9P41GM104601, 5R01GM098243-02