VMD: enabling preparation, visualization, and analysis of petascale and pre-exascale molecular dynamics simulations

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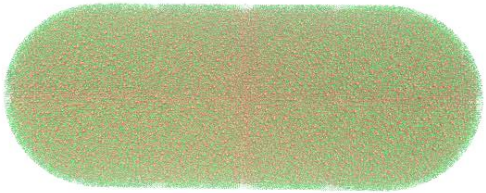
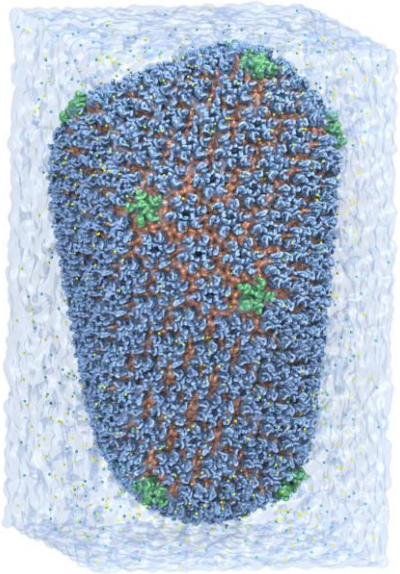
2pm, Armadillo Room (B453, R1001),
LLNL, Livermore, CA, Tuesday Jan 5, 2016

VMD – “Visual Molecular Dynamics”

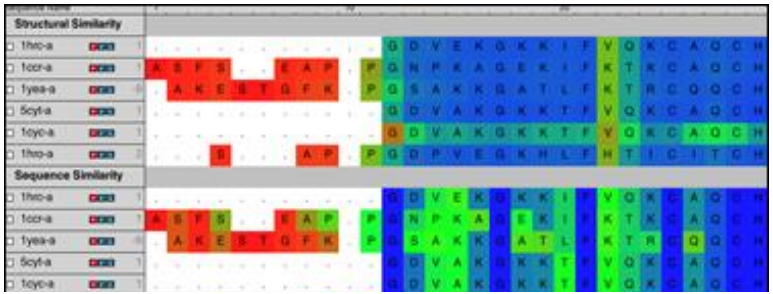
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



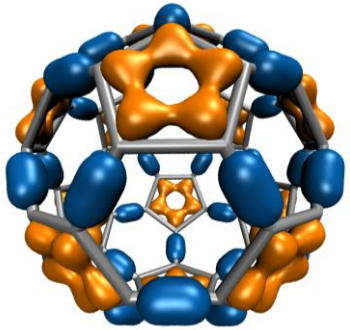
Whole Cell Simulation



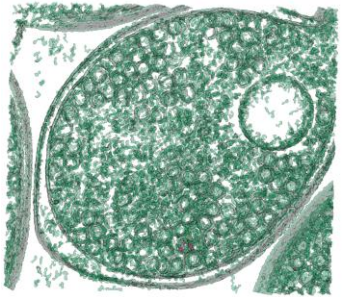
MD Simulations



Sequence Data



Quantum Chemistry

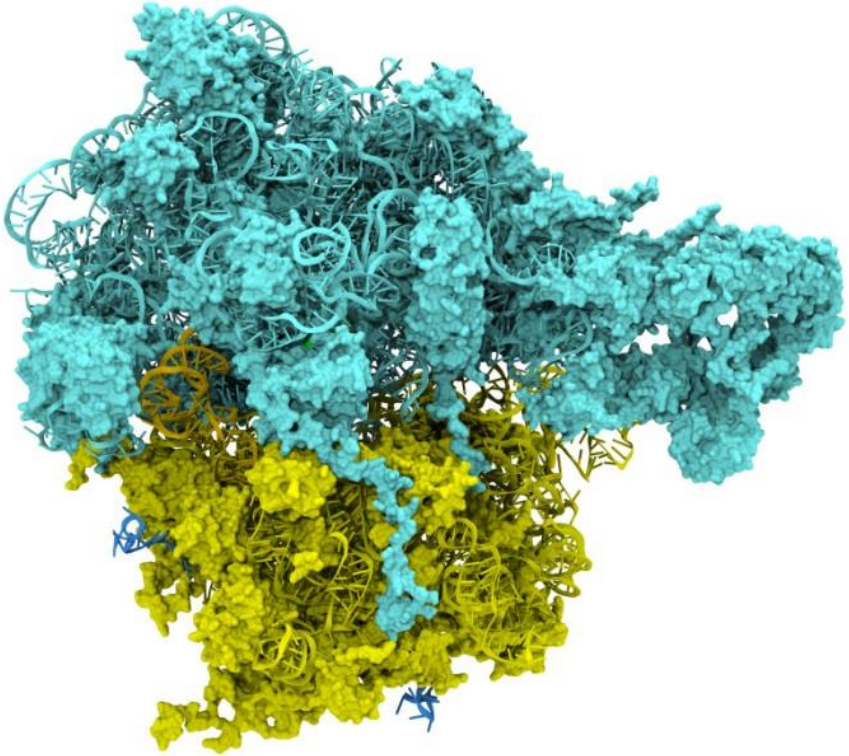


CryoEM, Cellular Tomography

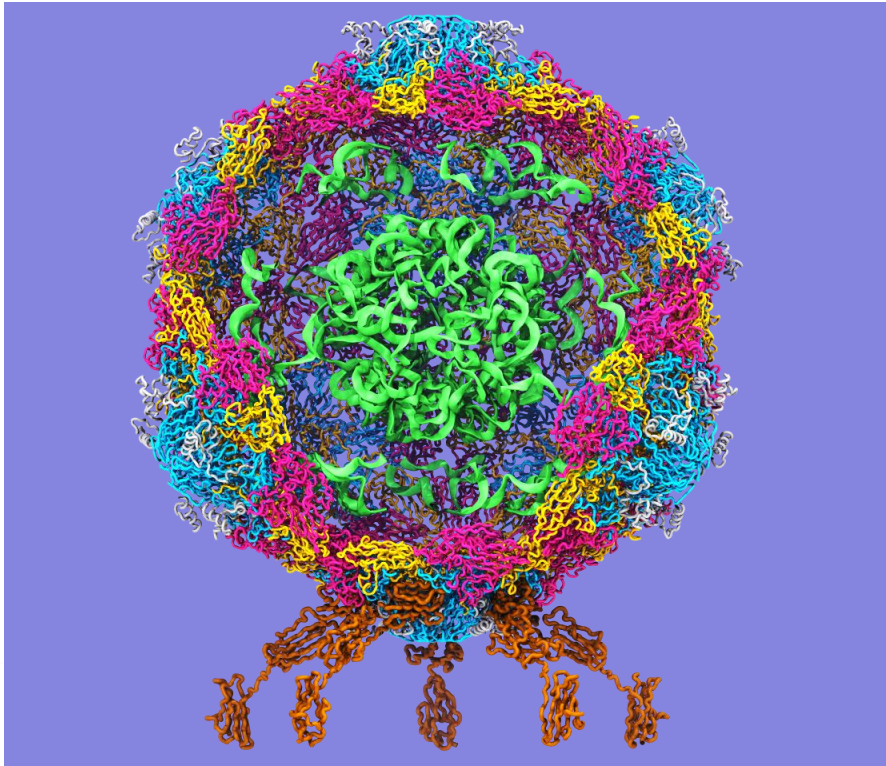
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

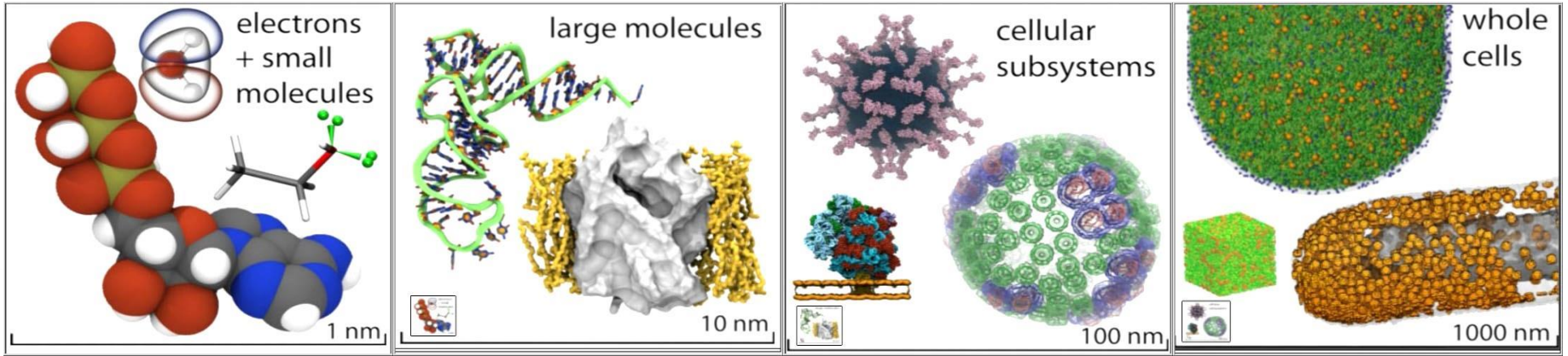


Poliovirus



VMD Interoperability Serves Many Communities

- Uniquely interoperable with a broad range of tools:
  - AMBER, CHARMM, CPMD, DL_POLY, GAMESS, GROMACS, HOOMD, LAMMPS, NAMD, and many more …
- Supports key data types, file formats, and databases
- Incorporates tools for simulation preparation, visualization, and analysis

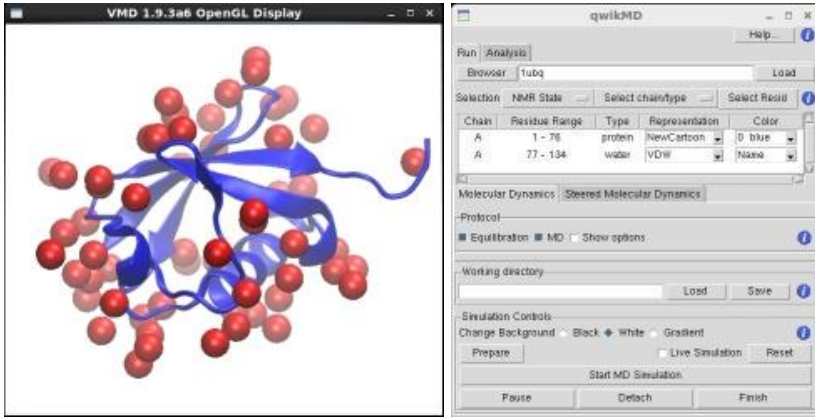


2015 VMD Achievements

1.9.1: 101,900 users, 16,800 NIH (Feb'12)
1.9.2: 50,000 users, 8,200 NIH (Dec'14)

1.9.3 coming soon (~Jan'16)

- Many visualization advances:
  - **Ray tracing advances, GPU 2x faster!**
  - NanoShaper: molecular surfaces, cavity calc.
  - Vector-field volumetric maps, variance maps, …
  - Parallel analysis infrastructure
- New, updated, user-contributed plugins:
  - **qwikMD simulation prep/analysis**
  - **ffTK force field parameterization**
  - Plumed – free energy + collective variable analysis
  - Multiseq – improved MAFFT alignment support
  - Many more….



New QwikMD simulation preparation plugin

Recent Publications:

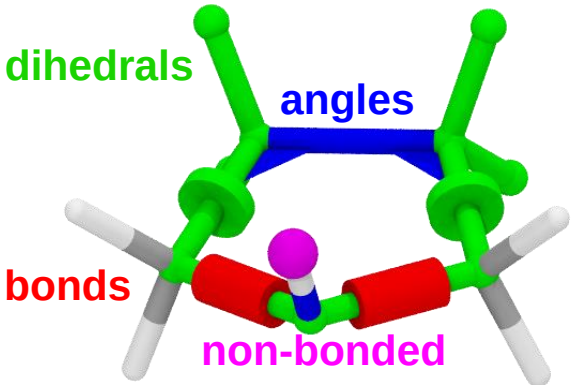
- J. Parallel Computing, 2016. (in-press)
- SC'15 Visualization and Data Analytics Showcase, 2015.
- J. Chemical Theory and Comp. 2015.
- IEEE Transactions on Parallel and Distributed Systems, 2015.

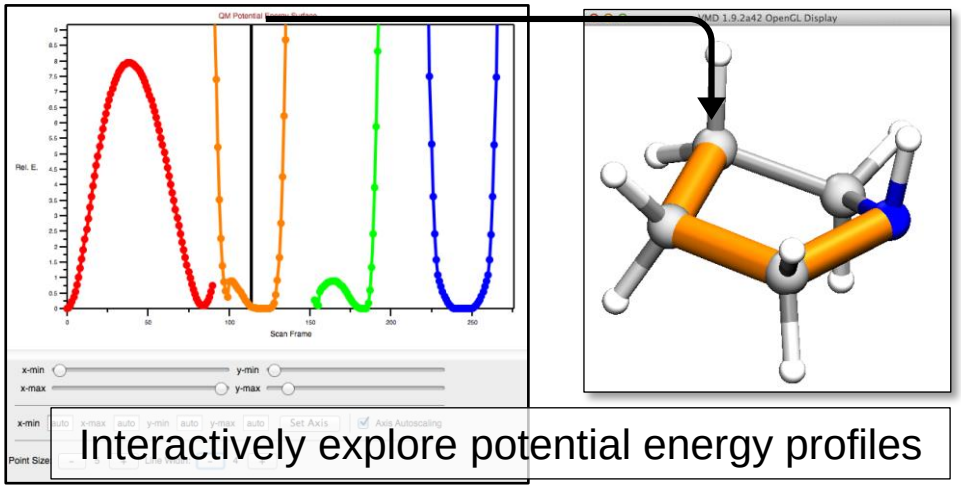
Parameterization with the Force Field Toolkit

Major updates for VMD 1.9.3:

- Read starting parameters computed by CGenFF
- Prepares initial structure files
- New ffTK parameterization tutorial

Visualize parameters directly in VMD



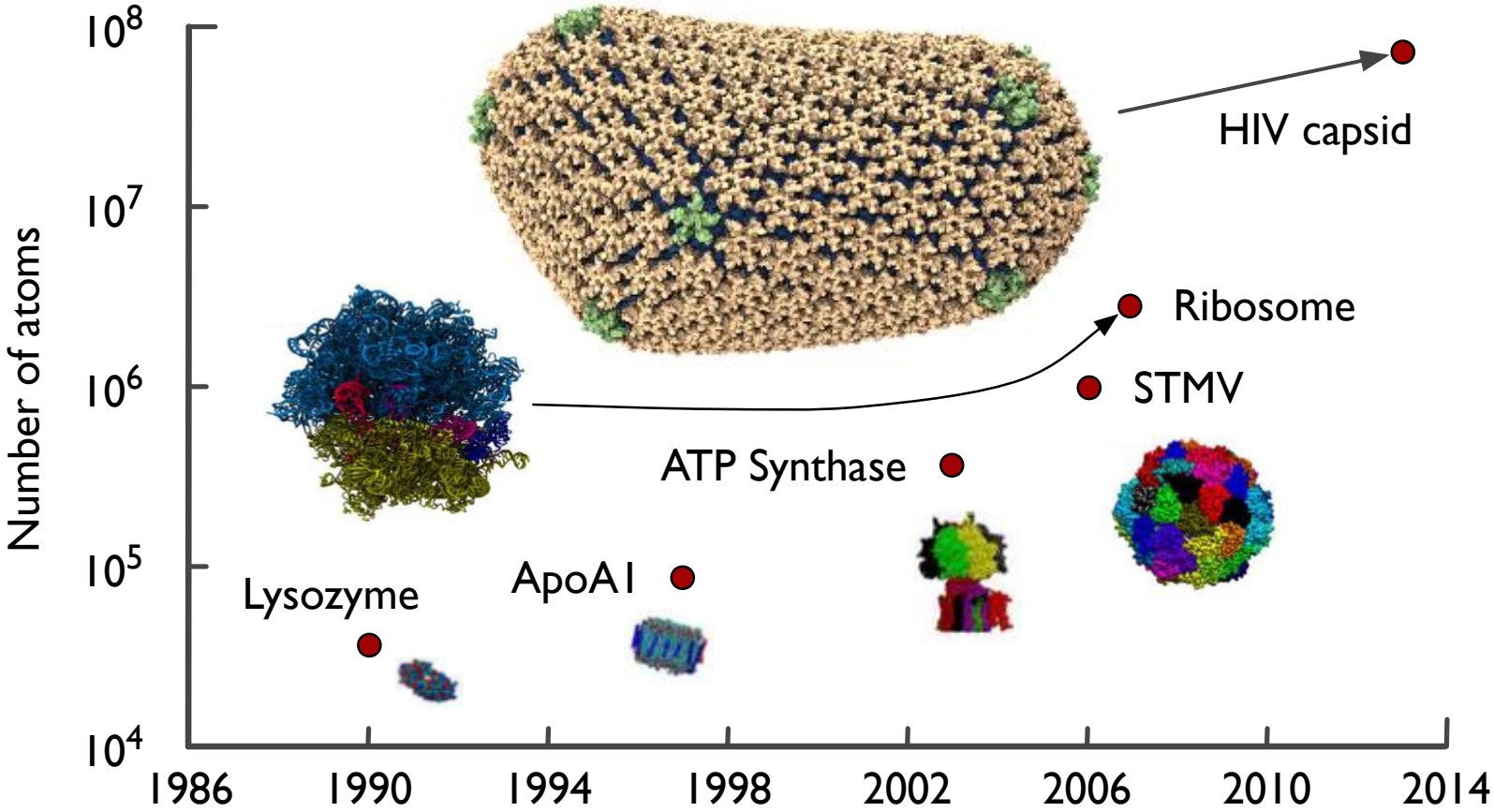


Interactively explore potential energy profiles

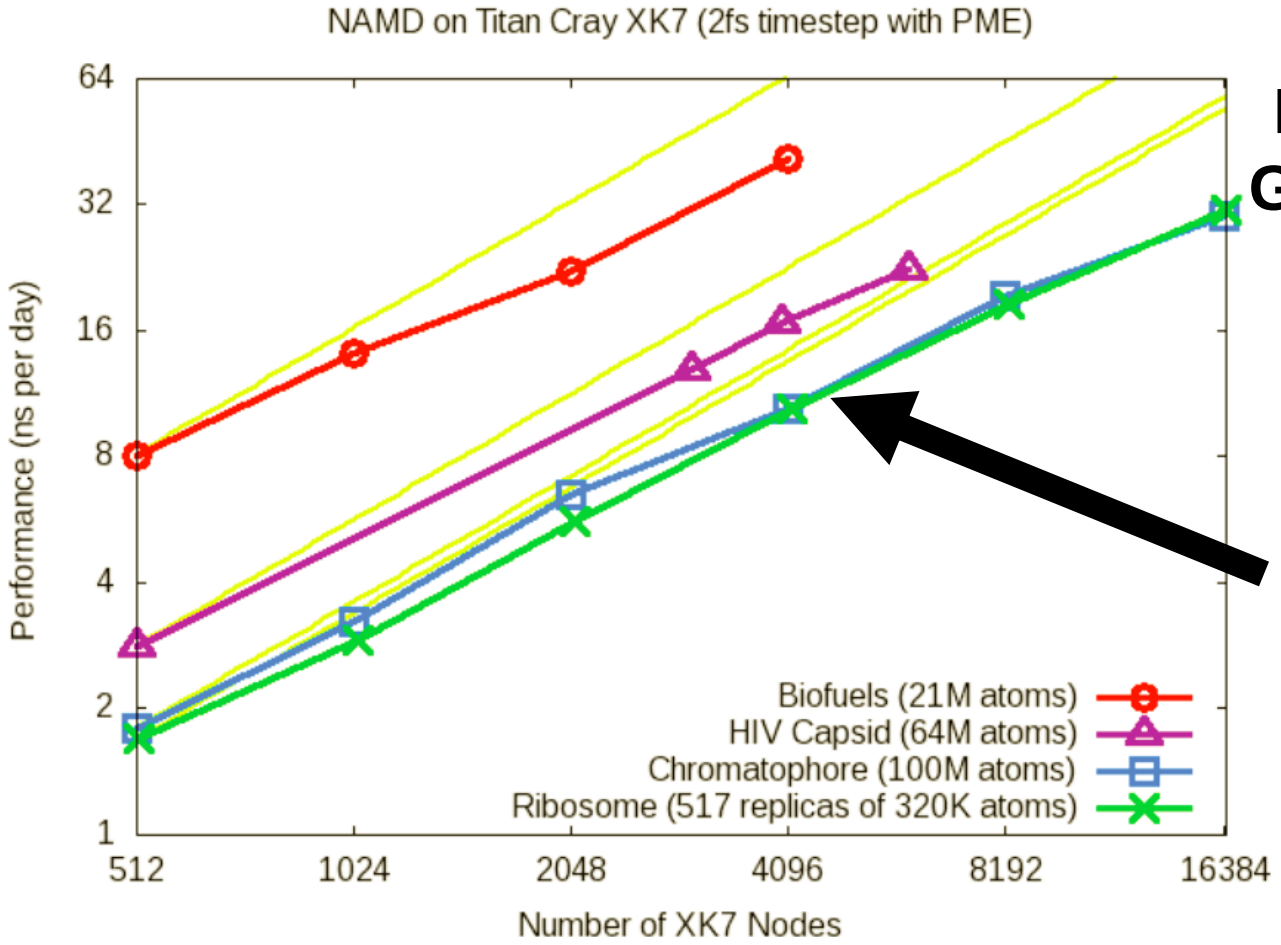
Future Plans:

- Energy evaluation engine in VMD
- Support additional and free-to-academic QM software

NAMD and VMD Use GPUs and Petascale Computing to Meet Computational Biology's Insatiable Demand for Processing Power



NAMD Titan XK7 Performance August 2013



NAMD XK7 vs. XE6 GPU Speedup: 2x-4x

HIV-1 Trajectory: ~1.2 TB/day @ 4096 XK7 nodes

VMD Petascale Visualization and Analysis

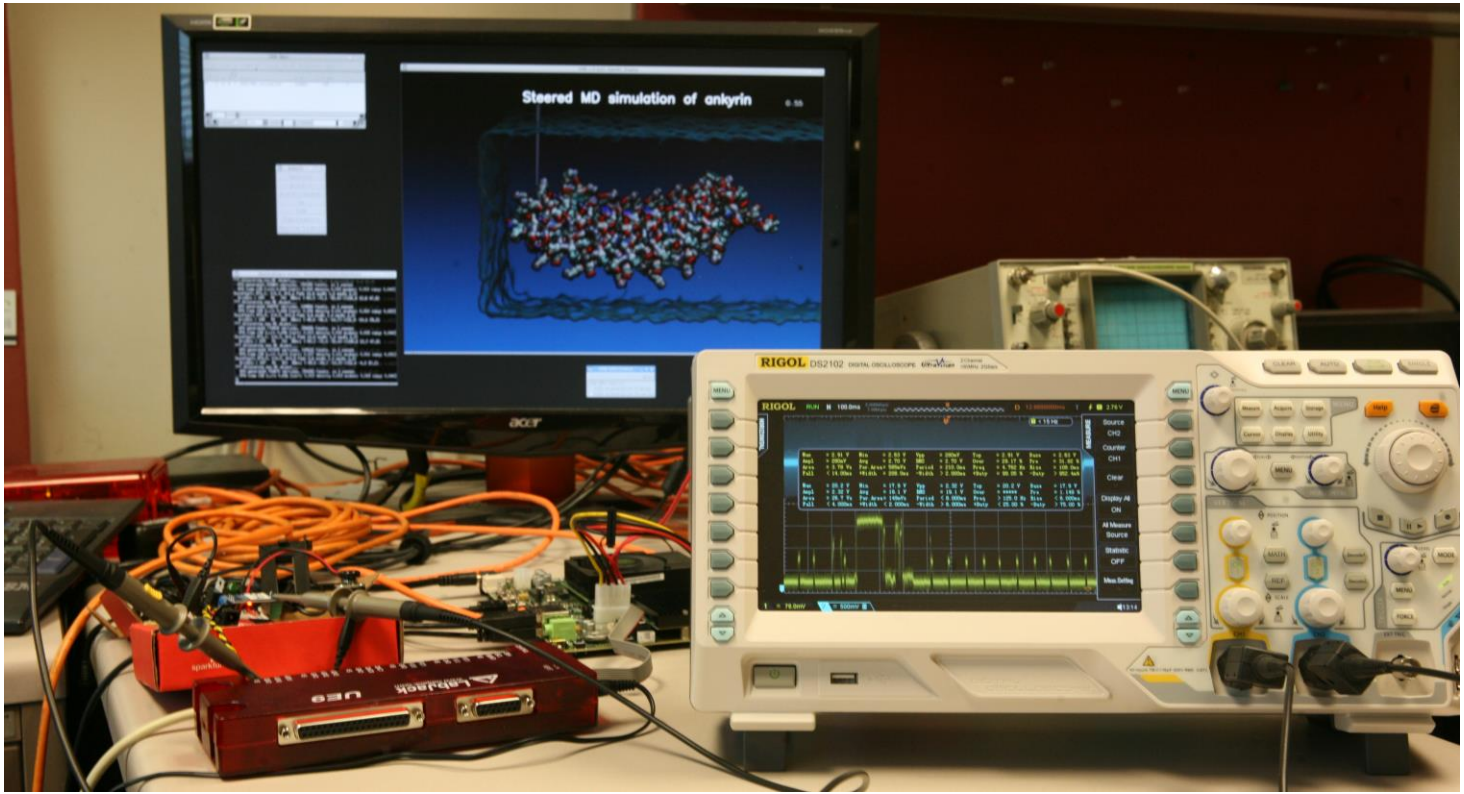
- Analyze/visualize large trajectories too large to transfer off-site:
  - User-defined parallel analysis operations, data types
  - Parallel rendering, movie making
- Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis:
  - **GPU accelerated trajectory analysis w/ CUDA**
  - **OpenGL and GPU ray tracing for visualization and movie rendering**
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 nodes – can read in **231 TB in 15 minutes!**

Parallel VMD currently available on:

ORNL Titan, NCSA Blue Waters, Indiana Big Red II, CSCS Piz Daint, and similar systems

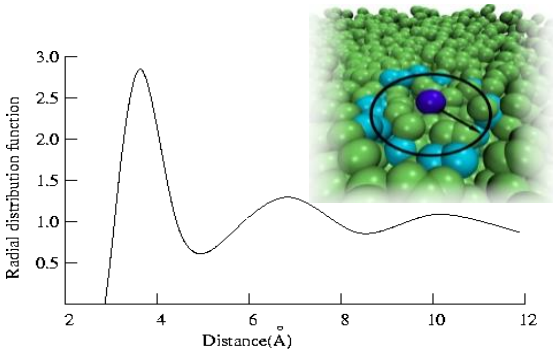
NCSA Blue Waters Hybrid Cray XE6 / XK7
22,640 XE6 dual-Opteron CPU nodes
4,224 XK7 nodes w/ Telsa K20X GPUs

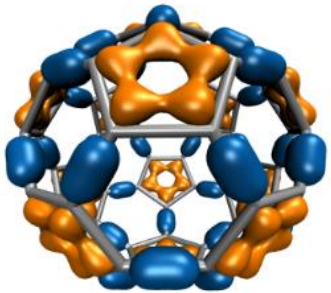
Optimizing VMD for Speed+Power Consumption



CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

VMD GPU-Accelerated Feature or GPU Kernel	Exemplary speedup vs. contemporary 4-core CPU
Molecular orbital display	**30x**
Radial distribution function	**23x**
Molecular surface display	**15x**
Electrostatic field calculation	**11x**
cryoEM cross correlation quality-of-fit	**7x**
Ion placement	6x
MDFF density map synthesis	6x
Implicit ligand sampling	6x
Root mean squared fluctuation	6x
Radius of gyration	5x
Close contact determination	5x
Dipole moment calculation	4x

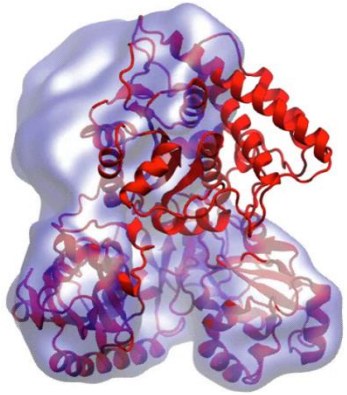




Molecular Dynamics Flexible Fitting (MDFF)

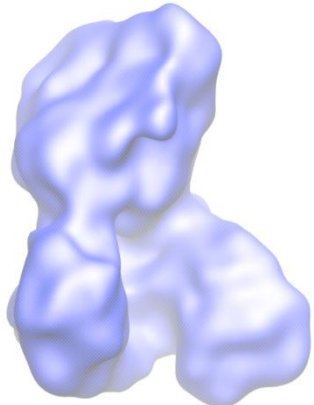
X-ray crystallography → MDFF ← Electron microscopy

APS at Argonne



FEI microscope

ORNL Titan



Flexible fitting of atomic structures into electron microscopy maps using molecular dynamics. L. Trabuco, E. Villa, K. Mitra, J. Frank, and K. Schulten. Structure, 16:673-683, 2008.

Molecular Dynamics Flexible Fitting - Theory

Two terms are added to the MD potential

$$U_{total} = U_{MD} + U_{EM} + U_{SS}$$

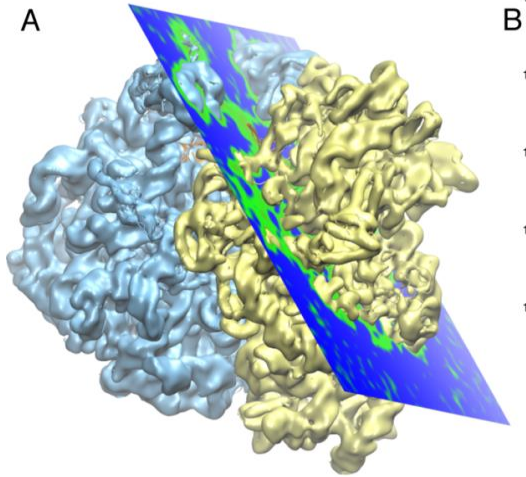
An external potential derived from the EM map is defined on a grid as

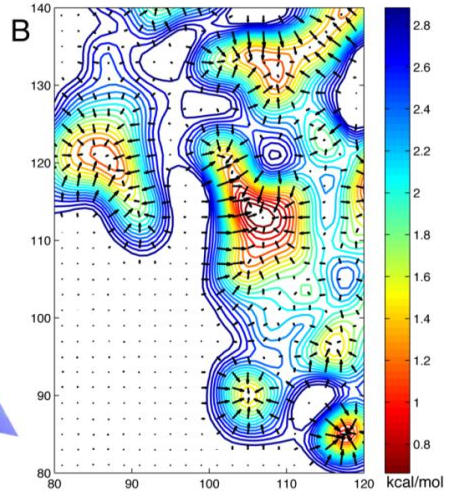
$$U_{EM}(\mathbf{R}) = \sum_j w_j V_{EM}(\mathbf{r}_j)$$

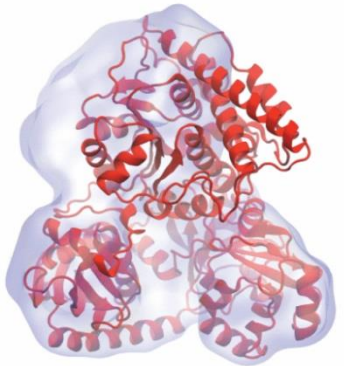
$$V_{EM}(\mathbf{r}) = \begin{cases} \xi \left(1 - \frac{\Phi(\mathbf{r}) - \Phi_{thr}}{\Phi_{max} - \Phi_{thr}}\right) & \text{if } \Phi(\mathbf{r}) \geq \Phi_{thr}, \\ \xi & \text{if } \Phi(\mathbf{r}) < \Phi_{thr}. \end{cases}$$

A mass-weighted force is then applied to each atom

$$\mathbf{f}_i^{EM} = -\nabla U_{EM}(\mathbf{R}) = -w_i \partial V_{EM}(\mathbf{r}_i)/\partial r_i$$

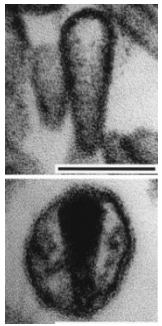


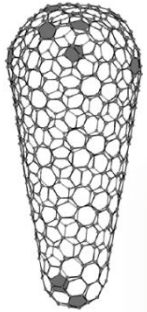




Structural Route to the all-atom HIV-1 Capsid

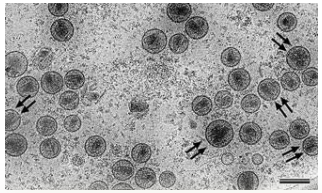
1st TEM (1999)

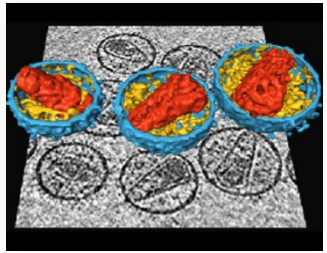




Ganser et al. *Science*, 1999

1st tomography (2003)

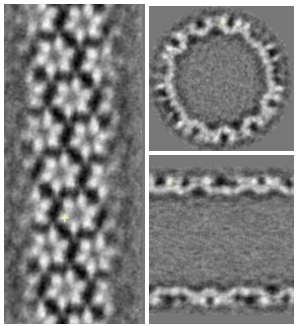




Briggs et al. *EMBO J*, 2003

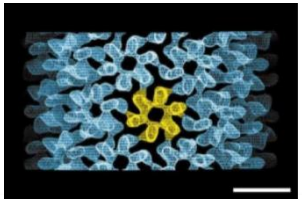
Briggs et al. *Structure*, 2006

cryo-ET (2006)



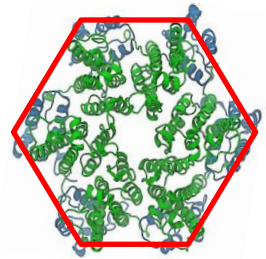
Byeon et al., *Cell* 2009

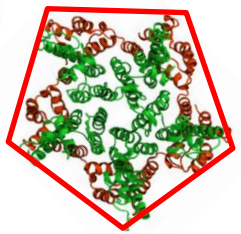
hexameric tubule

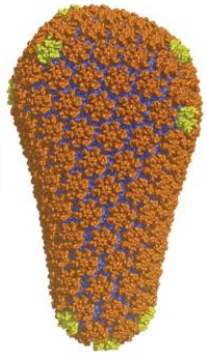


Li et al., *Nature*, 2000

Crystal structures of separated hexamer and pentamer

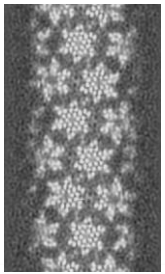


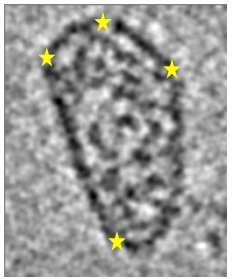


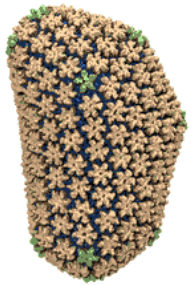


Pornillos et al. , *Cell* 2009, *Nature* 2011

High res. EM of hexameric tubule, tomography of capsid,
all-atom model of capsid by MDFF w/ NAMD & VMD, NSF/NCSA Blue Waters computer at Illinois



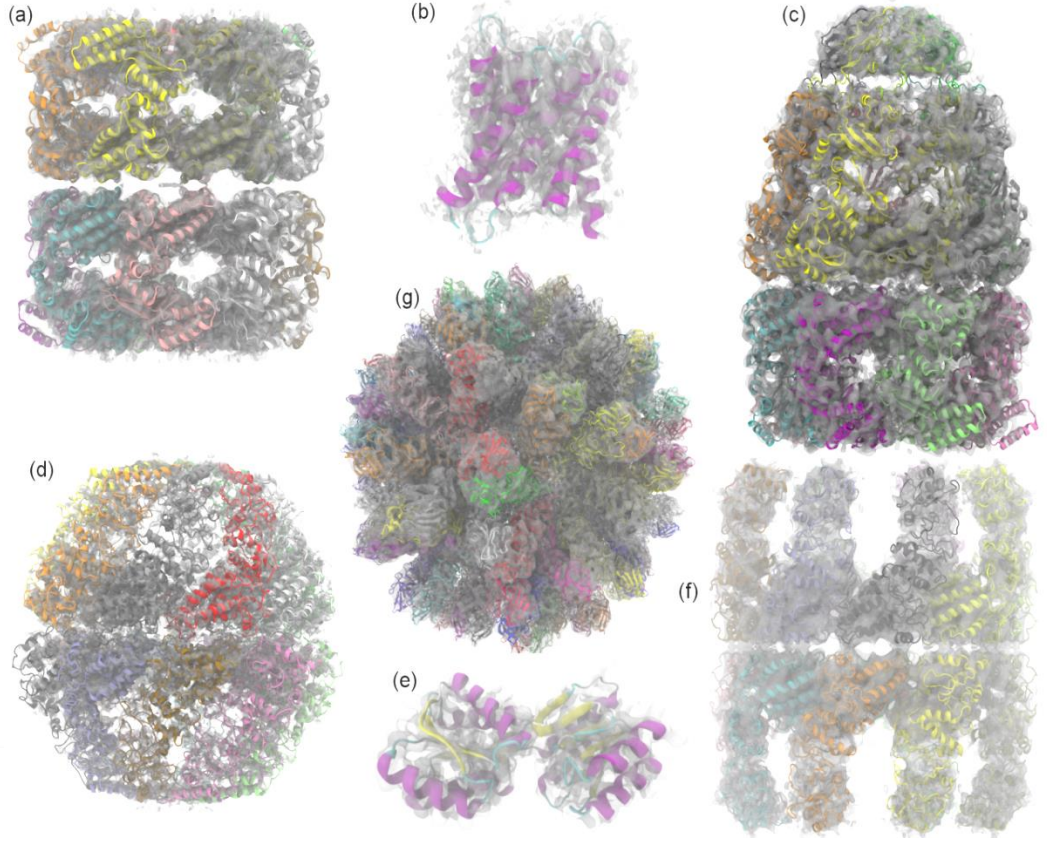




Zhao et al. , *Nature* 497: 643-646 (2013)

Evaluating Quality-of-Fit for Structures Solved by Hybrid Fitting Methods

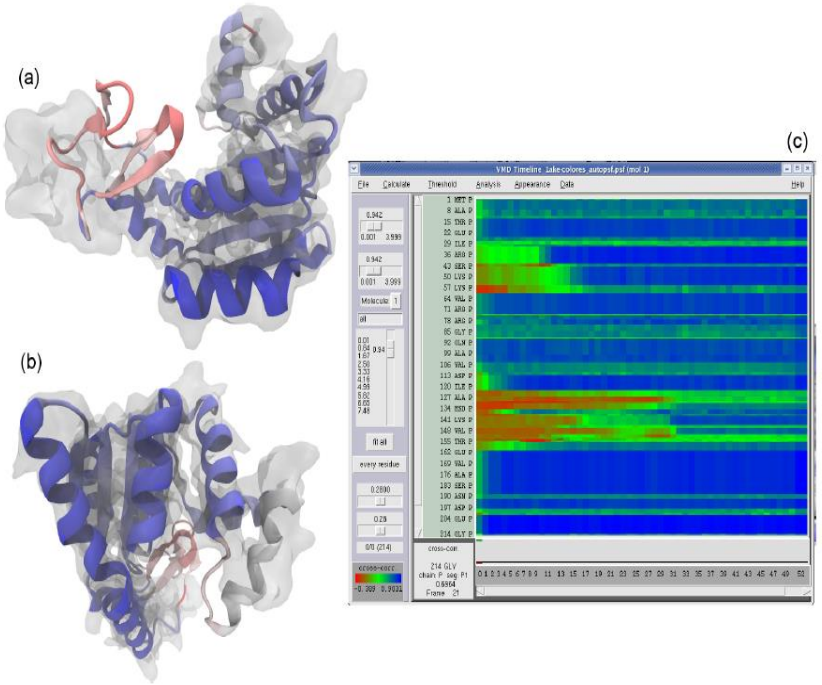
Compute Pearson correlation to evaluate the fit of a reference cryo-EM density map with a **simulated density map** produced from an **all-atom structure.**



GPUs Can Reduce MDFF Trajectory Analysis Runtimes from Hours to Minutes

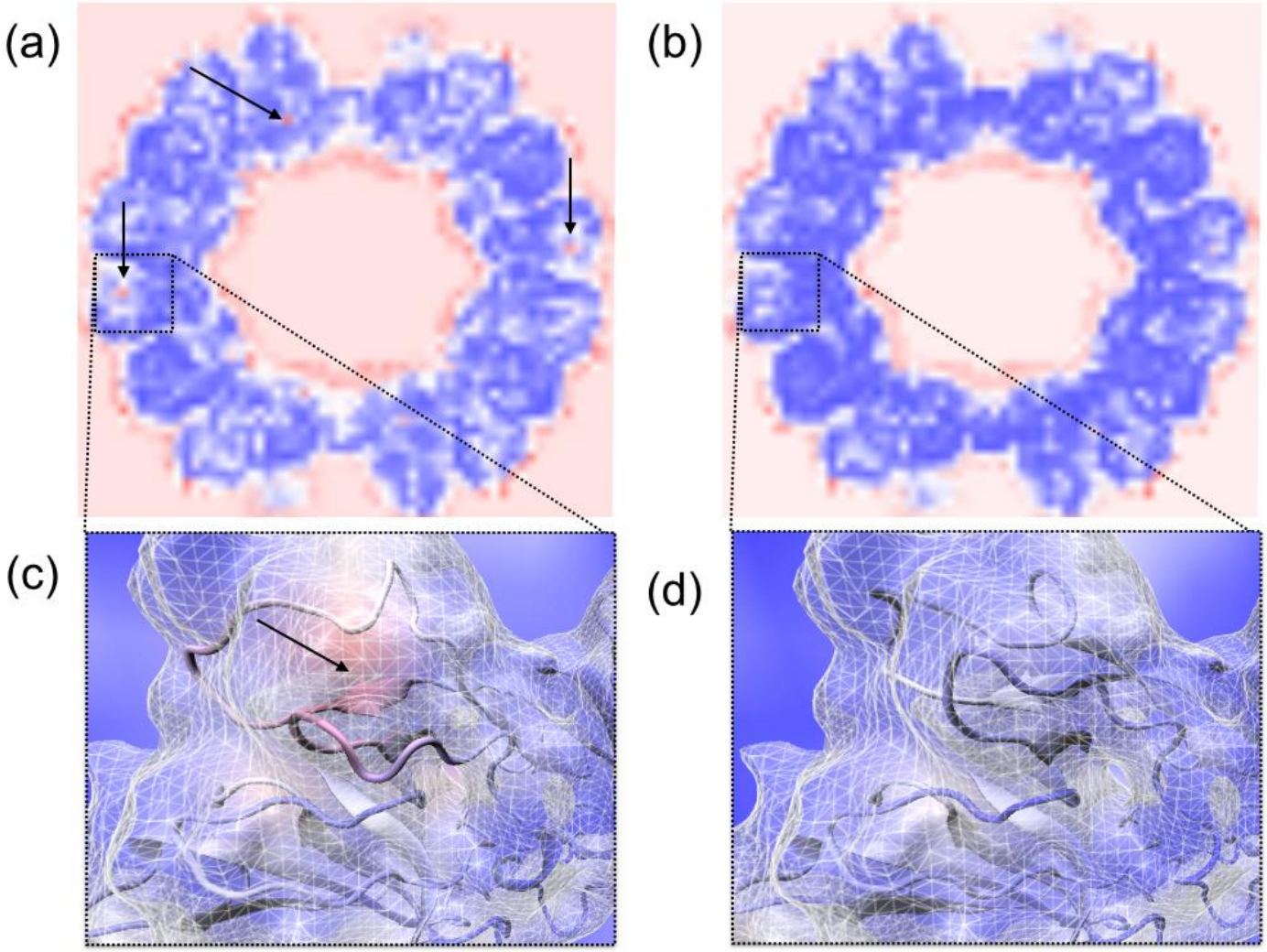
GPUs enable laptops and desktop workstations to handle tasks that would have previously required a cluster, or a *long wait*…

GPU-accelerated petascale supercomputers enable analyses that were previously impractical, allowing detailed study of very large structures such as viruses



GPU-accelerated MDFF Cross Correlation Timeline

Regions with poor fit **Regions with good fit**

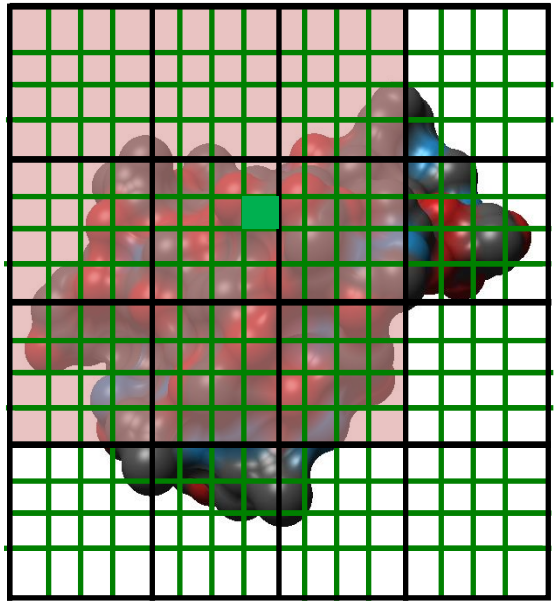

(a)
(b)
(c)
(d)

MDFF Density Map Algorithm

- Build spatial acceleration data structures, optimize data for GPU
- Compute 3-D density map:

$$\rho(\vec{r}; \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} e^{\frac{-|\vec{r}-\vec{r}_i|^2}{2\alpha^2}}$$

- Truncated Gaussian and spatial acceleration grid ensure linear time-complexity



3-D density map lattice point and the neighboring spatial acceleration cells it references

Single-Pass MDFF GPU Cross-Correlation

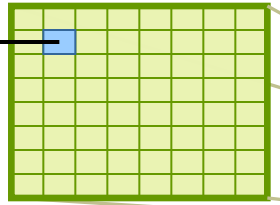
3-D density map decomposes into 3-D grid of 8x8x8 tiles containing CC partial sums and local CC values

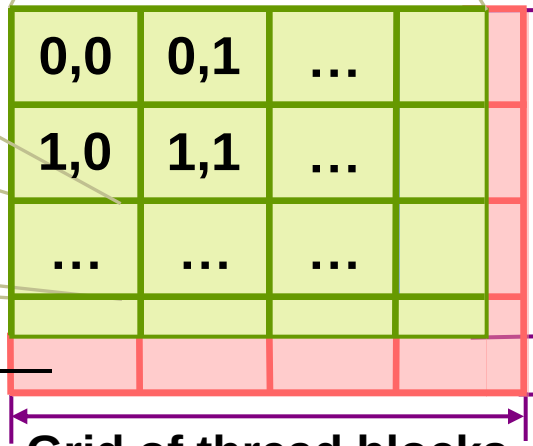
Fusion of density and CC calculations into a single CUDA kernel!!!

Spatial CC map and overall CC value computed in a single pass

Small 8x8x2 CUDA thread blocks afford large per-thread register count, shared memory

Each thread computes 4 z-axis density map lattice points and associated CC partial sums





Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

VMD GPU Cross Correlation Performance

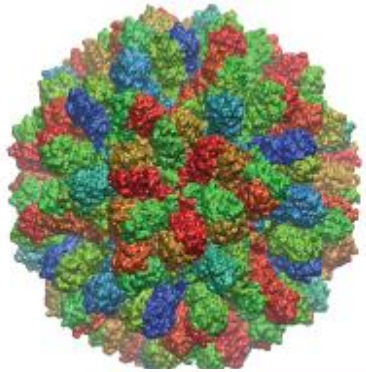
	RHDV	Mm-cpn open	GroEL	Aquaporin
Resolution (Å)	**6.5**	**8**	**4**	**3**
Atoms	**702K**	**61K**	**54K**	**1.6K**
VMD-CUDA Quadro K6000	**0.458s 34.6x**	**0.06s 25.7x**	**0.034s 36.8x**	**0.007s 55.7x**
VMD-CPU-SSE 32-threads, 2x Xeon E5-2687W	**0.779s 20.3x**	**0.085s 18.1x**	**0.159s 7.9x**	**0.033s 11.8x**
Chimera 1-thread Xeon E5-2687W	**15.86s 1.0x**	**1.54s 1.0x**	**1.25s 1.0x**	**0.39s 1.0x**

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.

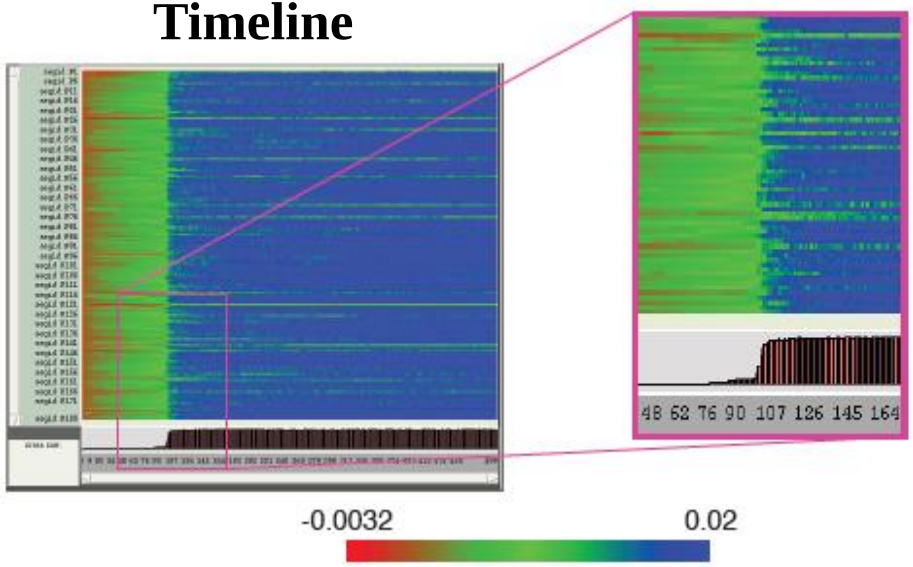
VMD RHDV Cross Correlation Timeline on Cray XK7

	RHDV
Atoms	702K
Traj. Frames	10,000
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 would take **5 years** using original serial CC calculation on a workstation!



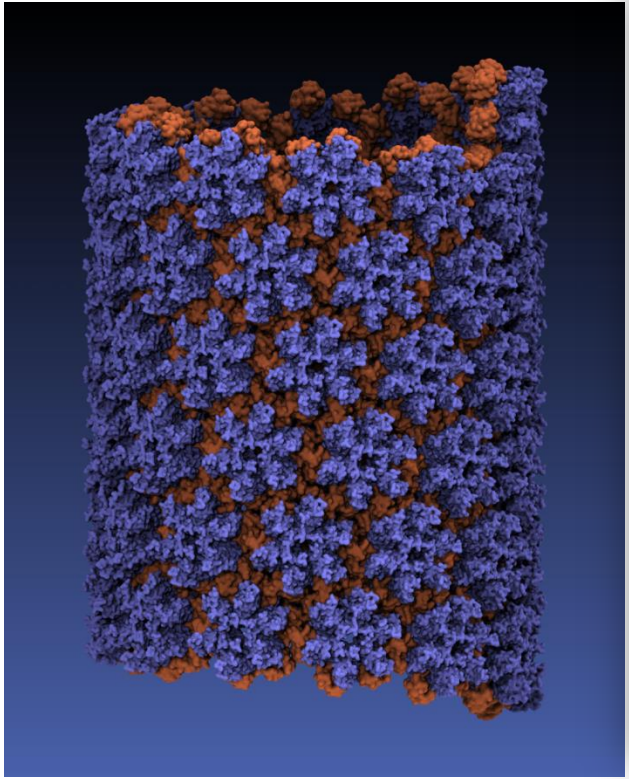
RHDV Group-relative CC Timeline

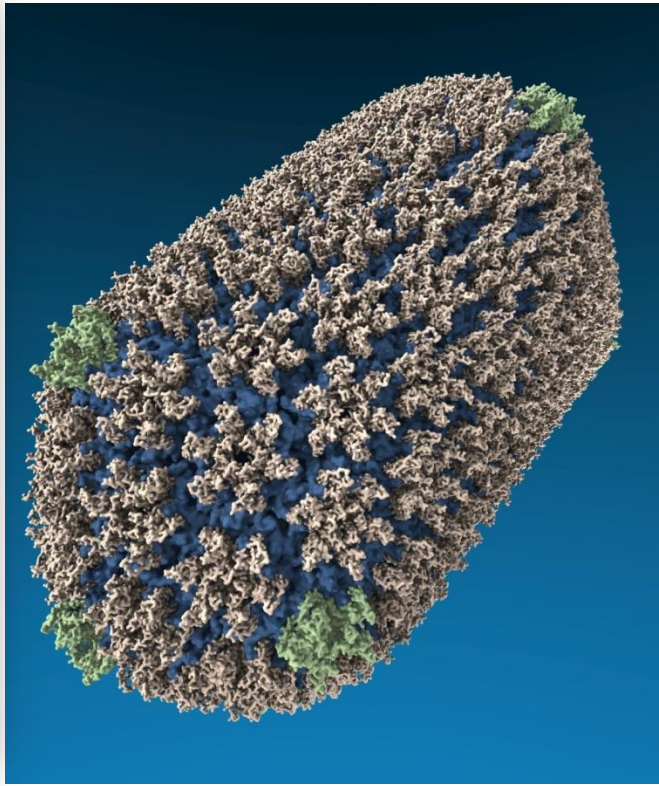


Visualization Goals, Challenges

- Increased CPU+GPU acceleration for visualization of **petascale molecular dynamics trajectories**
- **Overcome memory capacity limits**, enable high quality visualization of **100M atom to 1B atom systems**
- Use GPU to accelerate not only interactive-rate visualizations, but also photorealistic ray tracing with **artifact-free ambient occlusion lighting**, etc.
- Maintain **ease-of-use**, intimate link to VMD analytical features, atom selection language, etc.

VMD “QuickSurf” Representation, Ray Tracing

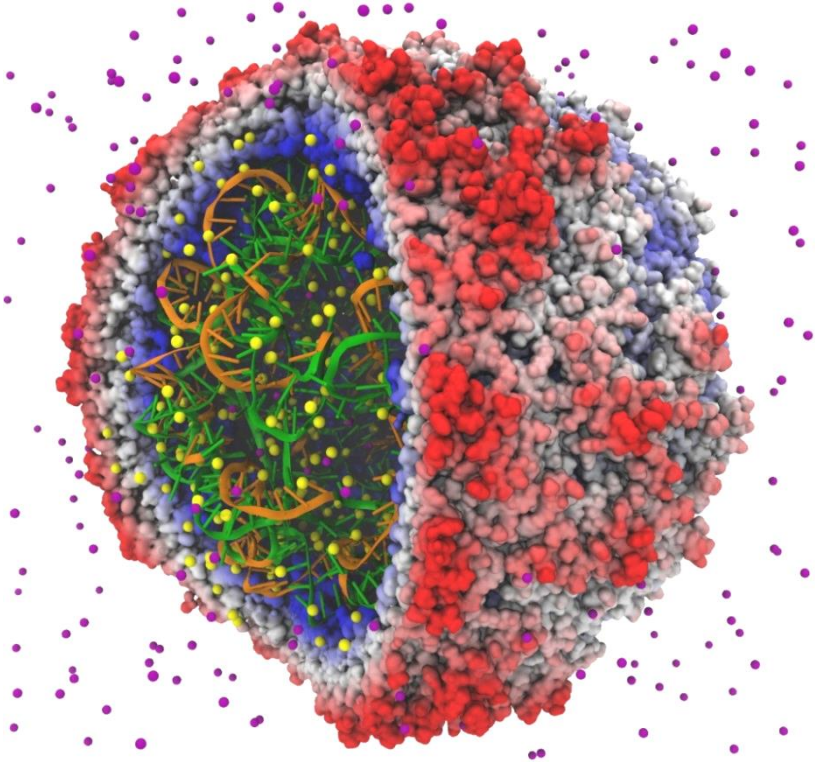




All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

VMD “QuickSurf” Representation

- Displays continuum of structural detail:
  - All-atom, coarse-grained, cellular models
  - Smoothly variable detail controls
- Linear-time algorithm, scales to millions of particles, as **limited by memory capacity**
- Uses multi-core CPUs and GPU acceleration to enable **smooth interactive animation** of molecular dynamics trajectories w/ up to ~1-2 million atoms
- **GPU acceleration yields 10x-15x speedup vs. multi-core CPUs**



Satellite Tobacco Mosaic Virus

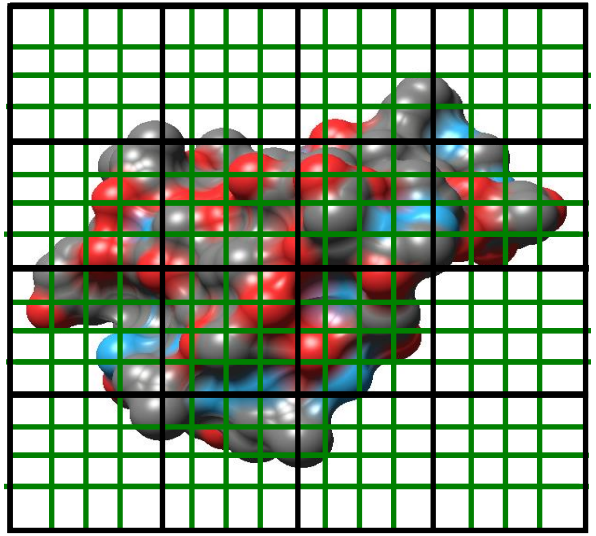
Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.
M. Krone, J. E. Stone, T. Ertl, K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012

VMD 1.9.x QuickSurf Algorithm Improvements

- **50%-66% memory use, 1.5x-2x speedup**
- Build spatial acceleration data structures, optimize data for GPU
- Compute 3-D density map, 3-D color texture map with **data-parallel *"gather"* algorithm**:

$$\rho(\vec{r}; \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} e^{\frac{-|\vec{r}-\vec{r}_i|^2}{2\alpha^2}}$$

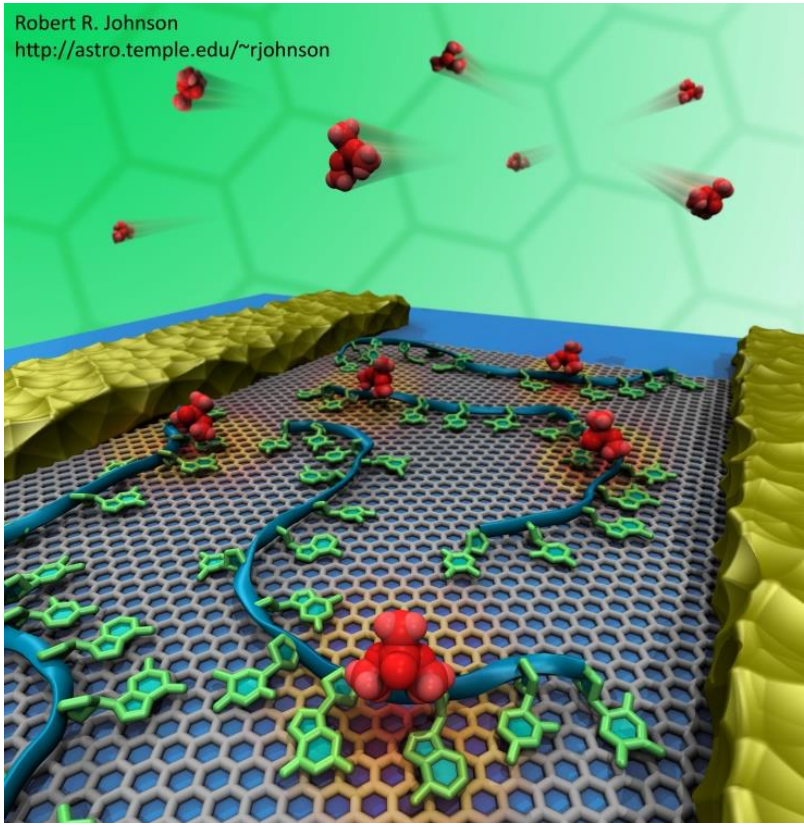
- **Normalize, quantize, and compress** density, color, surface normal data **while in registers**, before writing out to GPU global memory
- Extract isosurface, maintaining **quantized/compressed** data representation
- **Centralized GPU memory management** among all molecules+representations: enables graceful eviction of surface data for ray tracing, or other GPU-memory-capacity-constrained operations



3-D density map lattice, spatial acceleration grid, and extracted surface

Ray Tracing in VMD

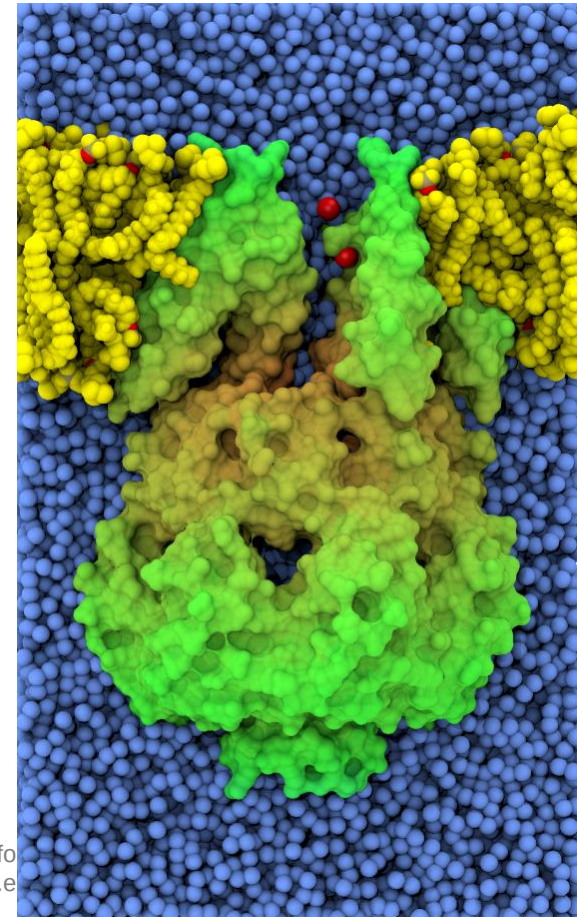
- Support for ray tracing of VMD molecular scenes began in 1995
- Tachyon parallel RT engine interfaced with VMD (1999)
- Tachyon embedded as an internal VMD rendering engine (2002)
- Built-in support for large scale parallel rendering (2012)
- Refactoring of VMD to allow fully interactive ray tracing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



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

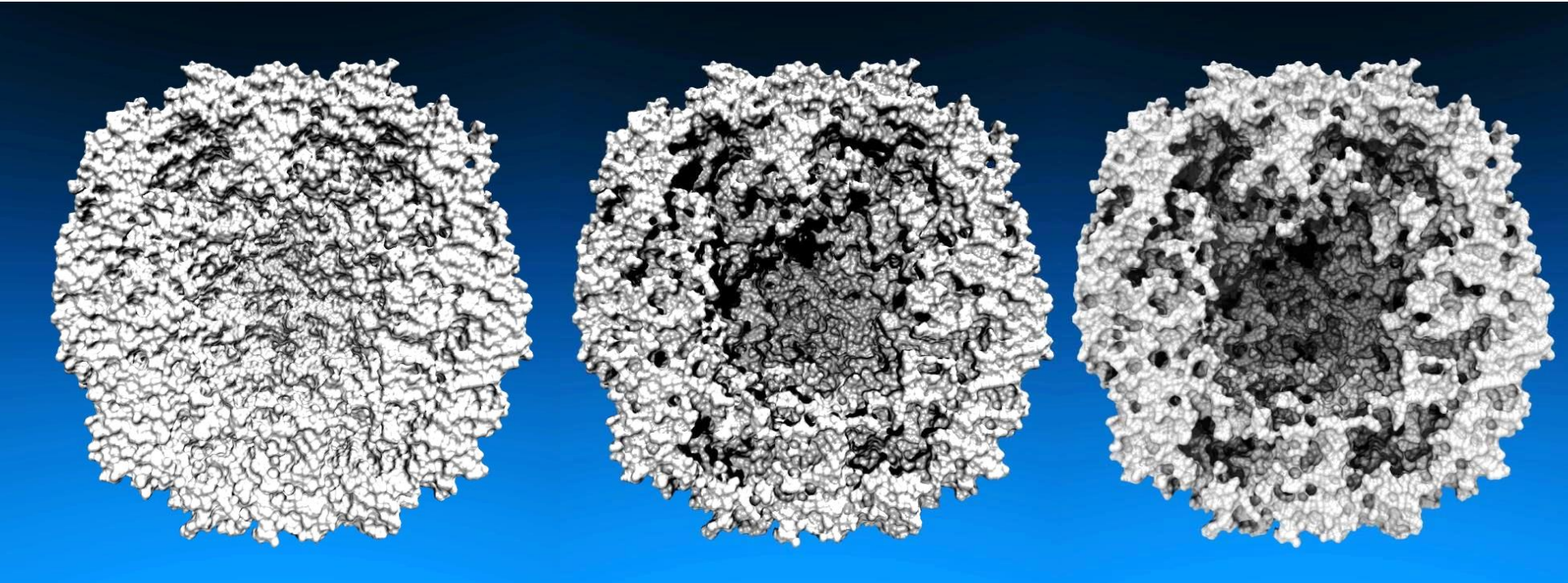


Lighting Comparison, STMV Capsid

Two lights, no shadows

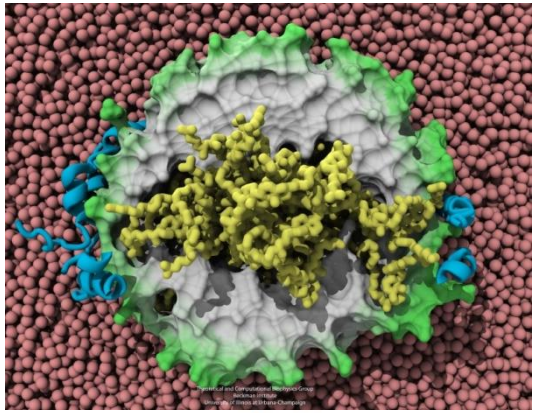
Two lights, hard shadows, 1 shadow ray per light

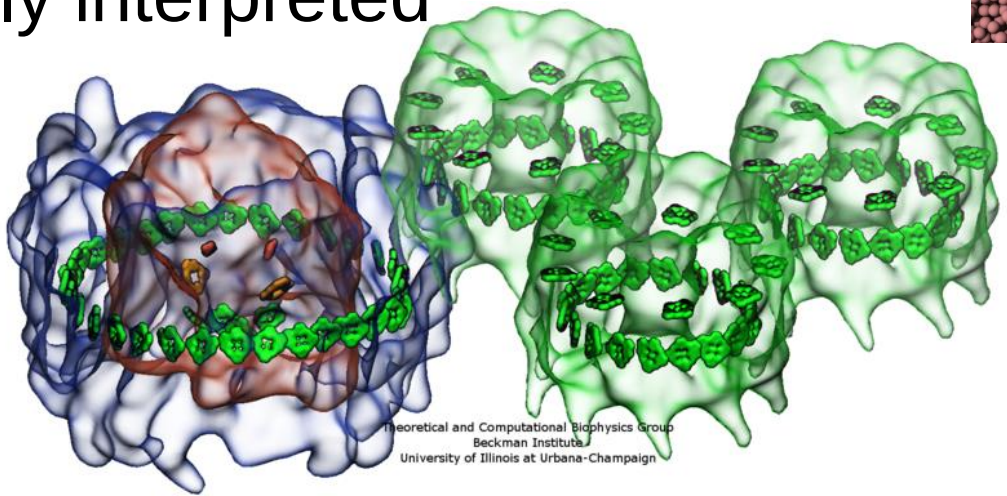
Ambient occlusion + two lights, 144 AO rays/hit

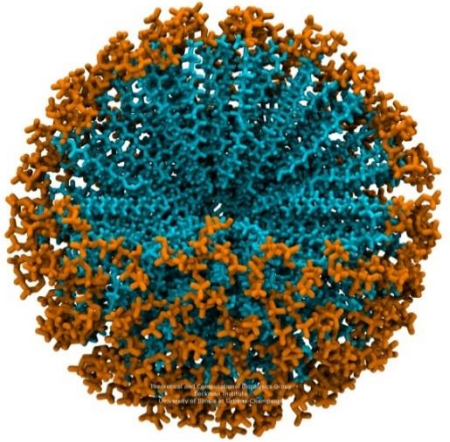


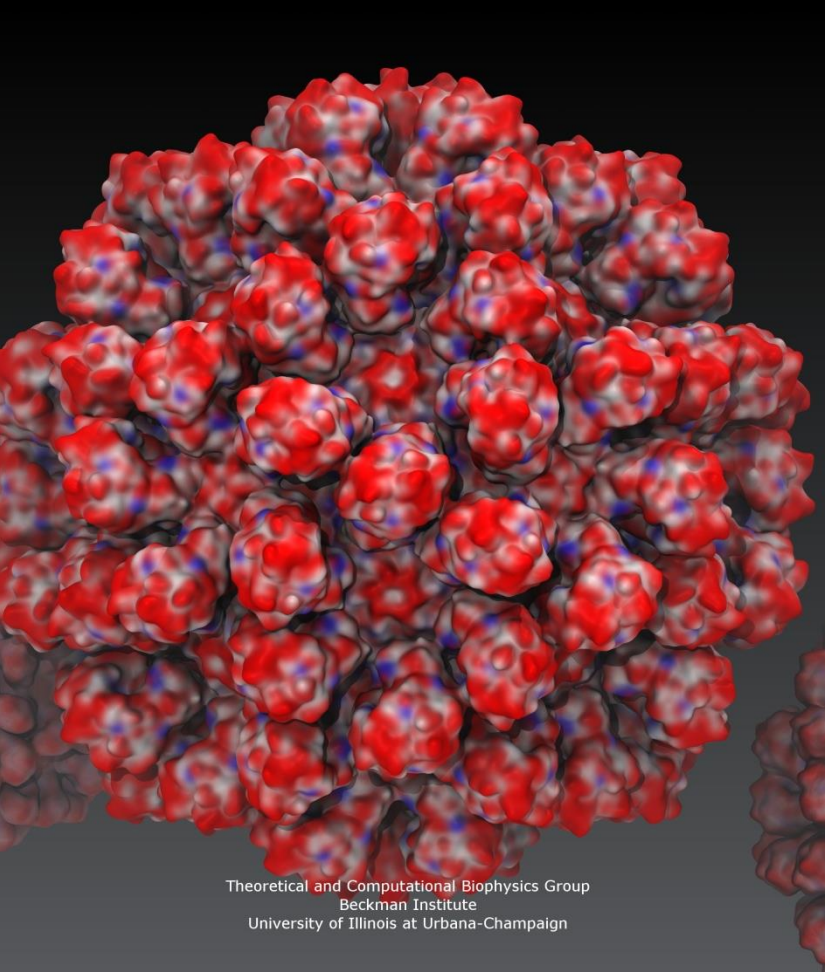
Benefits of Advanced Lighting and Shading Techniques

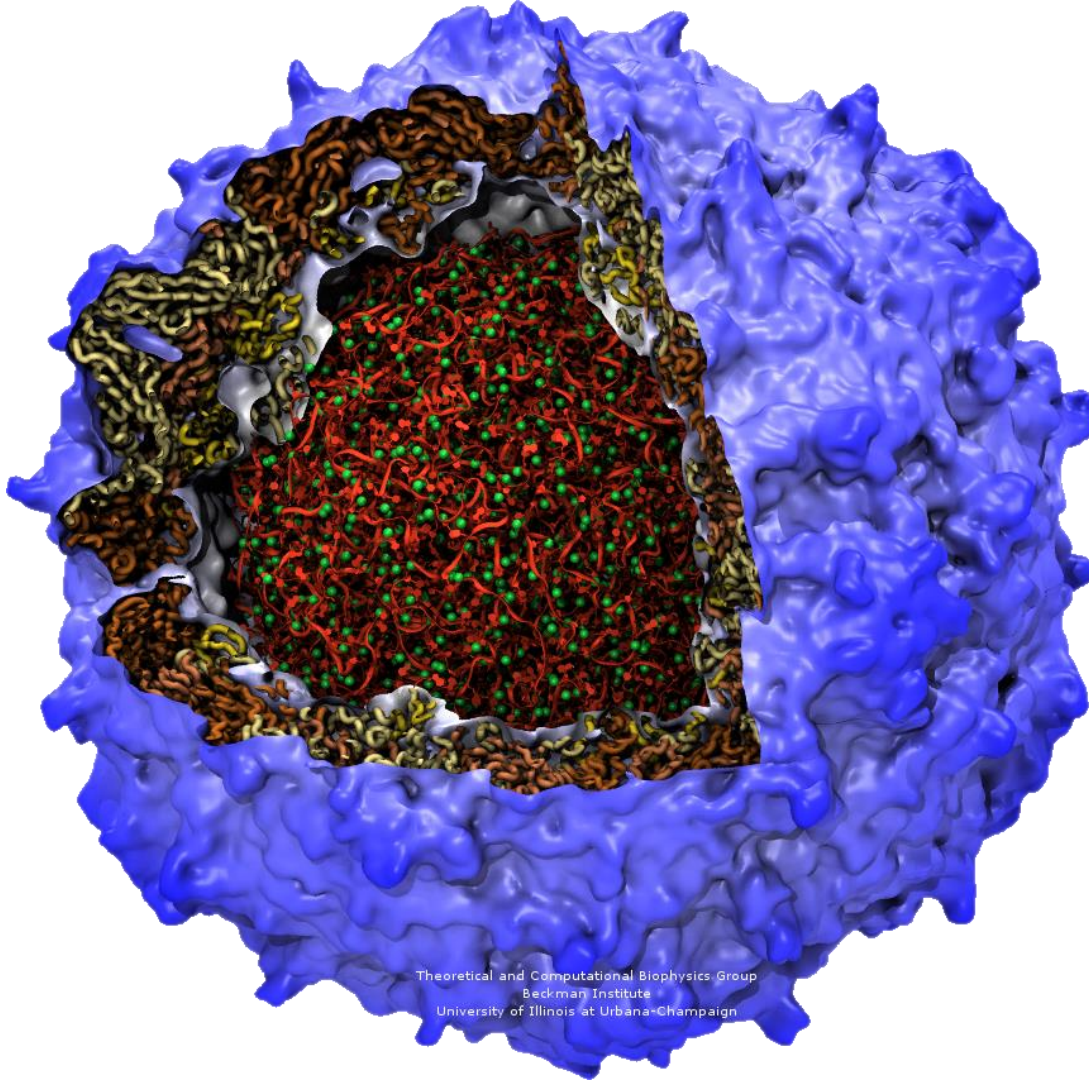
- Exploit visual intuition
- Spend computer time in exchange for scientists' time, make images that are more easily interpreted








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

Ray Tracing Performance

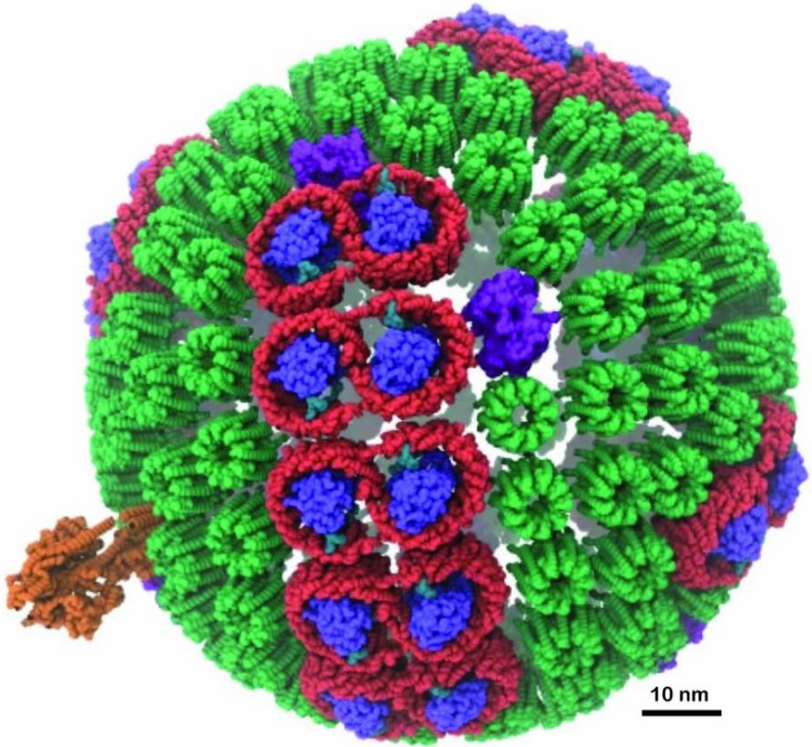
- Well suited to massively parallel hardware
- Peak performance requires full exploitation of SIMD/vectorization, multithreading, efficient use of memory bandwidth
- Traditional languages+compilers not yet up to the task:
  - Efficacy of compiler autovectorization for Tachyon and other classical RT codes is very low…
  - Core ray tracing kernels have to be explicitly designed for the target hardware, SIMD, etc.

Fast Ray Tracing Frameworks

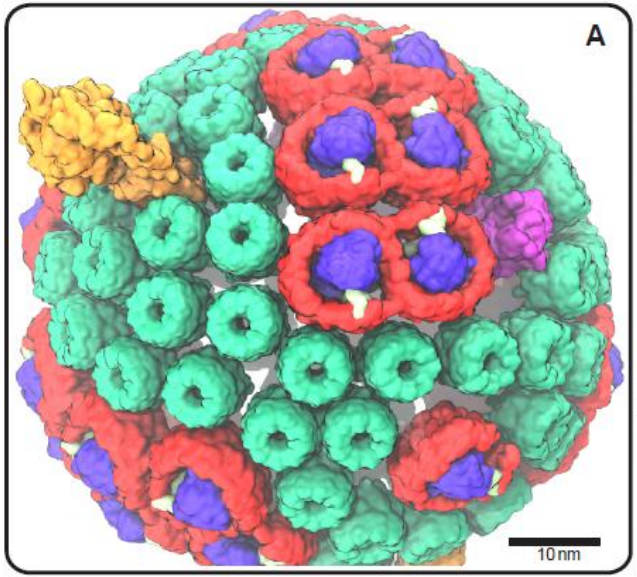
- Applications focus on higher level RT ops
- Parallel SPMD-oriented languages and compilers address the shortcomings of traditional tools
- RT frameworks provide performance-critical algorithms:
  - NVIDIA OptiX/CUDA: general RT framework for writing high performance GPU ray tracing engines
  - Intel OSPRay/Embree/ISPC: general RT framework and library, includes both basic kernels and full renderer implementations
  - AMD FireRays/OpenCL: library of high perf. GPU RT algorithms

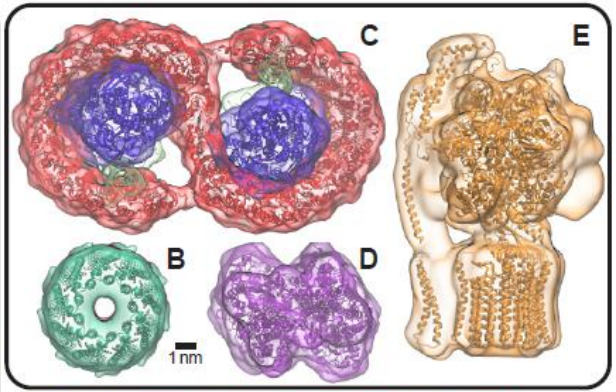
Photosynthetic Chromatophore of Purple Bacteria

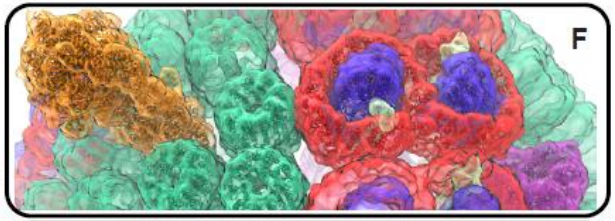
- Purple bacteria live in light-starved conditions at the bottom of ponds, with ~1% sunlight
- Chromatophore system
  - 100M atoms, 700 $Å^3$ volume
  - Contains over 100 proteins, ~3,000 bacteriochlorophylls for collection of photons
  - Energy conversion process synthesizes ATP, which fuels cells…

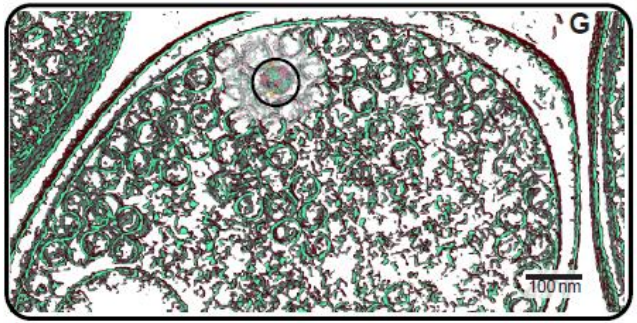


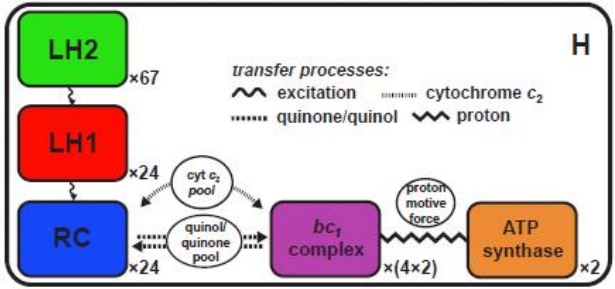
- Movie sums up ~40 papers and 37 years of work by Schulten lab and collaborators
- Driving NAMD and VMD software design:
  - Two decades of simulation, analysis, and visualization of individual chromatophore components w/ NAMD+VMD





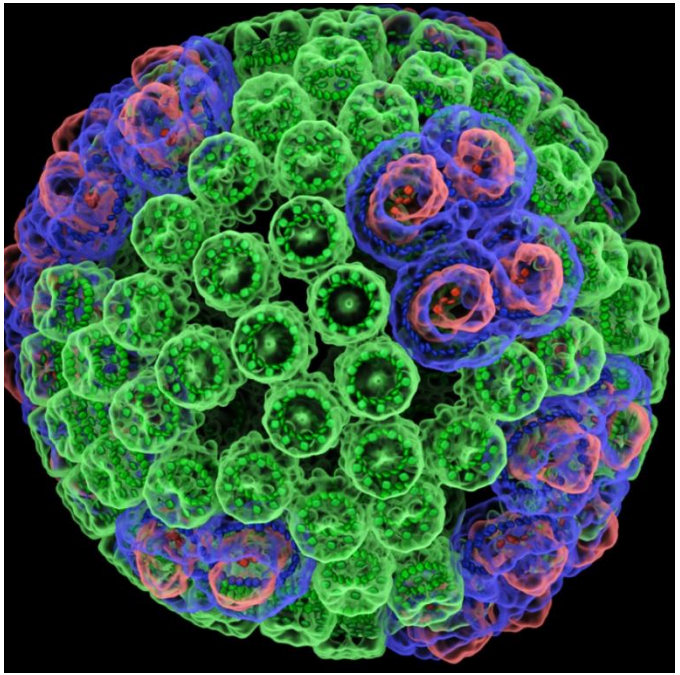






VMD Chromatophore Rendering on Blue Waters

- 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

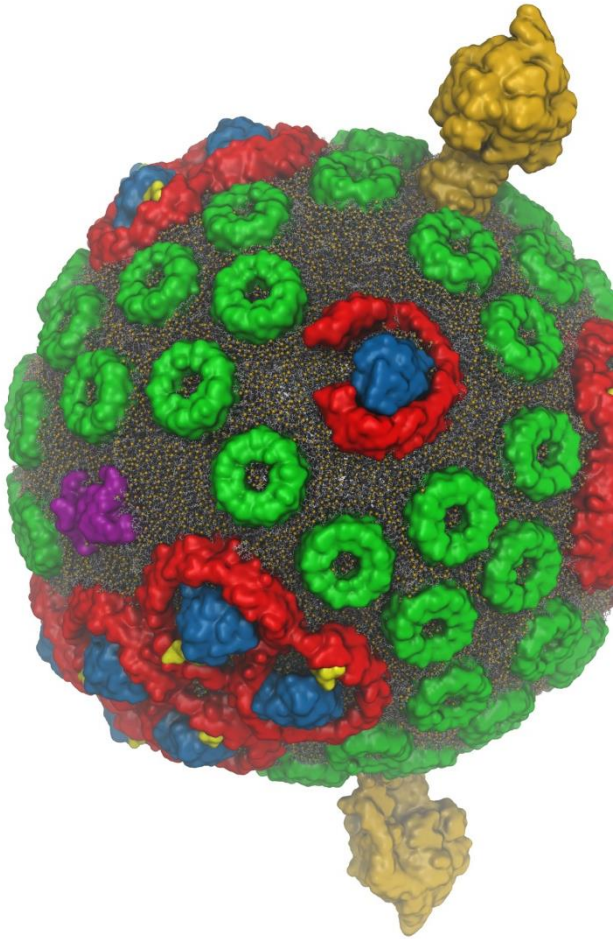


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

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**

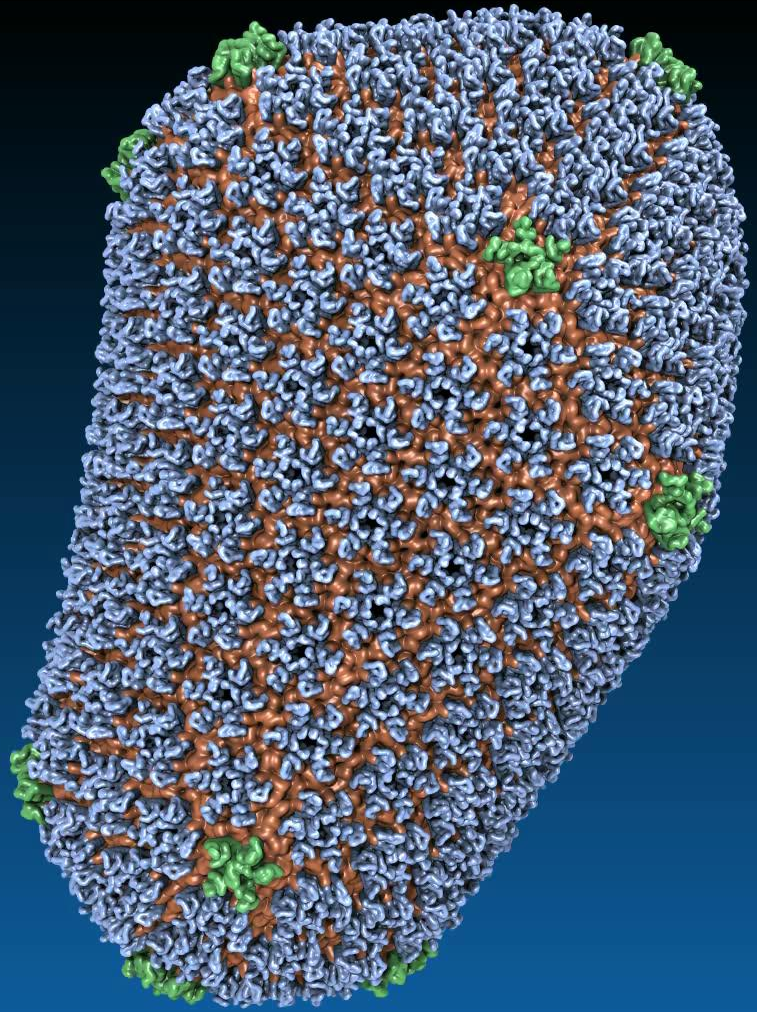
VMD 1.9.3+OptiX 3.8 – ~1.5x Performance Increase on Blue Waters Supercomputer

- 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**

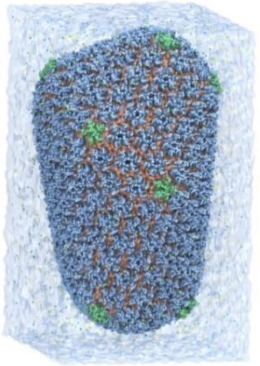


VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.

Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone et al., J. Parallel Computing, 2016.



VMD 1.9.3 HIV-1 Parallel Movie Rendering on Blue Waters Cray XE6/XK7



New VMD 1.9.3: TachyonL-OptiX on XK7 vs. Tachyon on XE6, K20X GPUs yield **up to twelve times** geom+ray tracing speedup

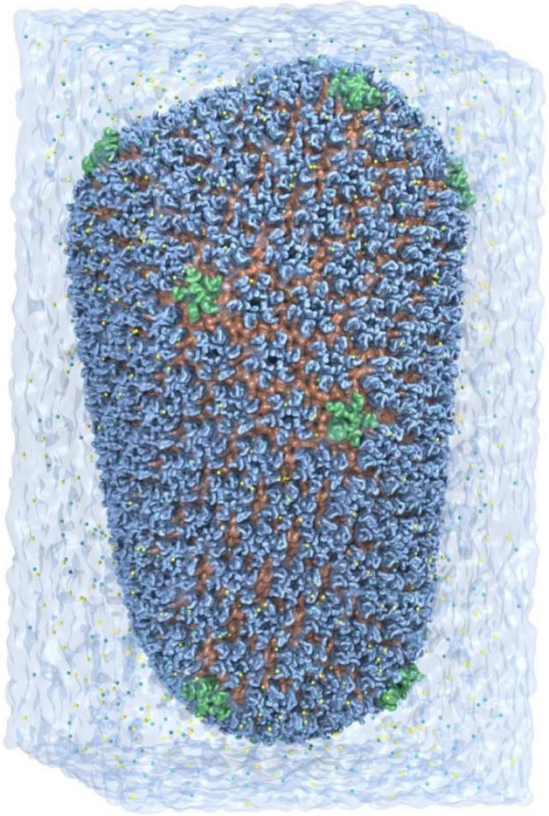
Ray Tracer Version	Node Type and Count	Script Load	State Load	Geometry + Ray Tracing	Total Time
New TachyonL-OptiX [2]	64 XK7 Tesla K20X GPUs	2 s	39 s	435 s	476 s
New TachyonL-OptiX [2]	**128 XK7 Tesla K20X GPUs**	**3 s**	**62 s**	**230 s**	**295 s**
TachyonL-OptiX [1]	64 XK7 Tesla K20X GPUs	2 s	38 s	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

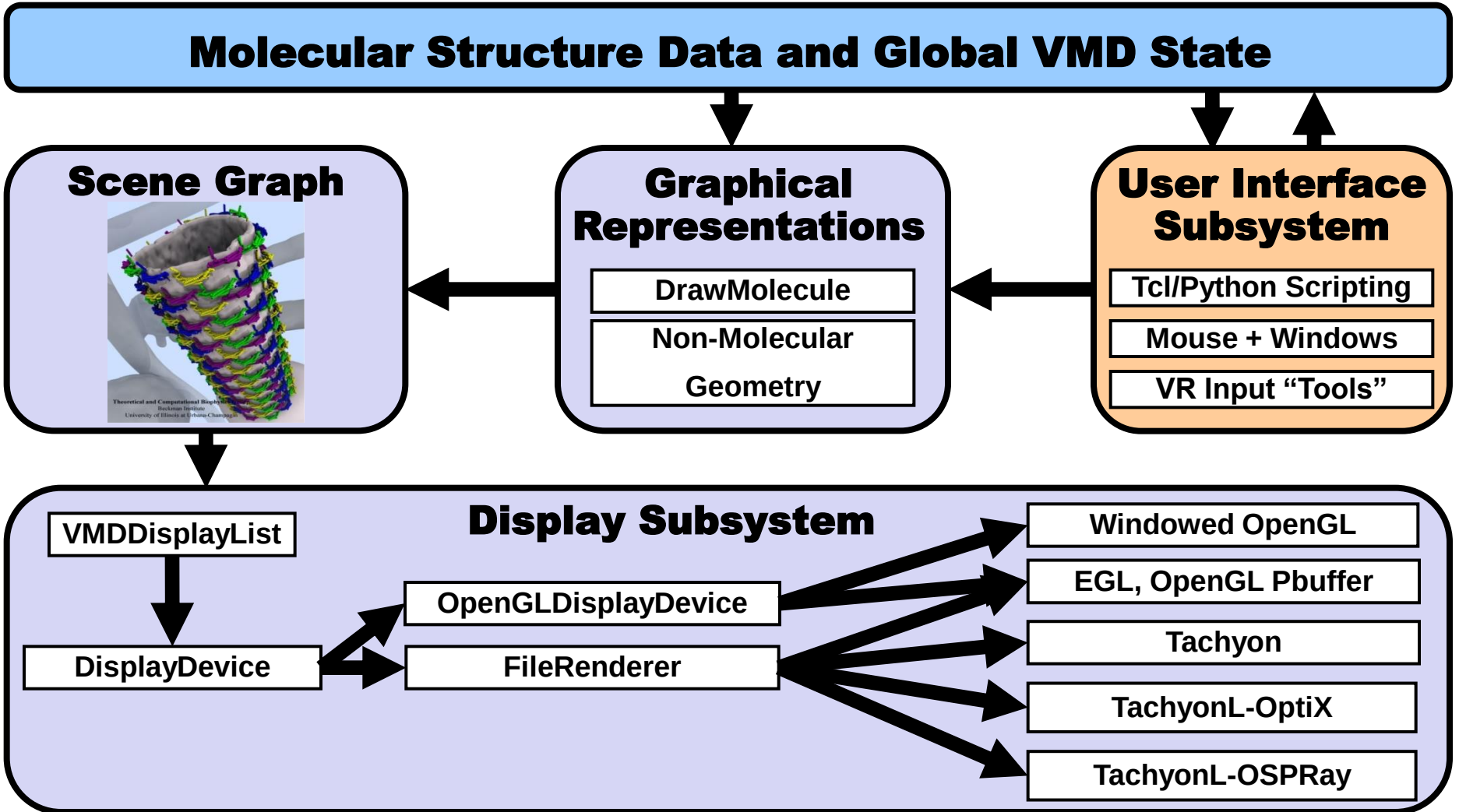
[1] GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms. J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13: Proceedings of the 8th International Workshop on Ultrascale Visualization, pp. 6:1-6:8, 2013.

[2] Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone et al., J. Parallel Computing, 2016 (in-press)

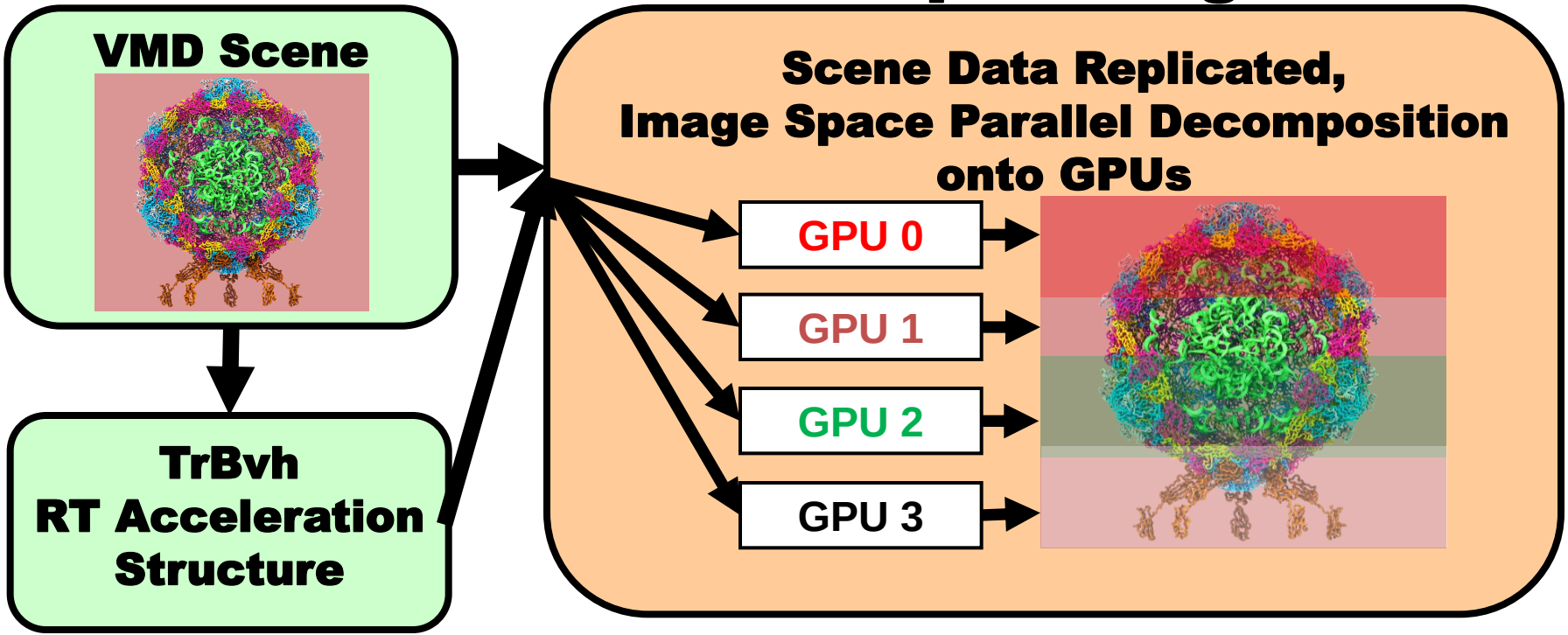
VMD 1.9.x Interactive Ray Tracing

- Ray tracing heavily used for VMD publication-quality images/movies
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides –***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers



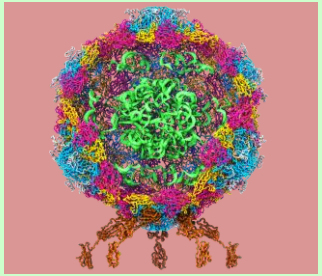

Molecular Structure Data and Global VMD State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input “Tools”
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL
EGL, OpenGL Pbuffer
Tachyon
TachyonL-OptiX
TachyonL-OSPRay

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



VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster

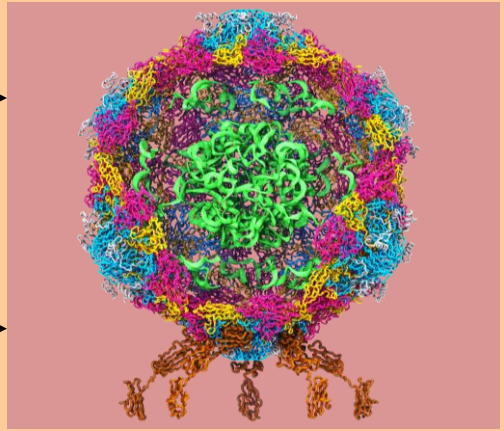
VMD Scene



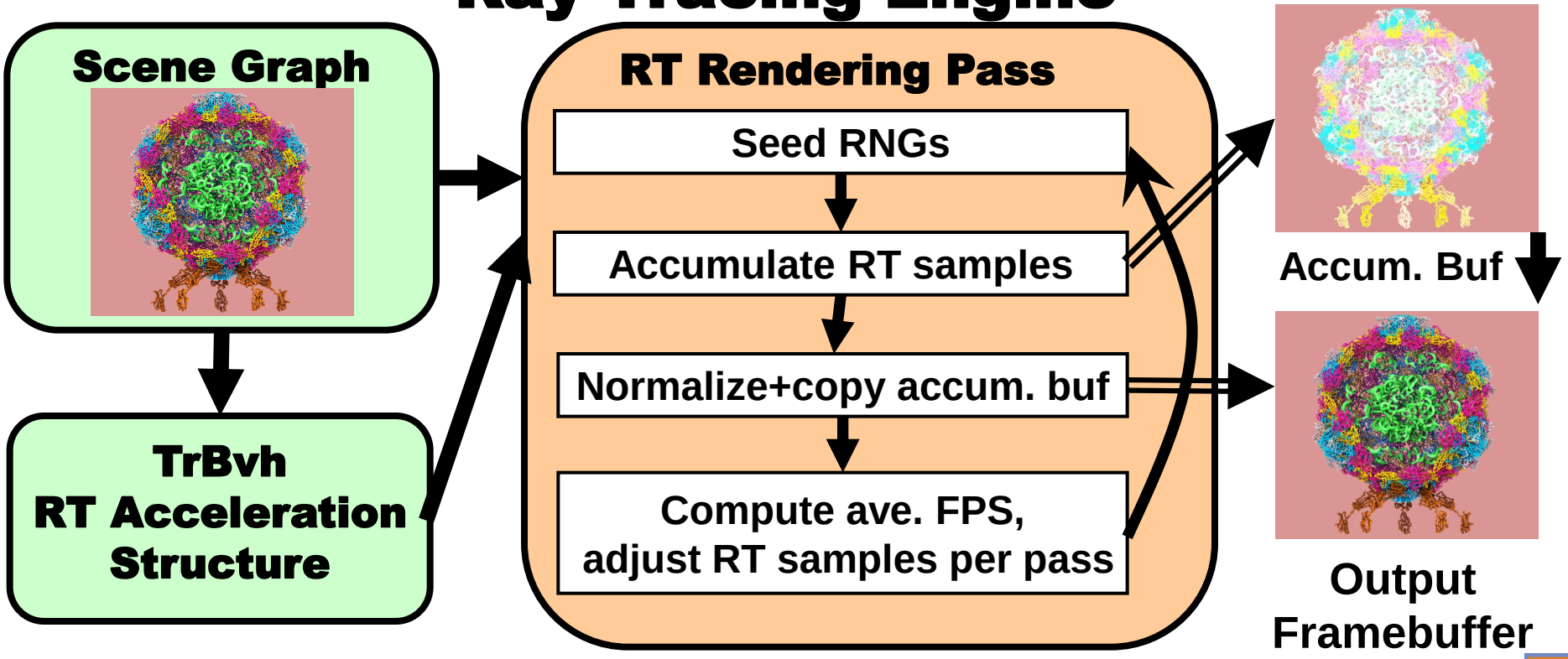
Scene Data Replicated, Image Space / Sample Space Parallel Decomposition onto GPUs

VCA 0:
8 K6000 GPUs

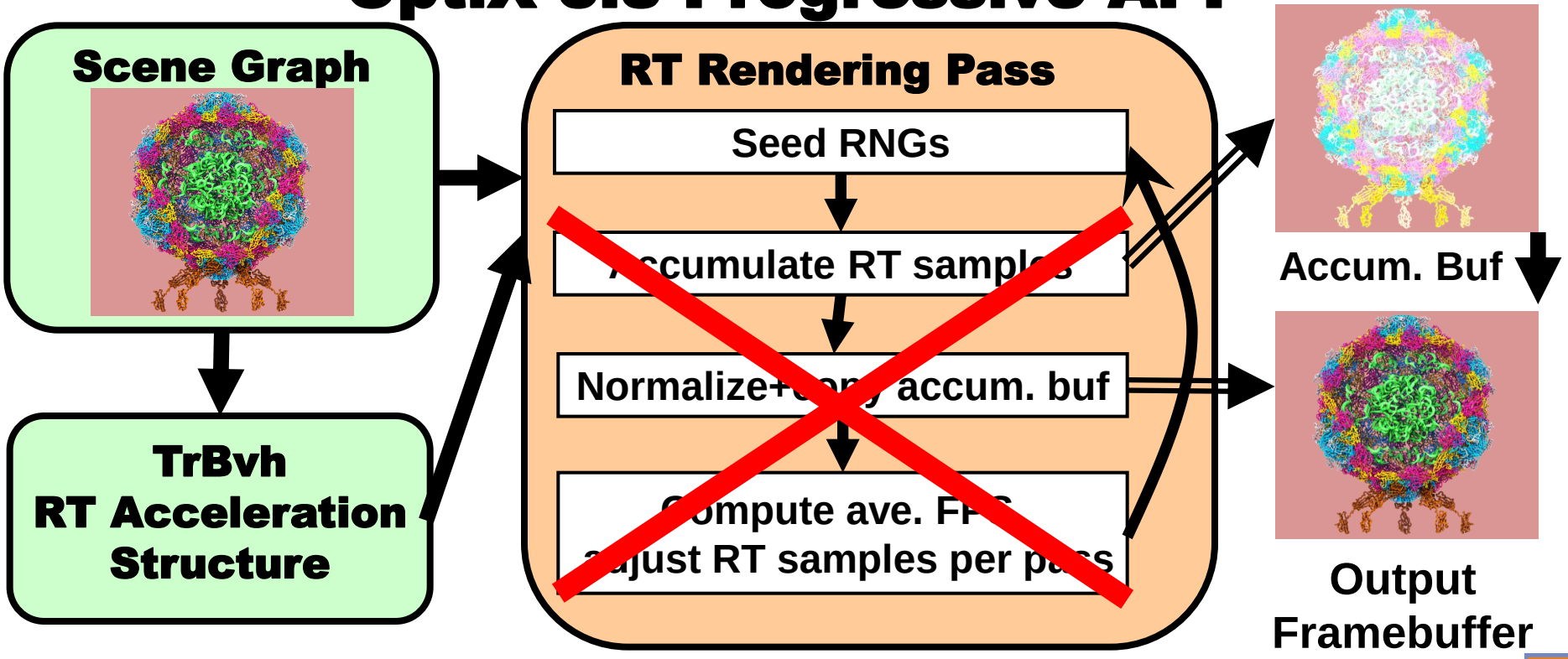
VCA N:
8 K6000 GPUs



VMD TachyonL-OptiX Interactive Ray Tracing Engine

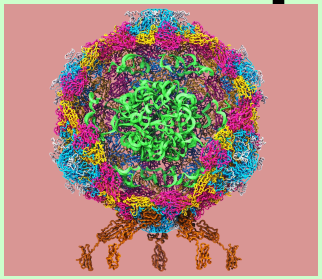


VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API

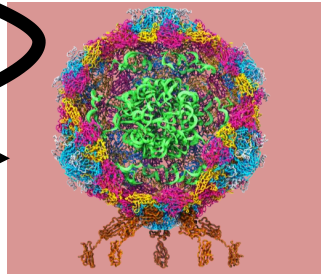
Scene Graph



TrBvh RT Acceleration Structure

RT Progressive Subframe

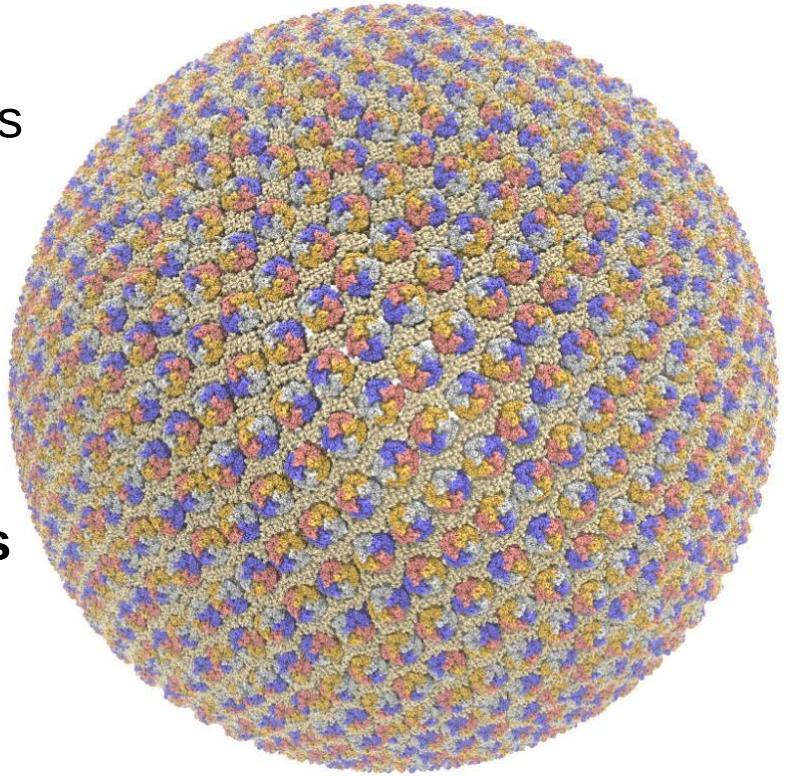
- rtContextLaunchProgressive2D()
- Check for User Interface Inputs, Update OptiX Variables
- rtBufferGetProgressiveUpdateReady()
- rtContextStopProgressive()



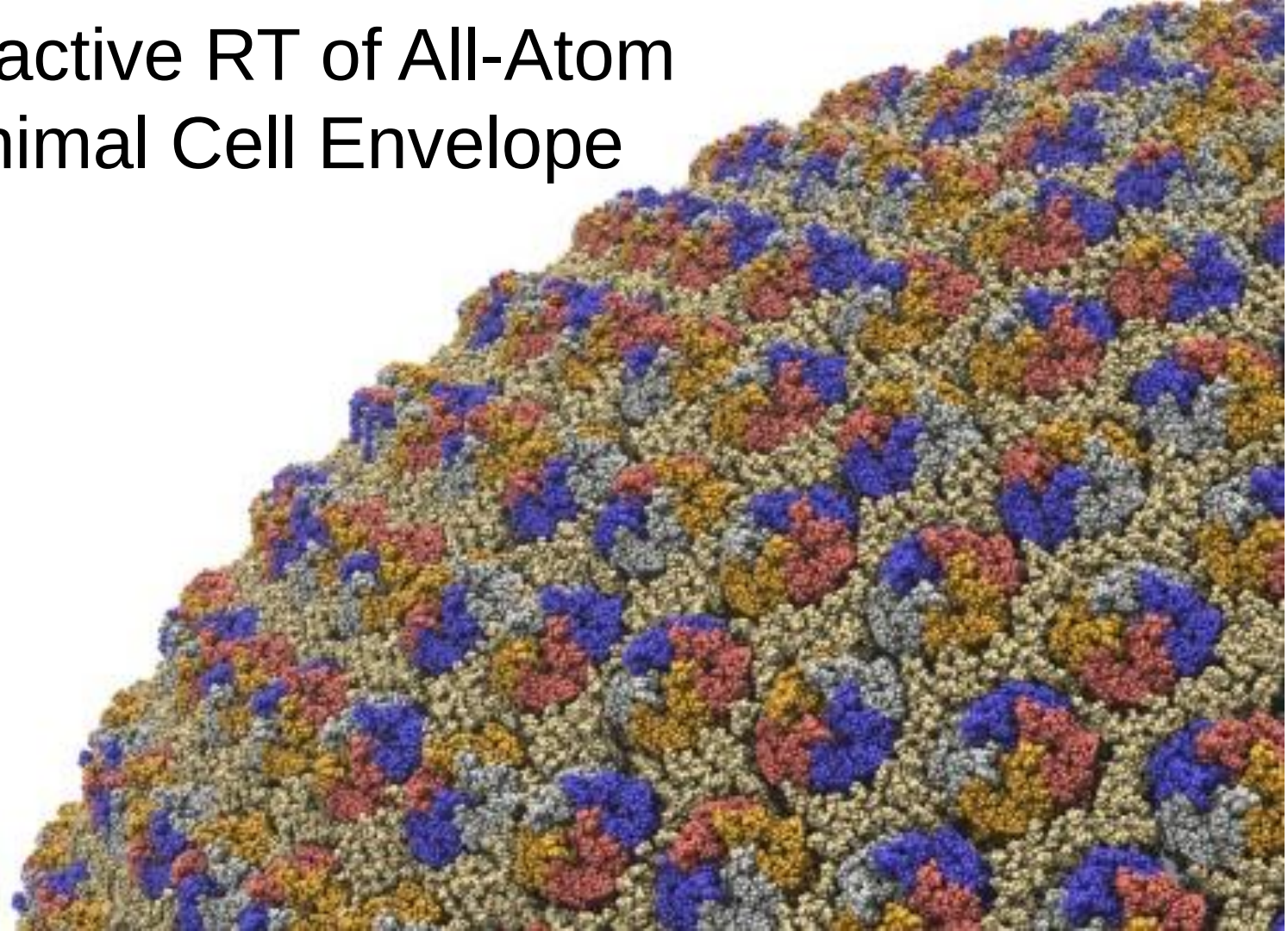
Draw Output Framebuffer

Interactive RT of All-Atom Minimal Cell Envelope

- 200 nm spherical envelope
- Membrane with ~50% occupancy by proteins (2000x Aquaporin channels)
- 42M atoms in membrane
- **Interactive RT w/ 2 dir. lights and AO on GeForce Titan X @ ~12 FPS**
- **Complete model with correct proteins, solvent, etc, will contain billions of atoms**

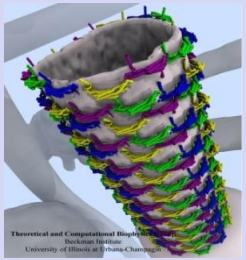


Interactive RT of All-Atom Minimal Cell Envelope



New: VMD-OSPRay Interactive CPU Ray Tracing with Progressive Refinement

Scene Graph and RT accel. data structures



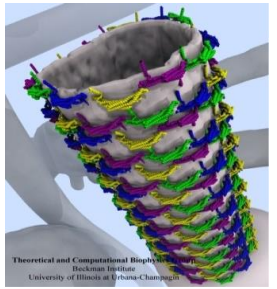
RT Progressive Refinement Loop

ospFrameBufferClear(OSP_FB_ACCUM**)**

ospRenderFrame(… OSP_FB_ACCUM**)**

Check for User Interface Inputs,
Update OSPRay Renderer State

ospMapFrameBuffer()
Draw…
ospUnmapFrameBuffer()



Draw Output Framebuffer

Interactive Remote Visualization and Analysis

- Enabled by hardware H.264/H.265 video encode/decode
- Enable visualization and analyses not possible with conventional workstations
- Access data located anywhere in the world
  - Same VMD session available to any device

Interactive Collaboration

- Enable interactive VMD sessions with multiple-endpoints
- Enable collaboration features that were previously impractical:
  - Remote viz. overcomes local computing and visualization limitations for interactive display

Supercomputer, MD Simulation

Experimentalist Collaborators Pittsburgh, PA

Urbana, IL

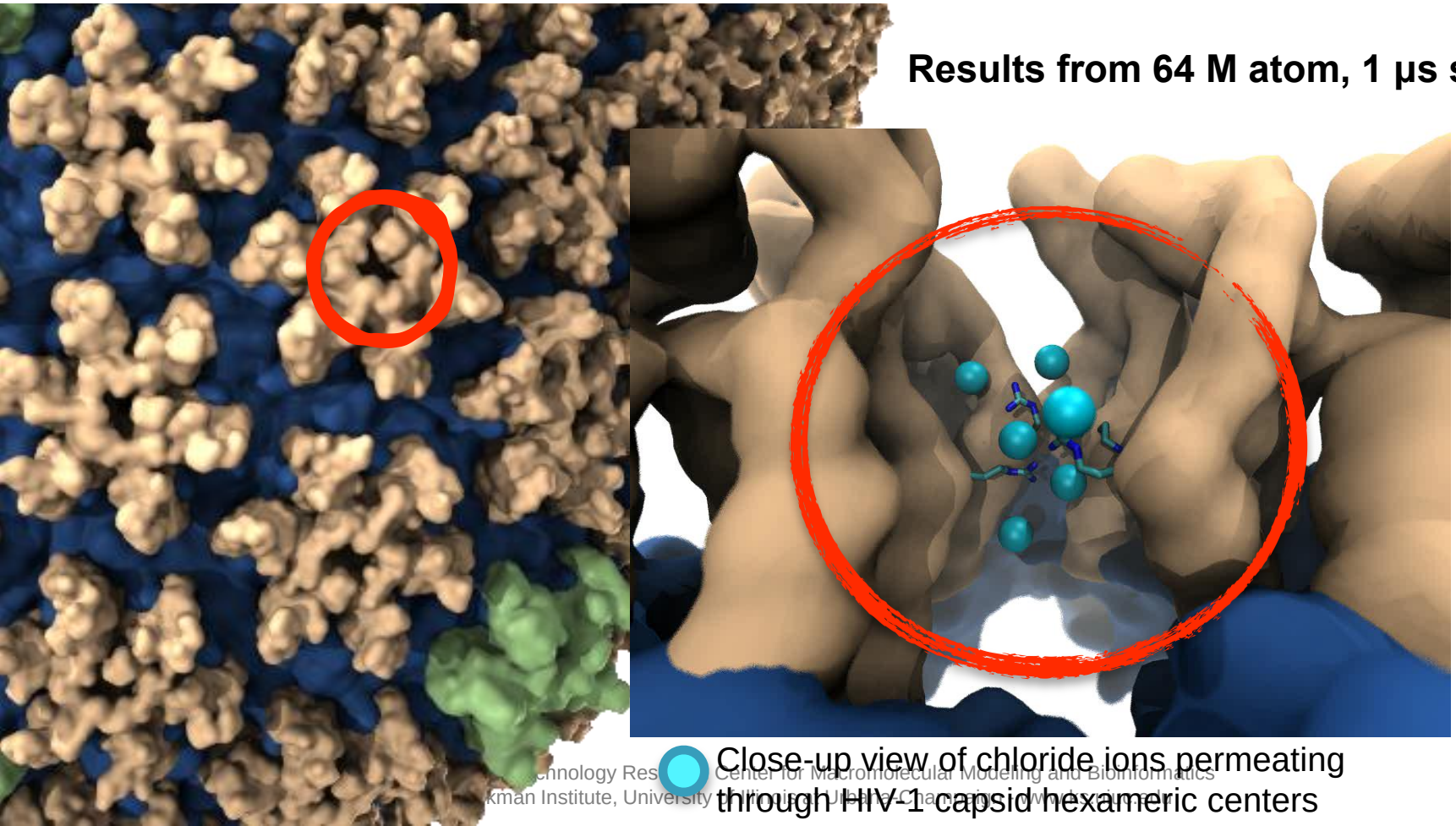
Immersive Viz. w/ VMD

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

VMD running in a CAVE

Goal: Intuitive interactive viz. in crowded molecular complexes

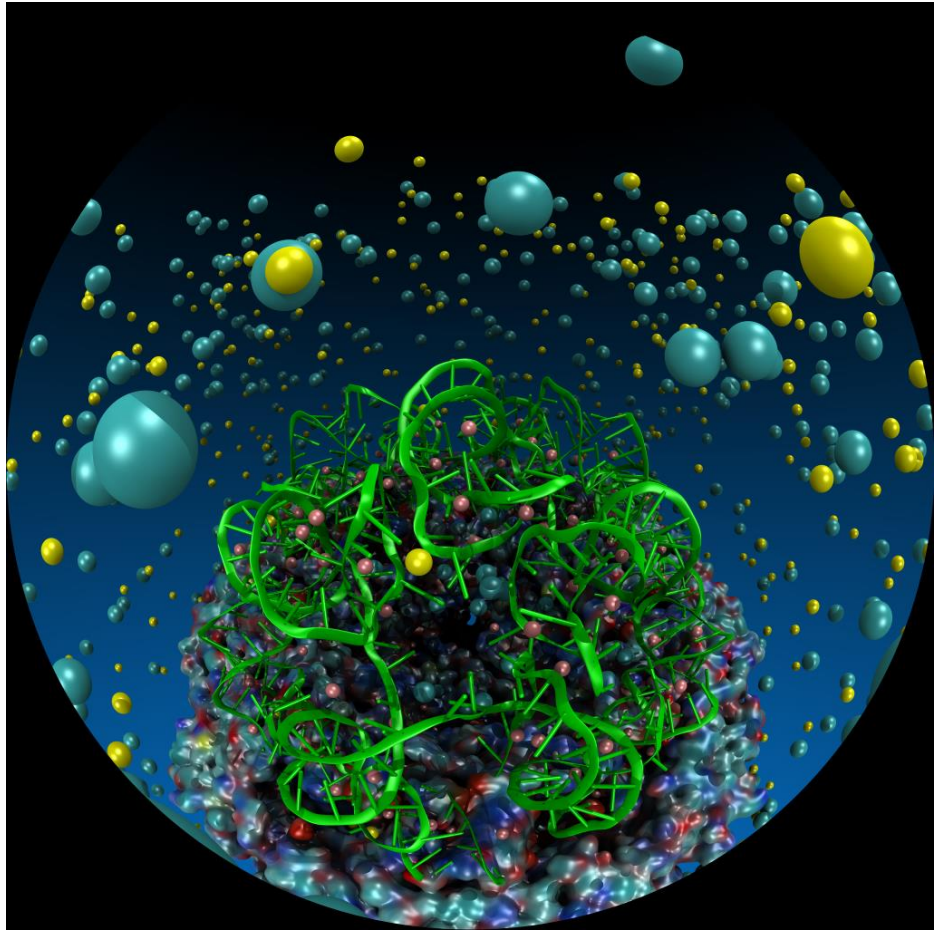
Results from 64 M atom, 1 μs sim!



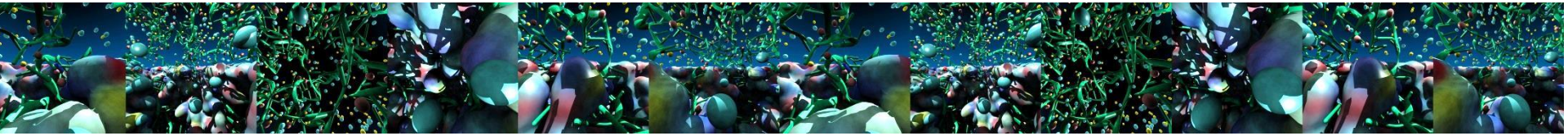
Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers

VMD Planetarium Dome Master Camera

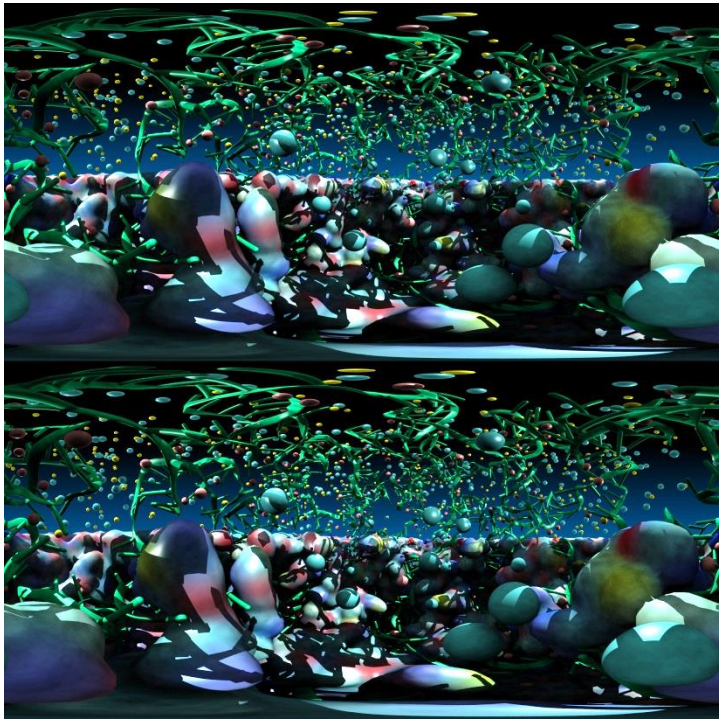
- RT-based dome projection -- rasterization poorly suited to non-planar projections
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required



Stereoscopic Panorama Ray Tracing w/ OptiX

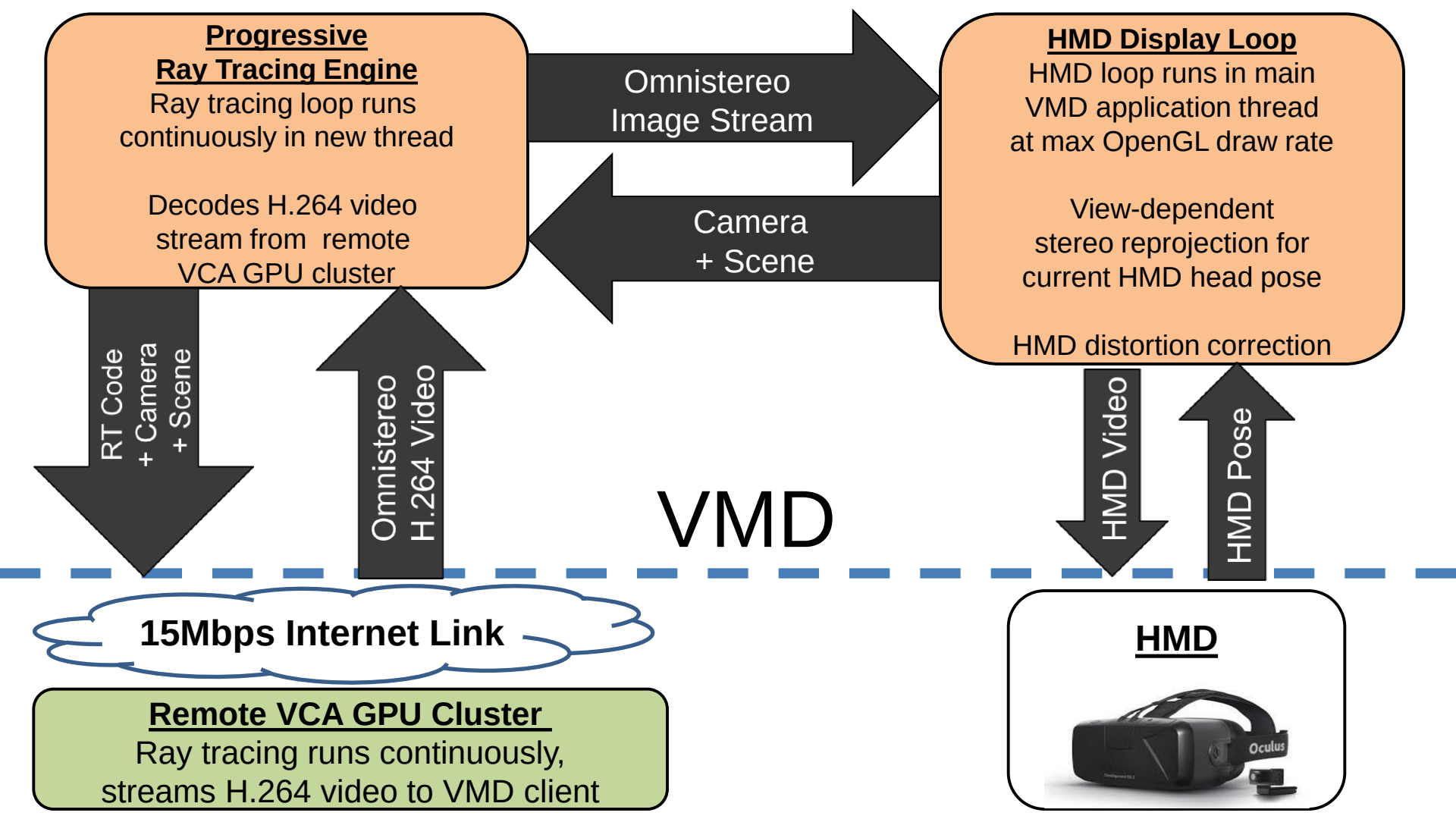


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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



HMD Ray Tracing Challenges

- HMDs require high frame rates **(90Hz or more)** and minimum latency between IMU sensor reads and presentation on the display
- Multi-GPU workstations fast enough to direct-drive HMDs at required frame rates for simple scenes with direct lighting, hard shadows
- Advanced RT effects such as AO lighting, depth of field require much **larger sample counts**, impractical for direct-driving HMDs
- **Remote viz. required for** many HPC problems due to **large data**
- **Remote viz. latencies too high for direct-drive of HMD**
- **Our two-phase approach: moderate-FPS remote RT combined with local high-FPS view-dependent HMD reprojection w/ OpenGL**


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
Oculus

HMD View-Dependent Reprojection with OpenGL

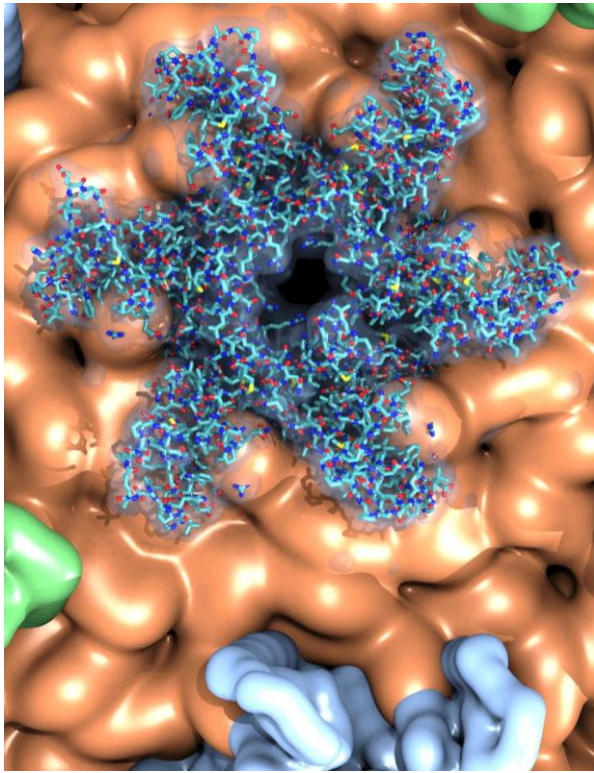
- Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface
- HMD sees standard perspective frustum view of the textured surface
- Commodity HMD optics require **software lens distortion and chromatic aberration correction** prior to display, implemented with multi-pass FBO rendering
- Low-latency redraw as HMD head pose changes

Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing

VMD-Next: Coming Soon

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

- Improved movie making tools, off-screen OpenGL movie rendering, parallel movie rendering:
  - EGL for parallel graphics w/o X11 server
  - Built-in (basic) interactive remote visualization on HPC clusters and supercomputers
- Much work to do on VR user interfaces, multi-user collaborative visualization, …



GPU Ray Tracing of HIV-1 Capsid Detail

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Related Publications

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

- **Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering.** John E. Stone, William R. Sherman, and Klaus Schulten.High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
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- **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. *International Conference on Green Computing,* pp. 317-324, 2010.
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