Frontiers of Molecular Visualization: Interactive Ray Tracing, Panoramic Displays, VR HMDs, and Remote Visualization

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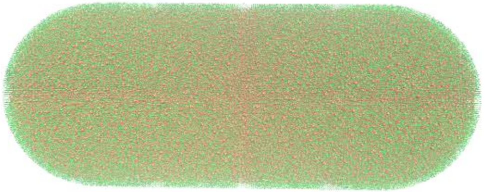
2:30pm, Hilton Salon B, Sunday Nov 15, 2015

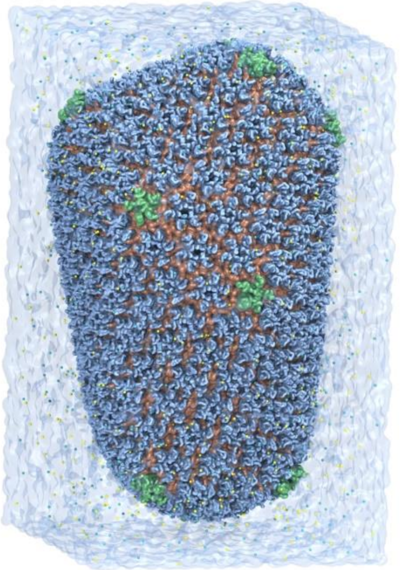
Supercomputing 2015, Austin, TX

VMD – “Visual Molecular Dynamics”

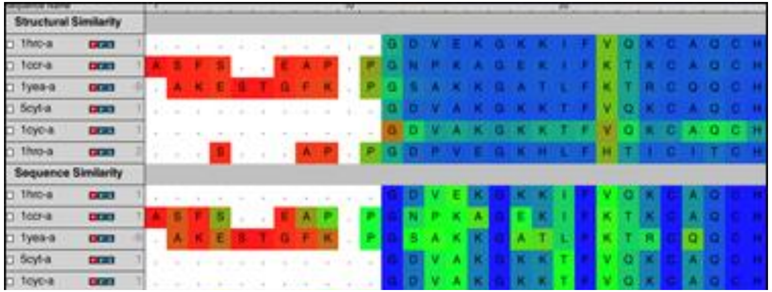
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



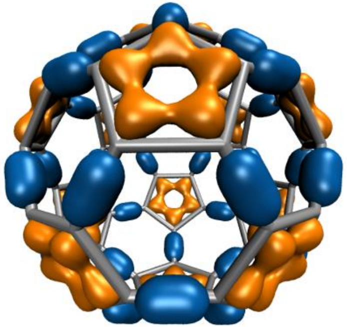
Whole Cell Simulation



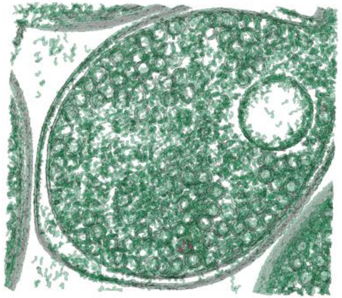
MD Simulations



Sequence Data



Quantum Chemistry

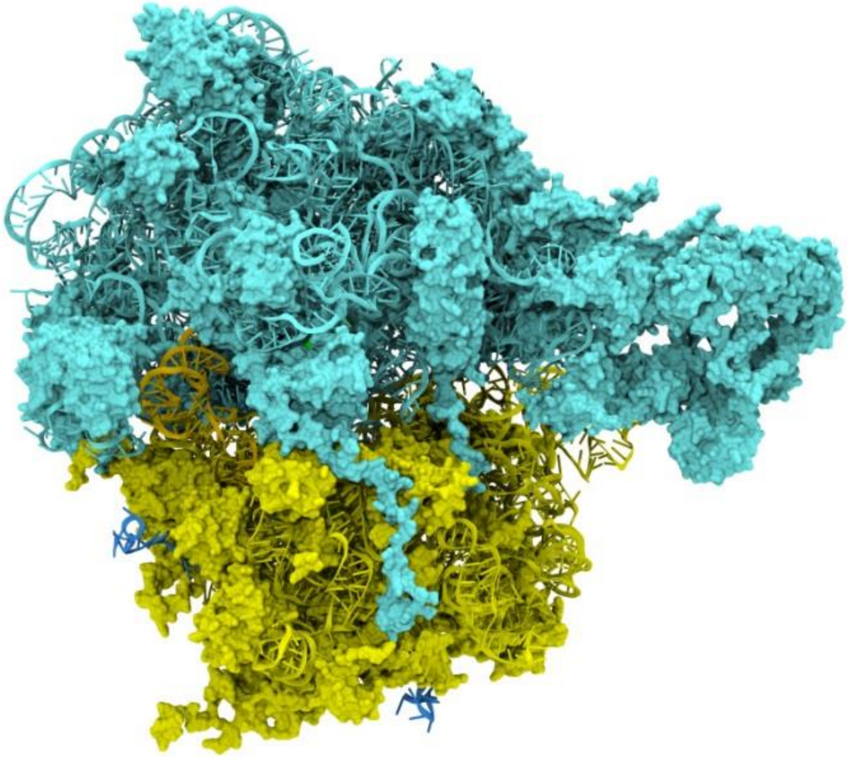


CryoEM, Cellular Tomography

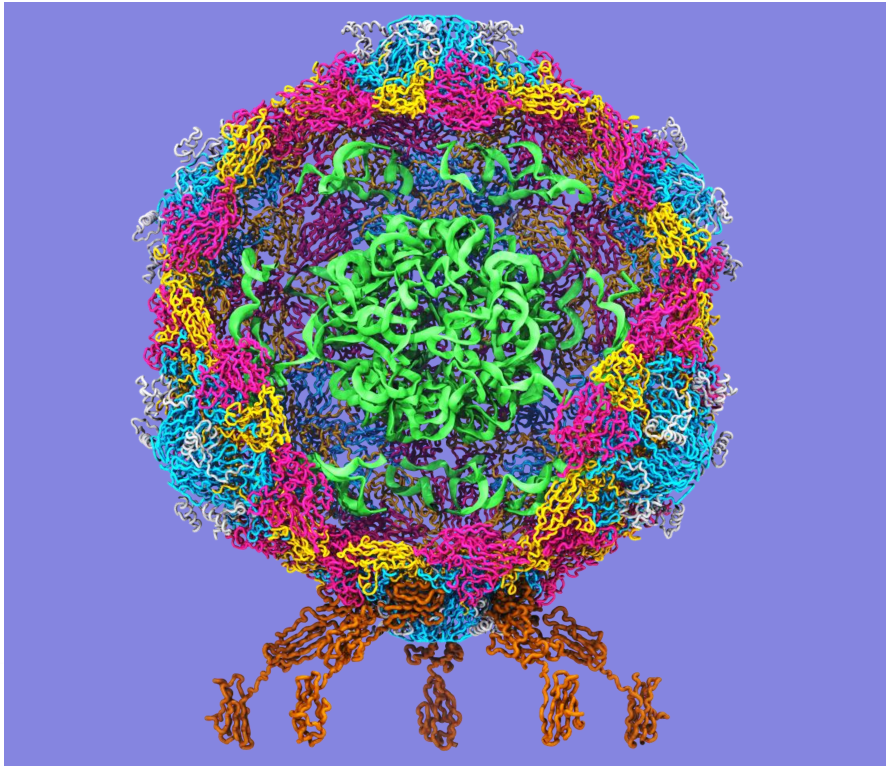
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

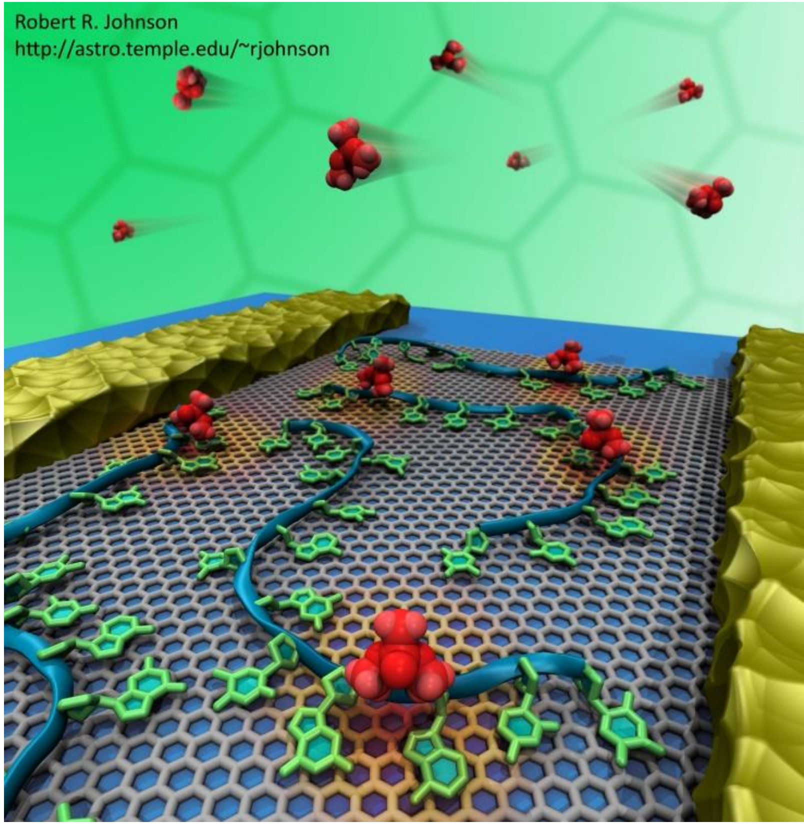


Poliovirus



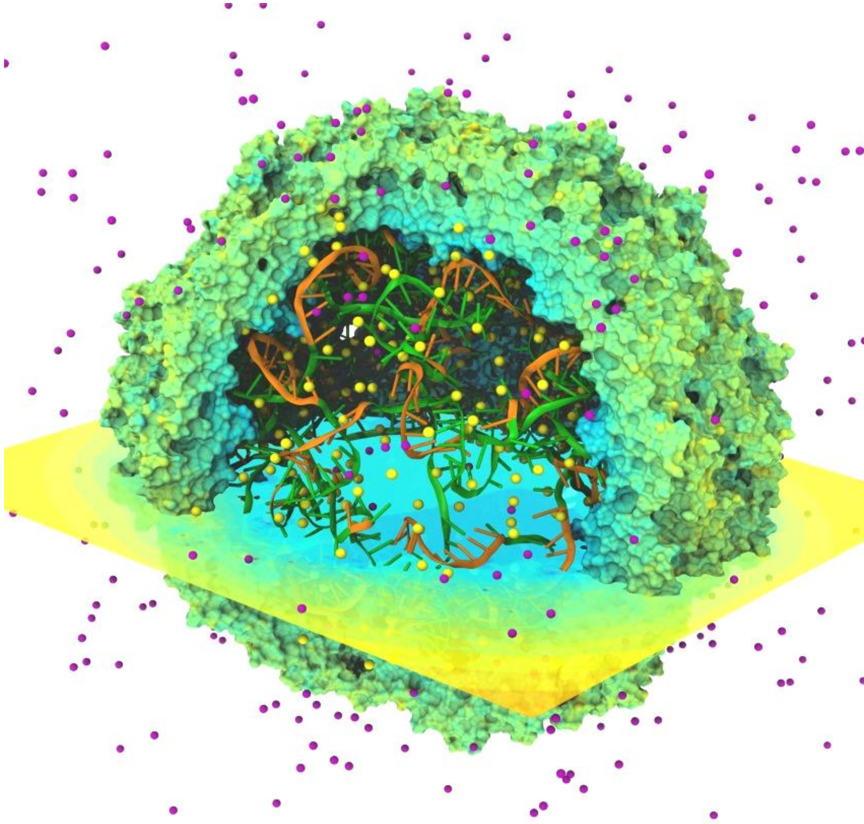
Ray Tracing in VMD

- 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)



Biomolecular Visualization Challenges

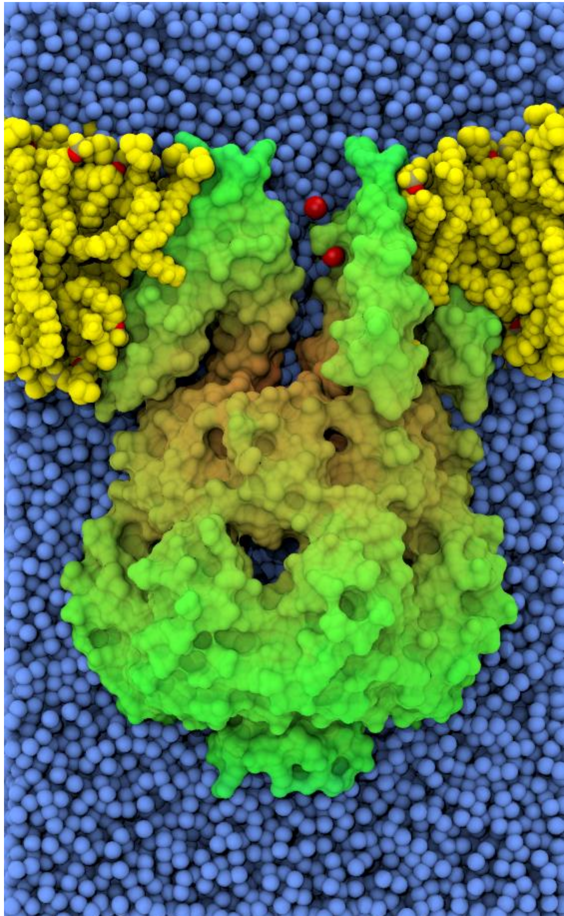
- Geometrically complex scenes
- Spatial relationships important to see clearly: fog, shadows, AO helpful
- Often show a mix of structural and spatial properties
- Time varying!



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

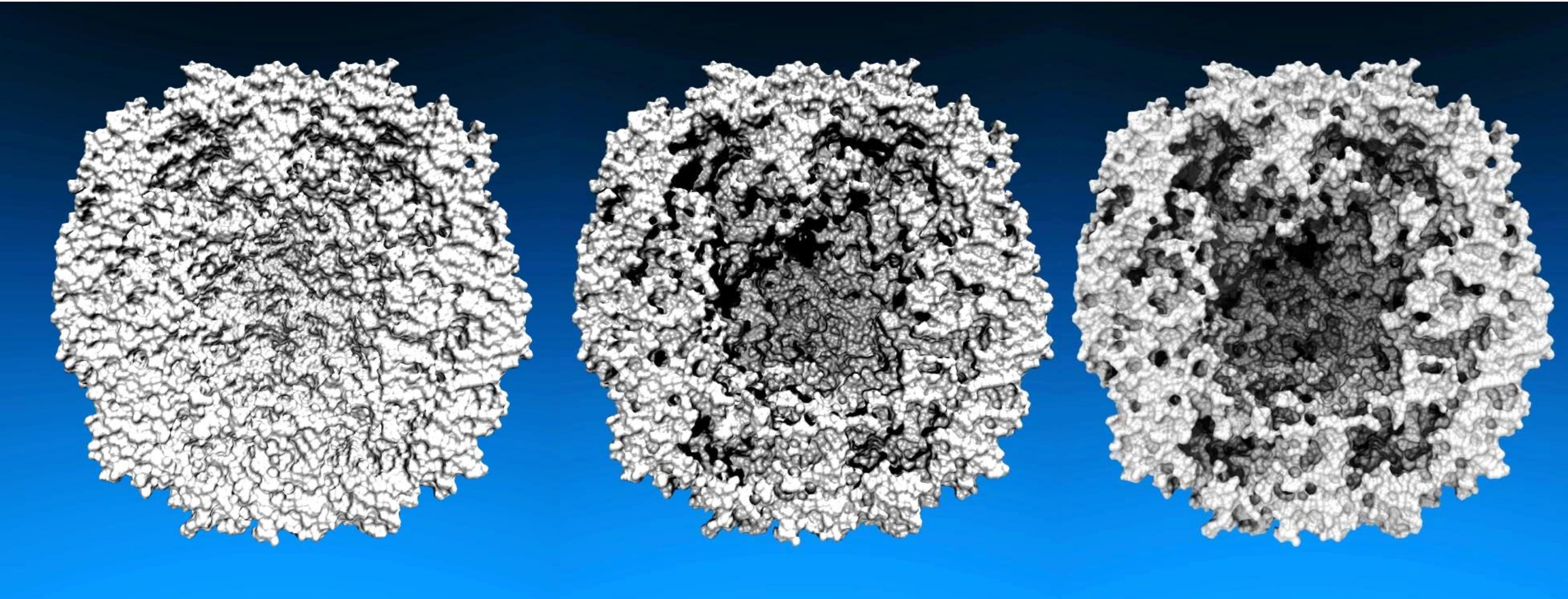


Lighting Comparison

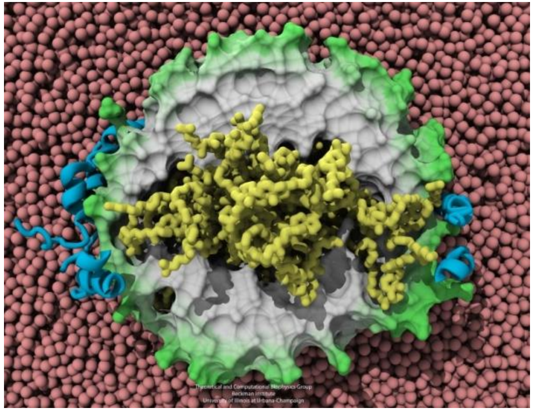
Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

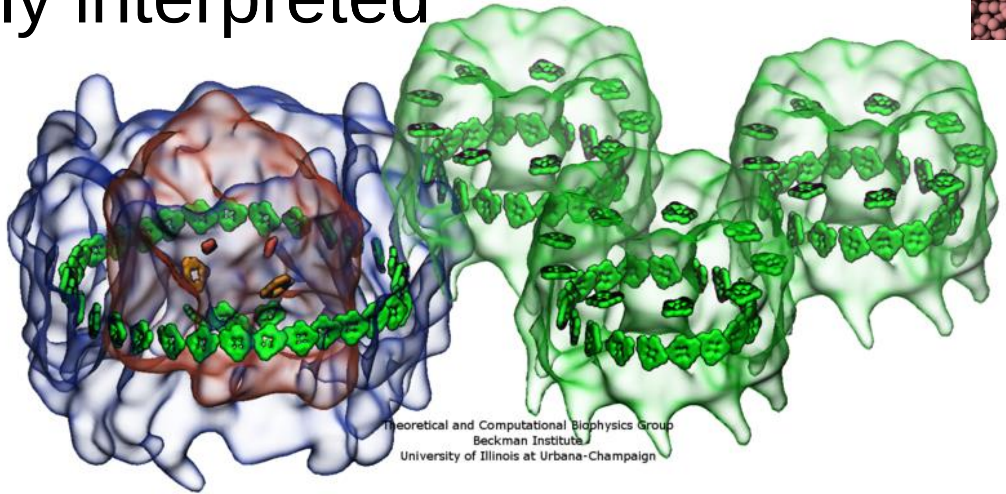
Ambient occlusion + two lights, 144 AO rays/hit

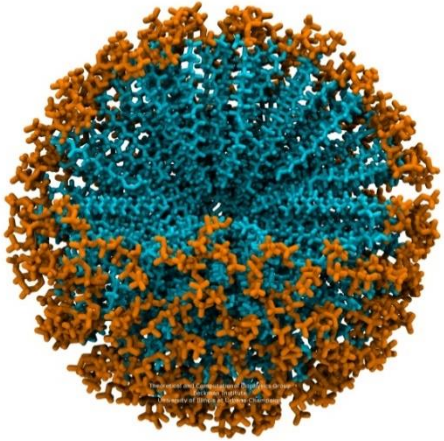


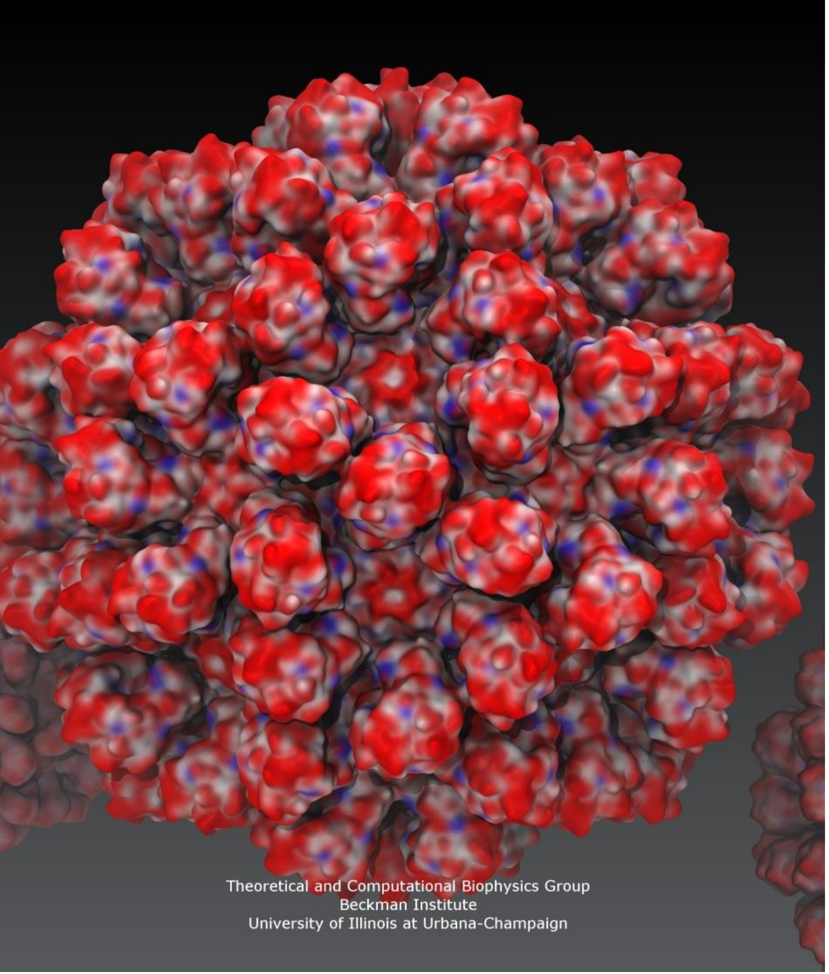
Benefits of Advanced Lighting and Shading Techniques



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



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Beckman Institute
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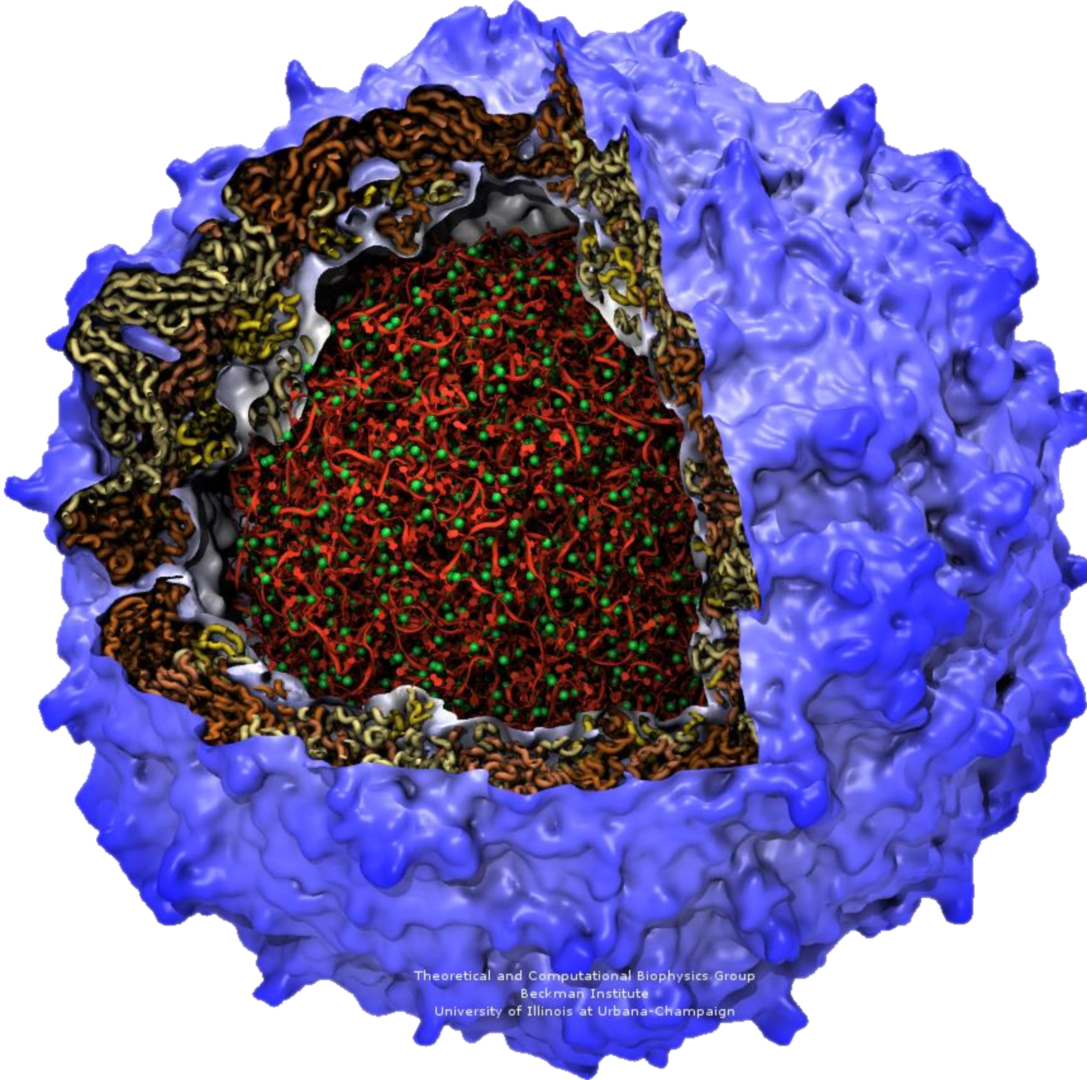
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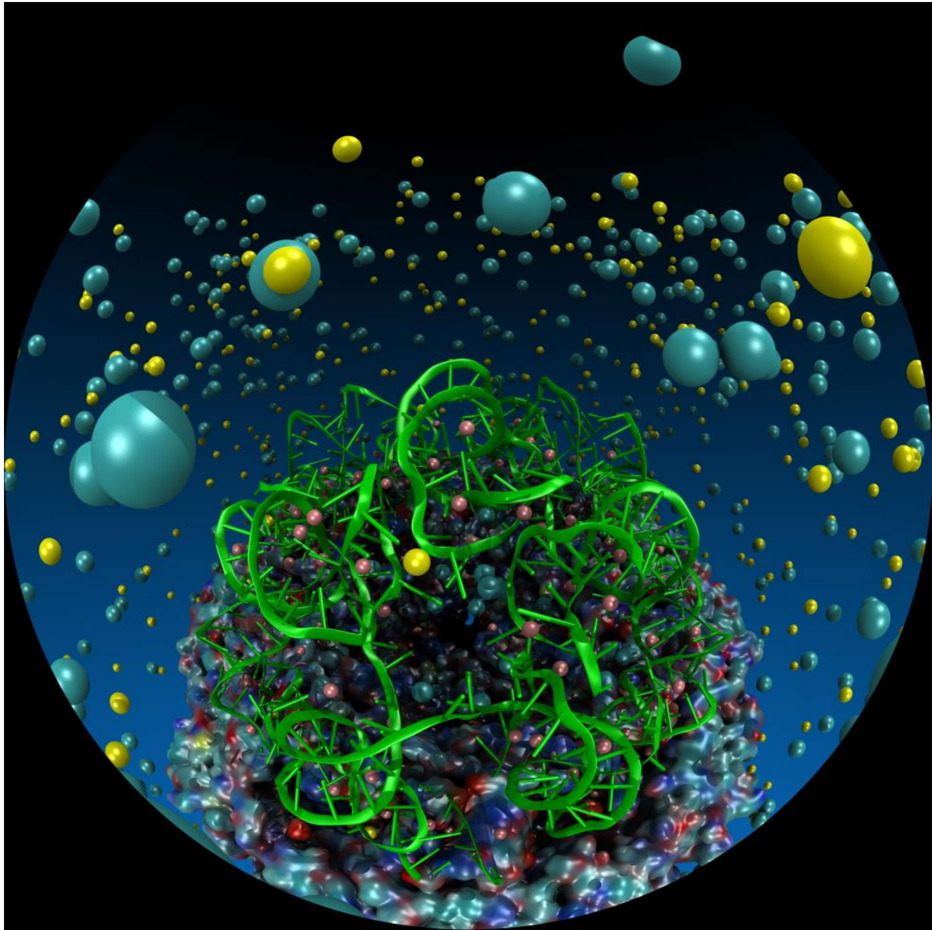
VMD Planetarium Dome Master Camera

- 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

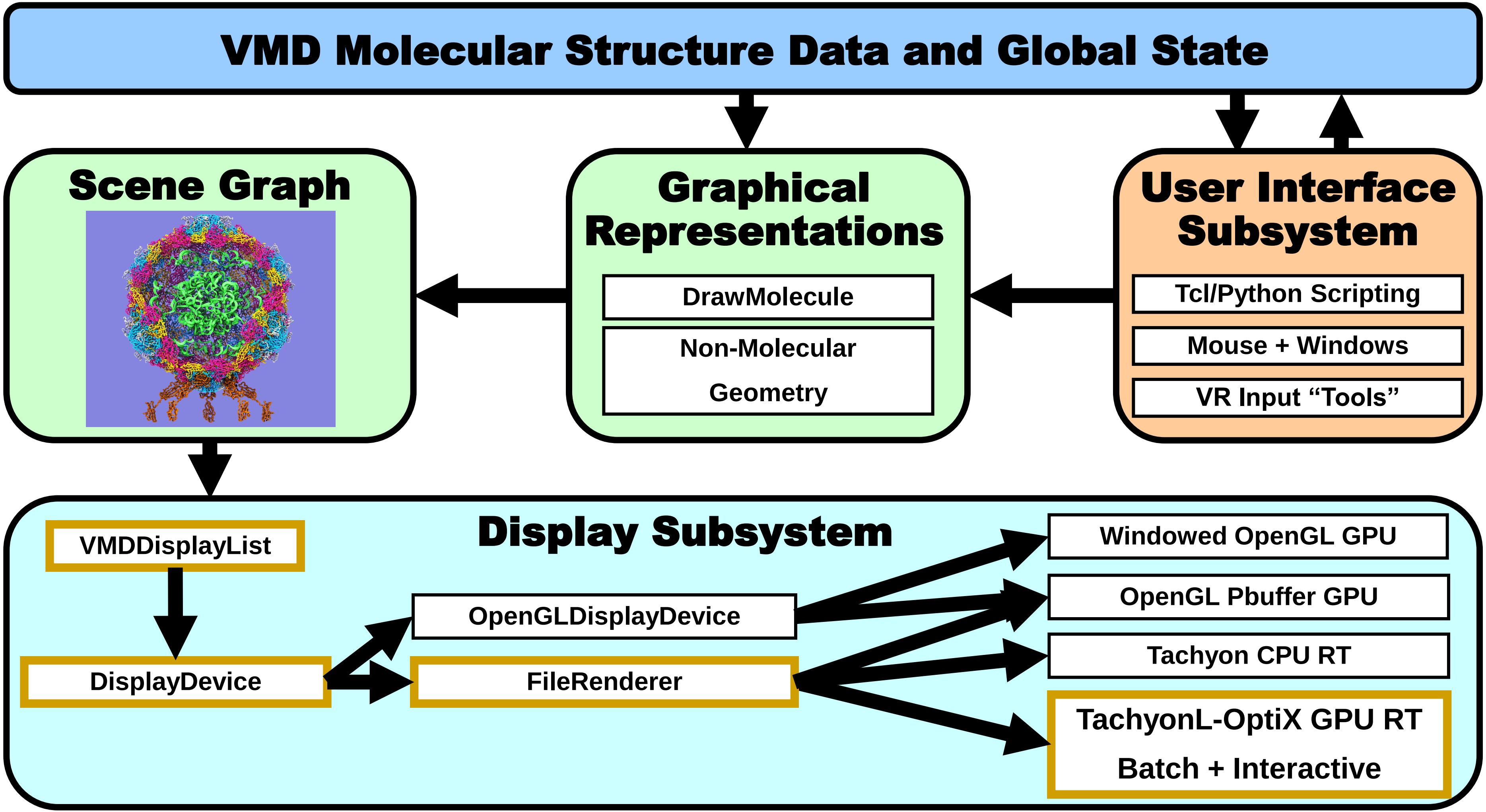


Ray Tracing Performance

- 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 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.

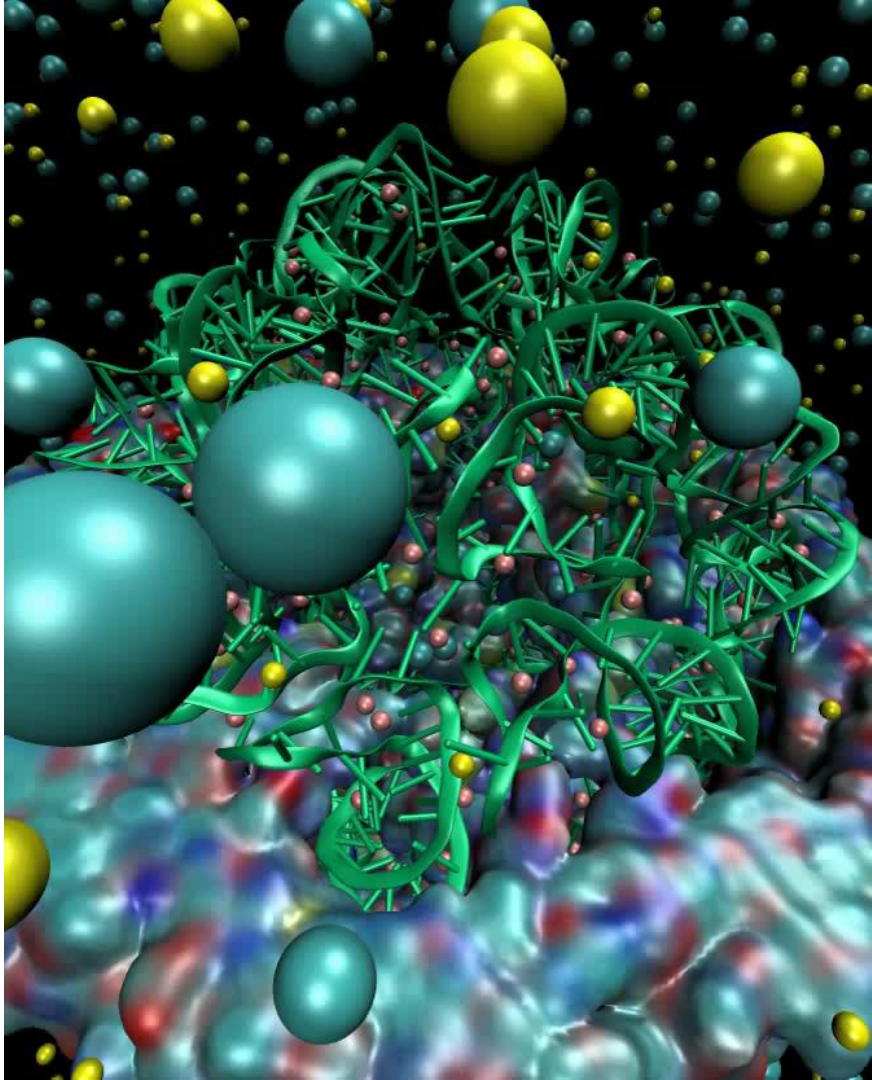
Fast Ray Tracing Frameworks

- 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/ISPC: general RT framework and library, includes not only basic kernels but also complete renderer implementations
  - AMD FireRays/OpenCL: library of high perf. GPU RT algorithms

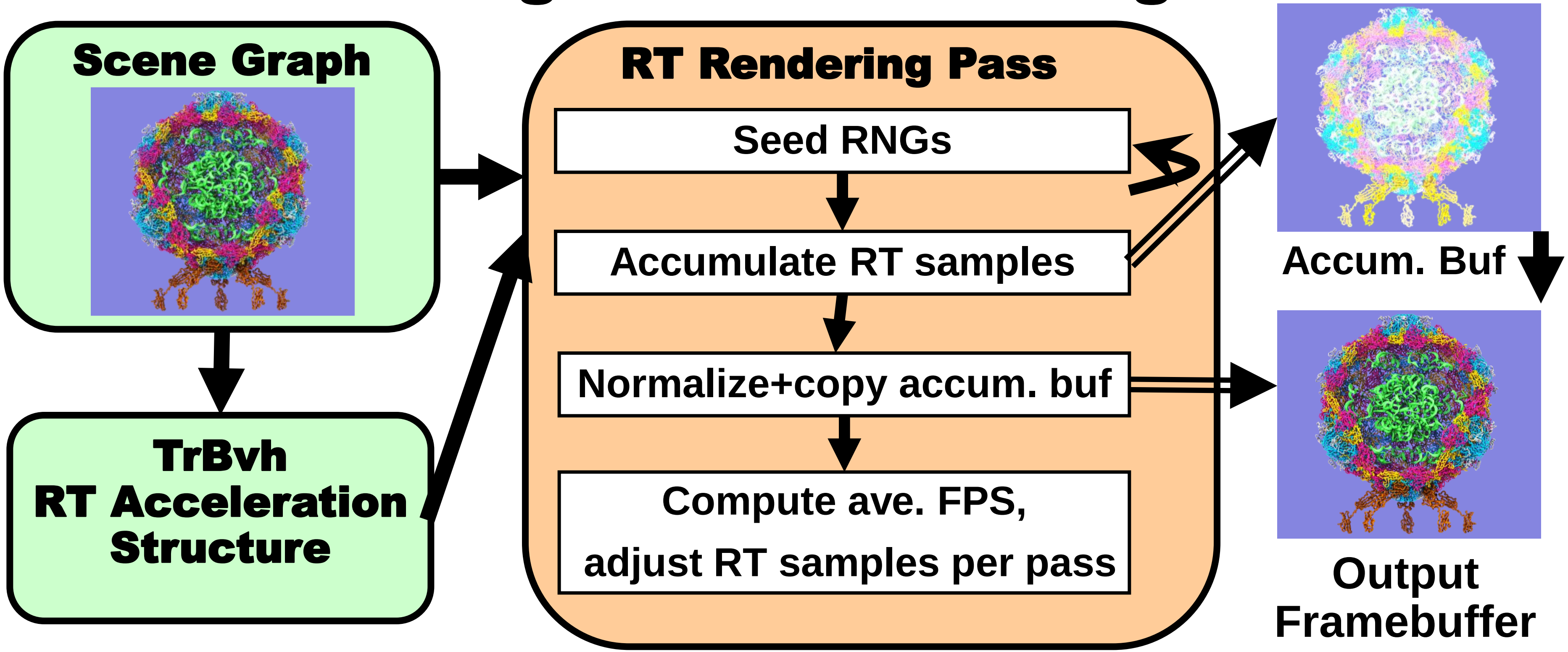

VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input “Tools”
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL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

VMD Interactive GPU Ray Tracing

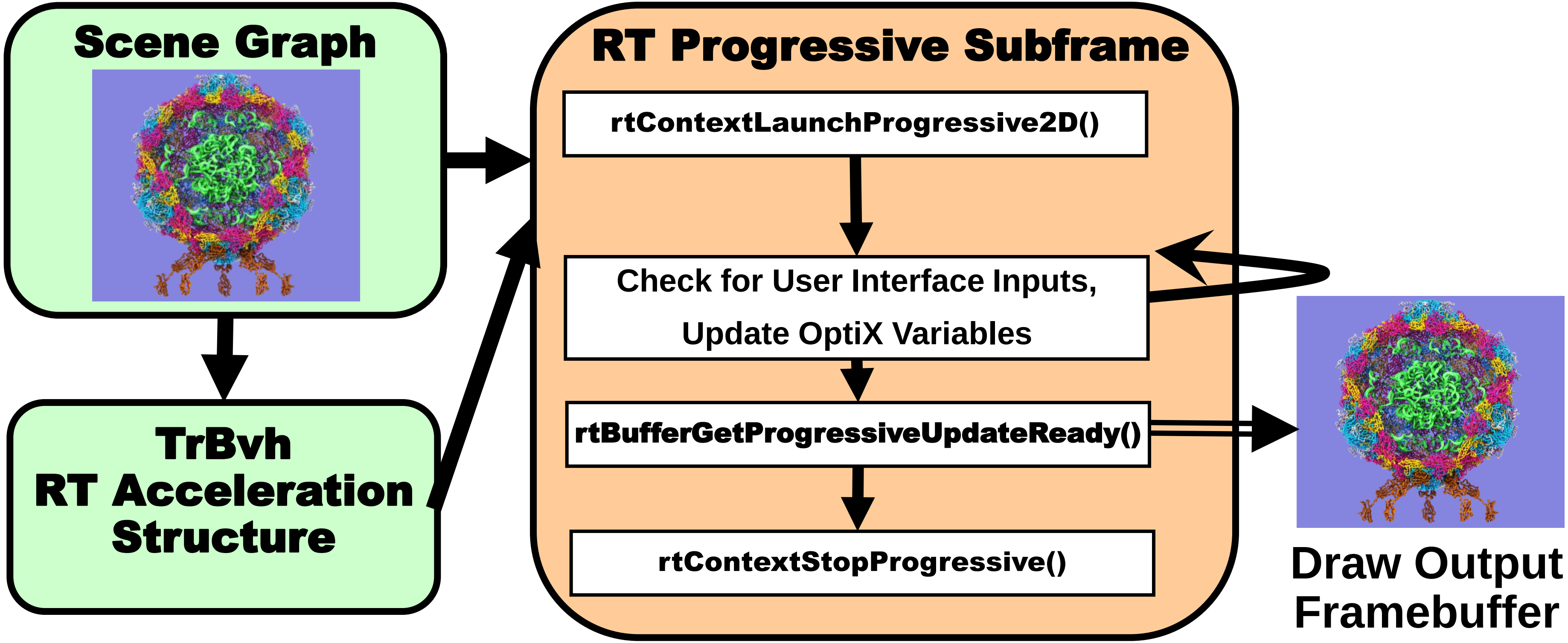
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides – ***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers
- **Movie was recorded live while using remote visualization**



VMD TachyonL-OptiX Interactive RT w/ Progressive Rendering

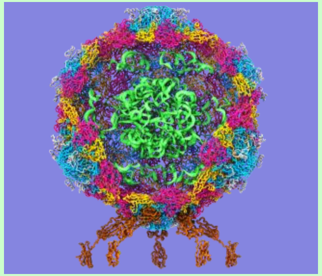


VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



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

VMD Scene



TrBvh RT Acceleration Structure

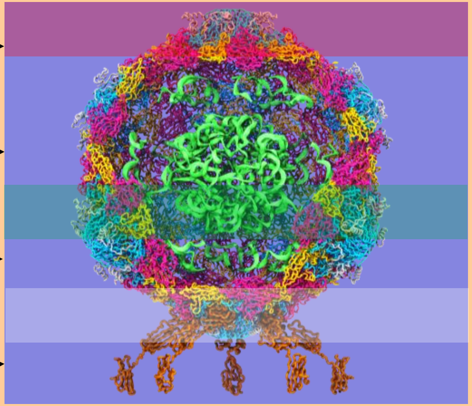
Scene Data Replicated, Image Space Parallel Decomposition onto GPUs

GPU 0

GPU 1

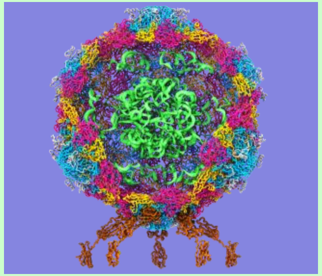
GPU 2

GPU 3



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

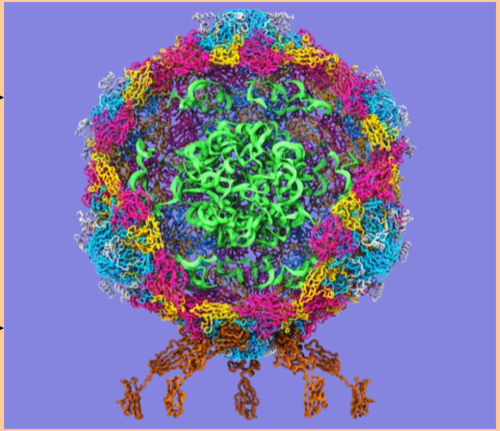
VMD Scene

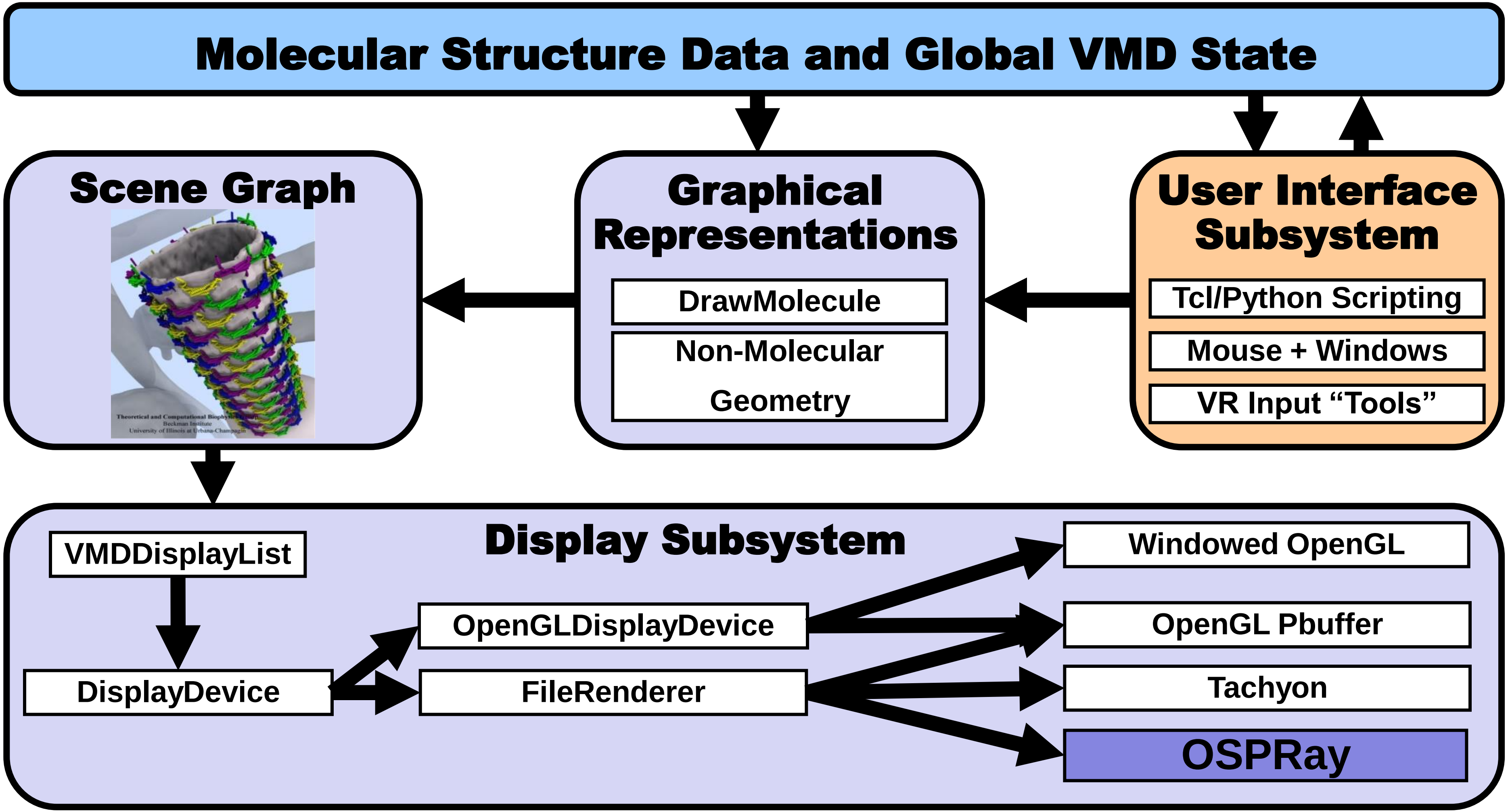


Scene Data Replicated, Image Space / Sample Space Parallel Decomposition onto GPUs

VCA 0:
8 M6000 GPUs

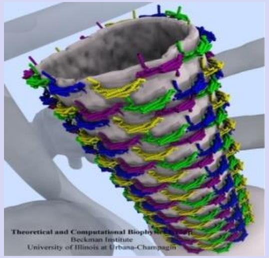
VCA N:
8 M6000 GPUs




Molecular Structure Data and Global VMD State
Scene Graph
Beckman Institute
University of Illinois at Urbana-Champagin
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
OpenGL Pbuffer
Tachyon
OSPRay

VMD-OSPRay Interactive CPU Ray Tracing with Progressive Refinement

Scene Graph and RT accel. data structures



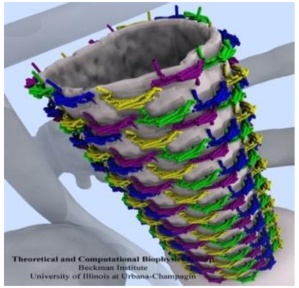
RT Progressive Refinement Loop

ospFrameBufferClear(OSP_FB_ACCUM**)**

ospRenderFrame(… OSP_FB_ACCUM**)**

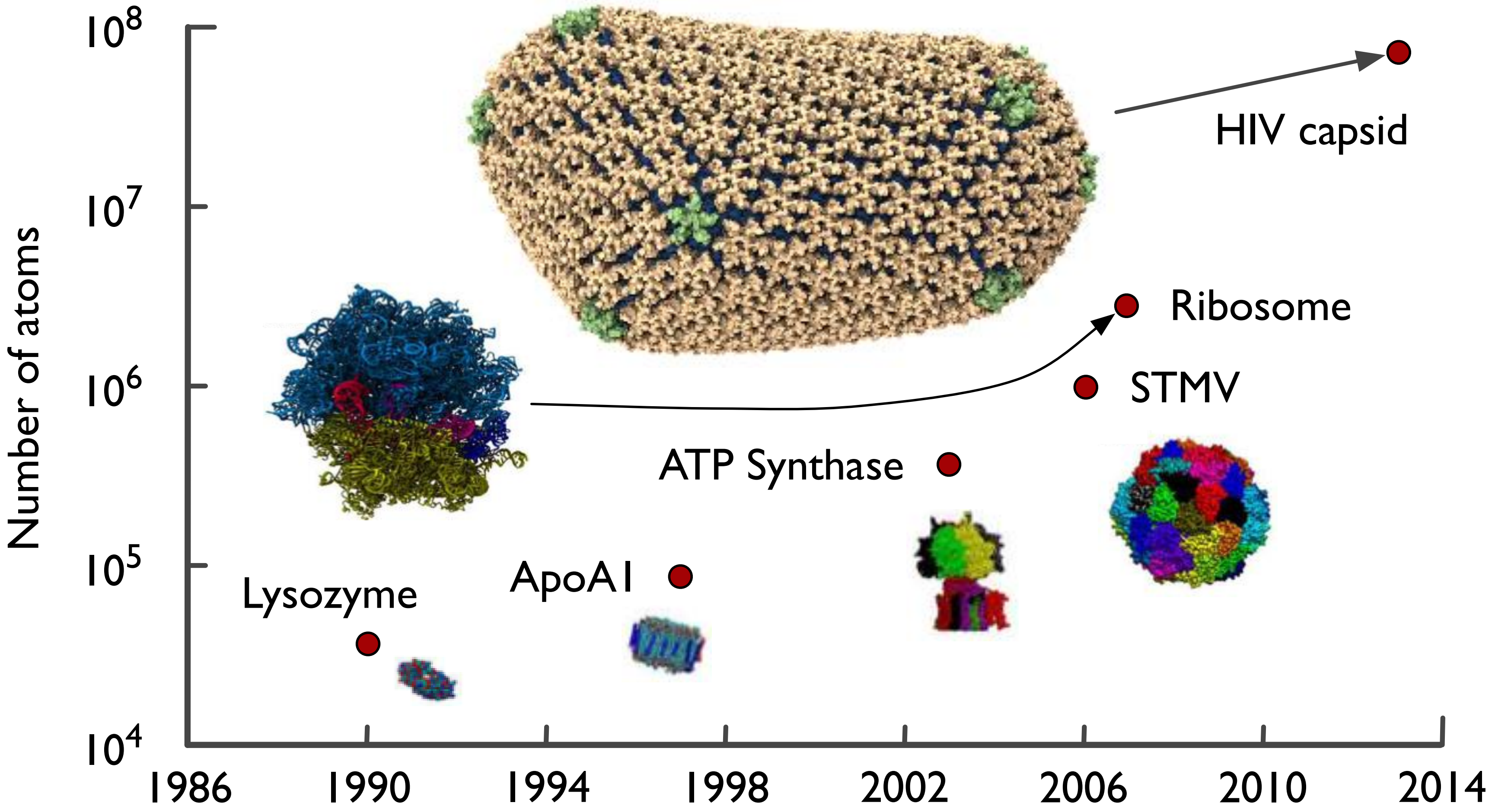
Check for User Interface Inputs,
Update OSPRay Renderer State

ospMapFrameBuffer()
Draw…
ospUnmapFrameBuffer()



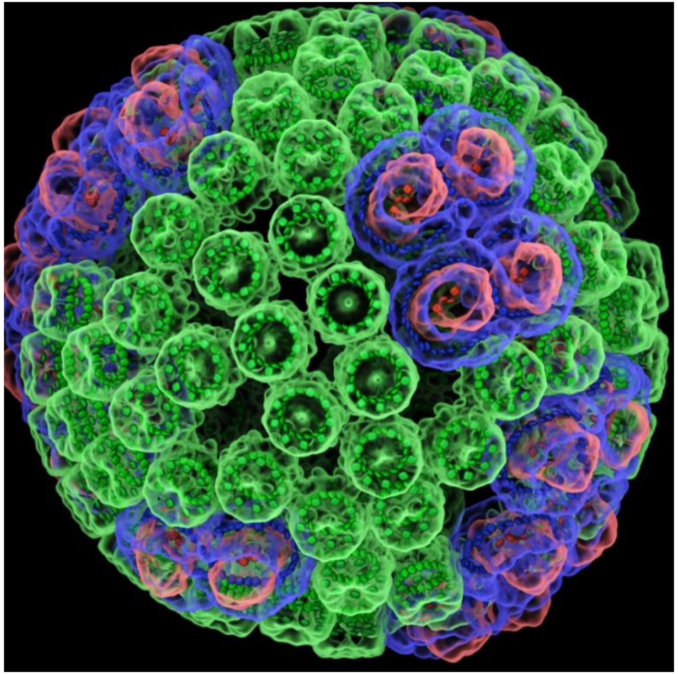
Draw Output Framebuffer

Computational Biology's Insatiable Demand for Processing Power



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

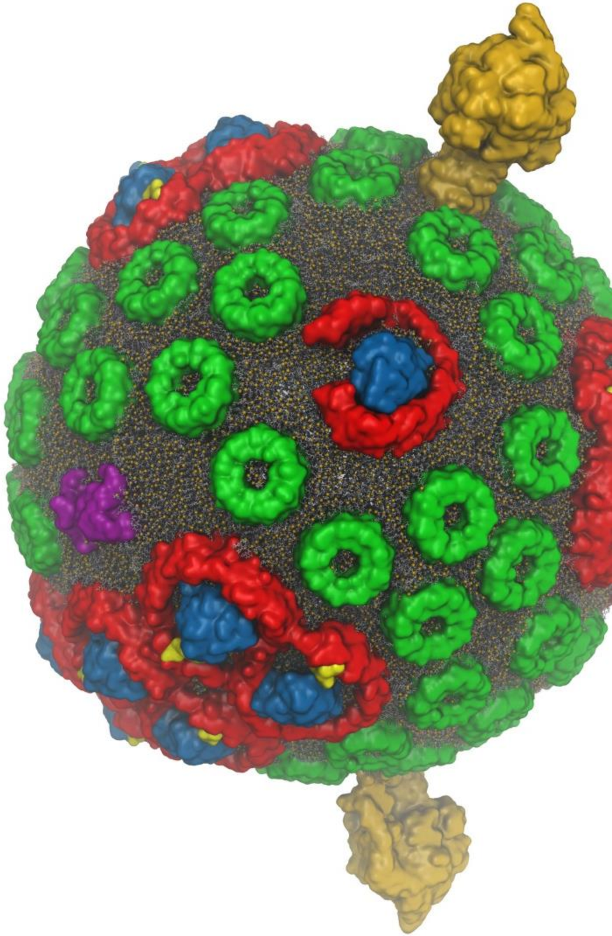


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

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

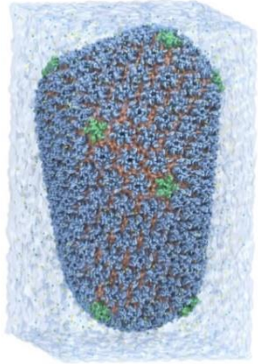
VMD 1.9.3+OptiX 3.8 – ~1.5x Performance Increase on Blue Waters Supercomputer

- 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.

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



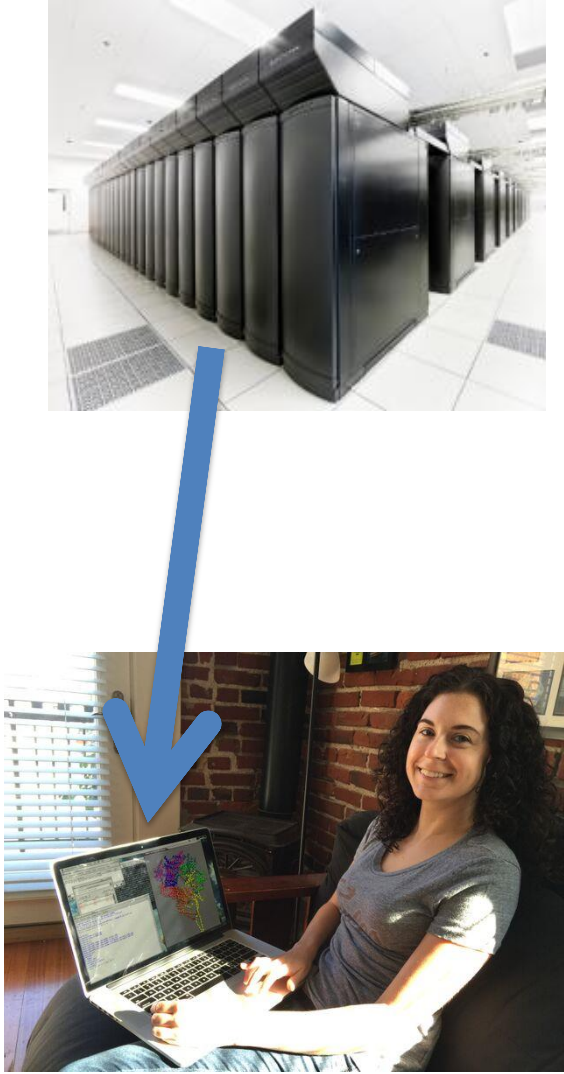
New VMD TachyonL-OptiX on XK7 vs. Tachyon on XE6:
K20X GPUs yield **up to twelve times** geom+ray tracing speedup

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.

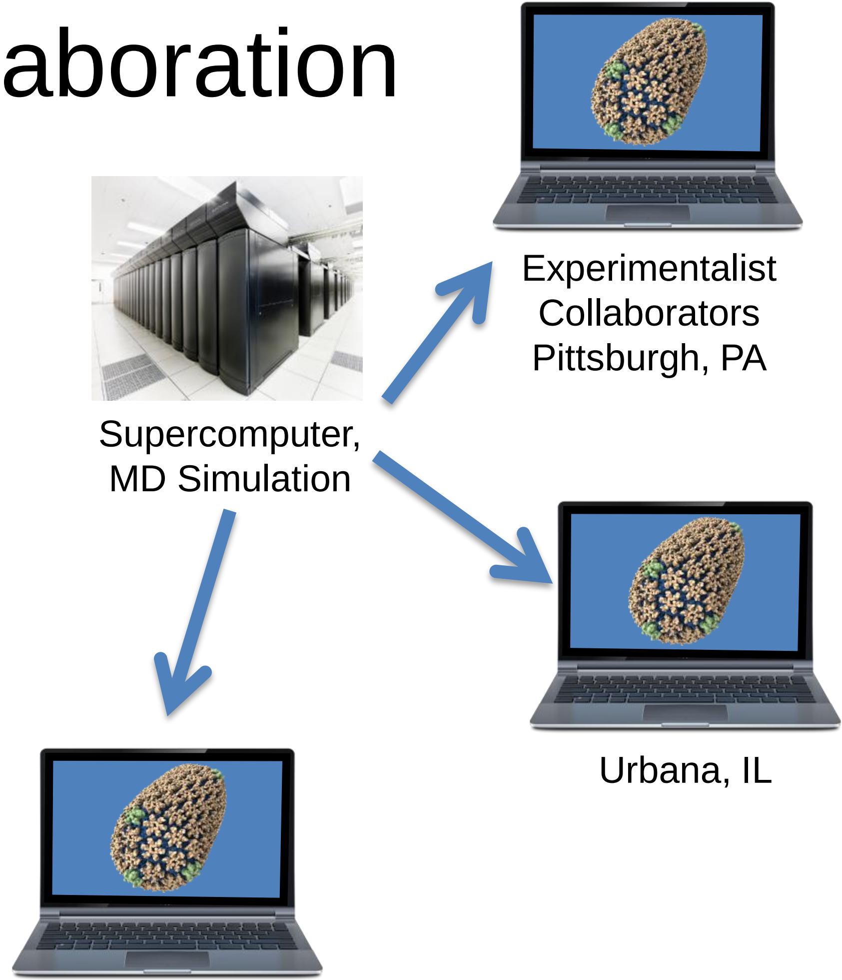
Interactive Remote Visualization and Analysis

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



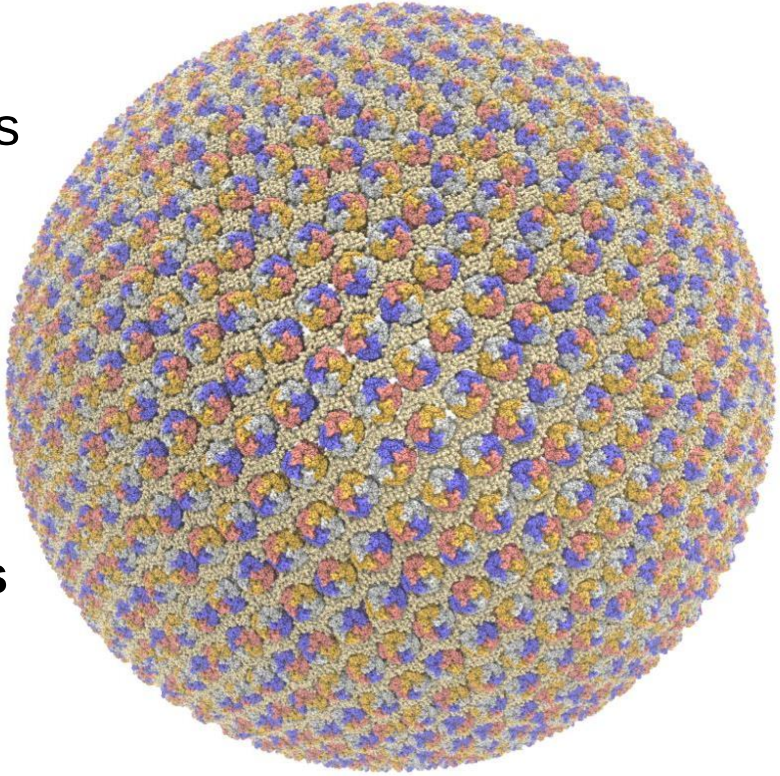
Interactive Collaboration

- 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

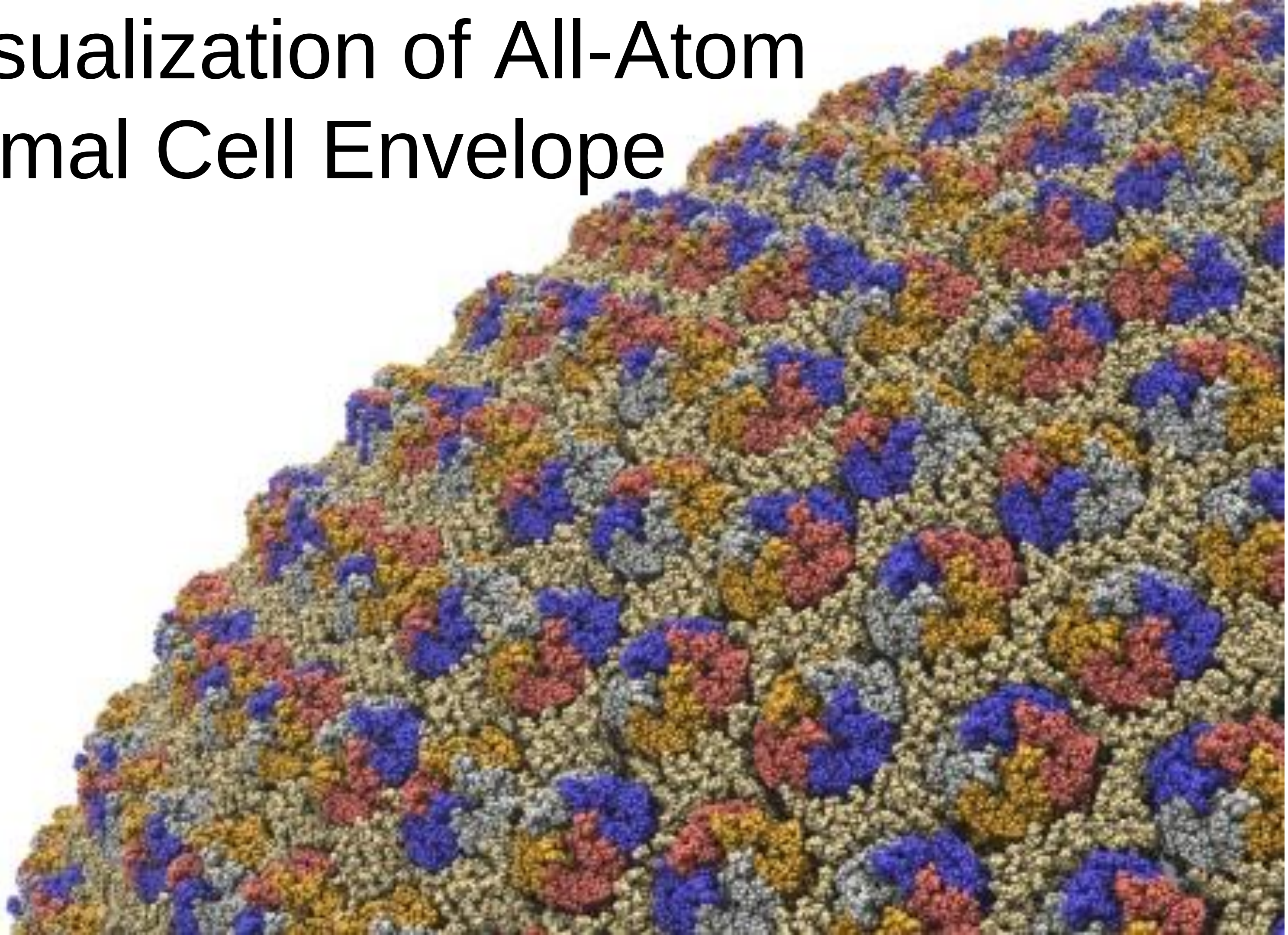


VMD Visualization of All-Atom Minimal Cell Envelope

- 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**



VMD Visualization of All-Atom Minimal Cell Envelope

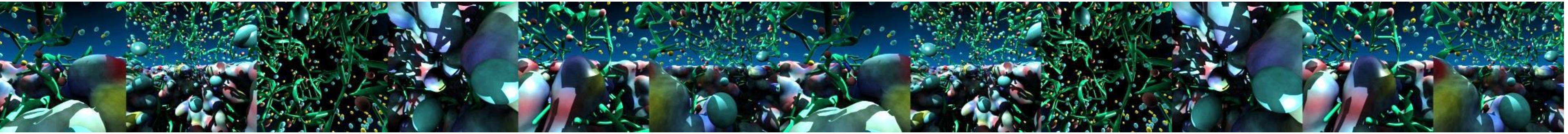


Immersive Viz. w/ VMD

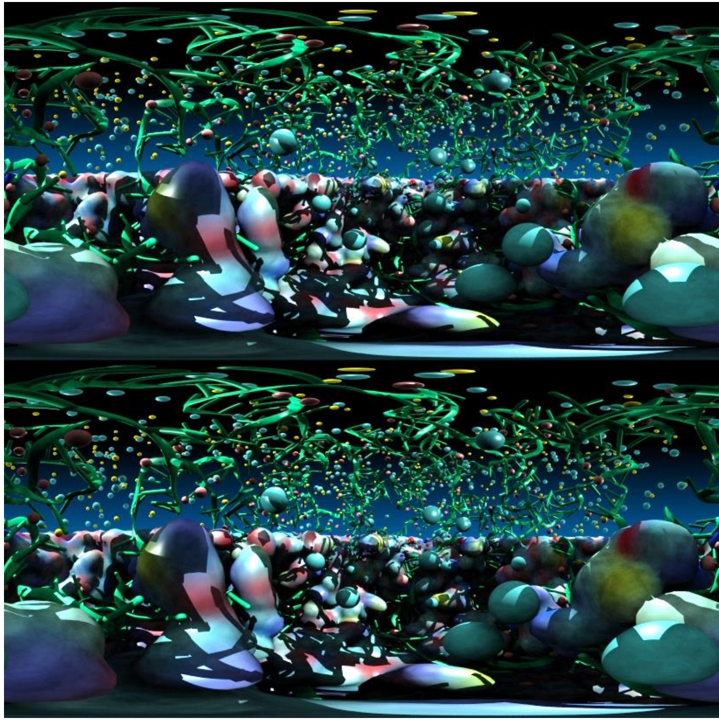
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support for remote visualization
  - 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

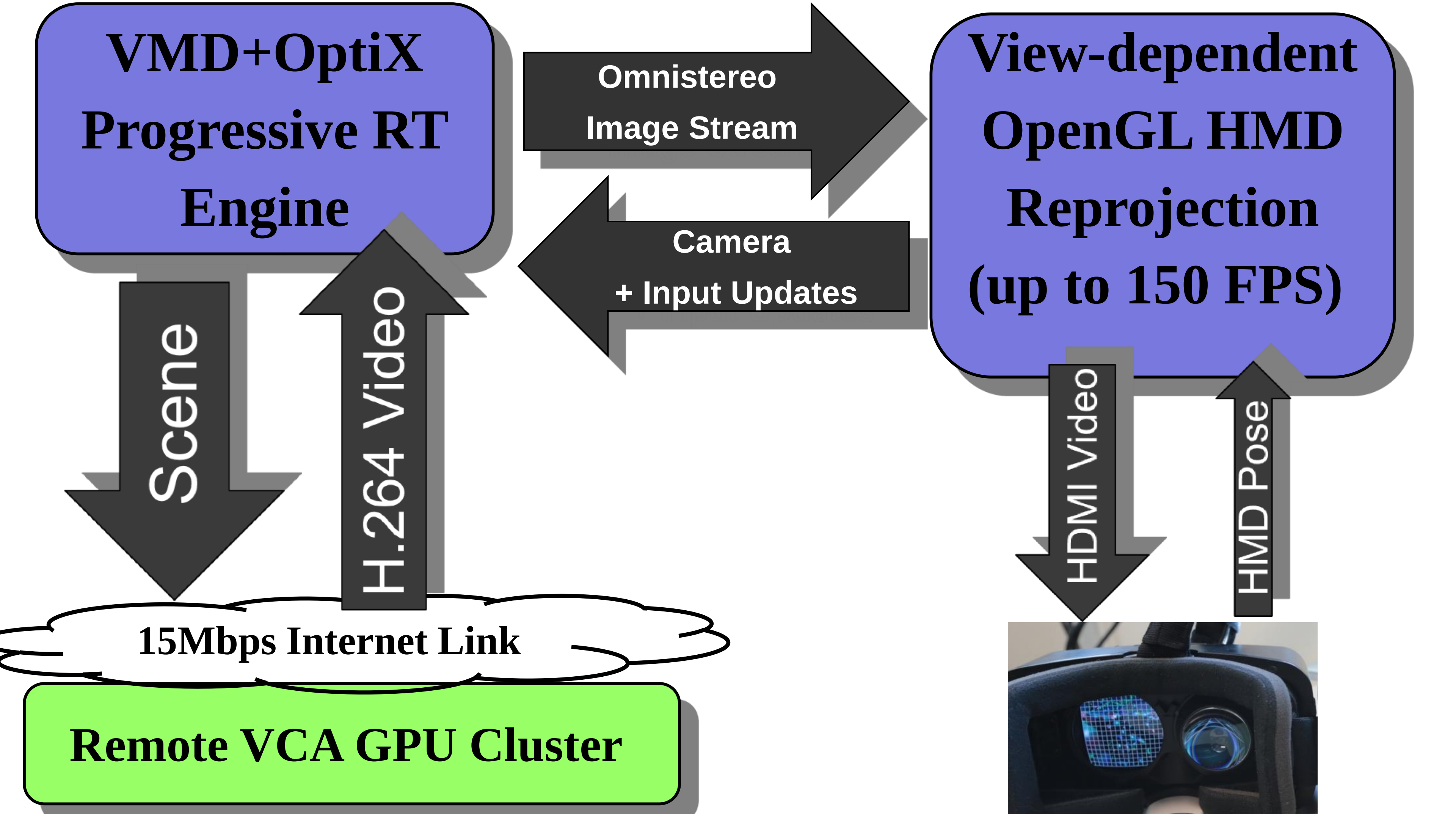


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace omnidirectional stereo spheremaps or cubemaps for very high-frame-rate reprojection and display via OpenGL texturing
- Stereo requires spherical camera projections **poorly suited to rasterization**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



HMD Ray Tracing Challenges

- HMDs require high frame rates **(90Hz or more)** and low latency between 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**
- **Split two-phase approach: moderate frame rate remote RT combined with local high frame rate view-dependent HMD rendering**


VMD+OptiX Progressive RT Engine
Omnistereo Image Stream
Camera + Input Updates
View-dependent OpenGL HMD Reprojection (up to 150 FPS)
Scene
H.264 Video
HDMI Video
HMD Pose
15Mbps Internet Link
Remote VCA GPU Cluster

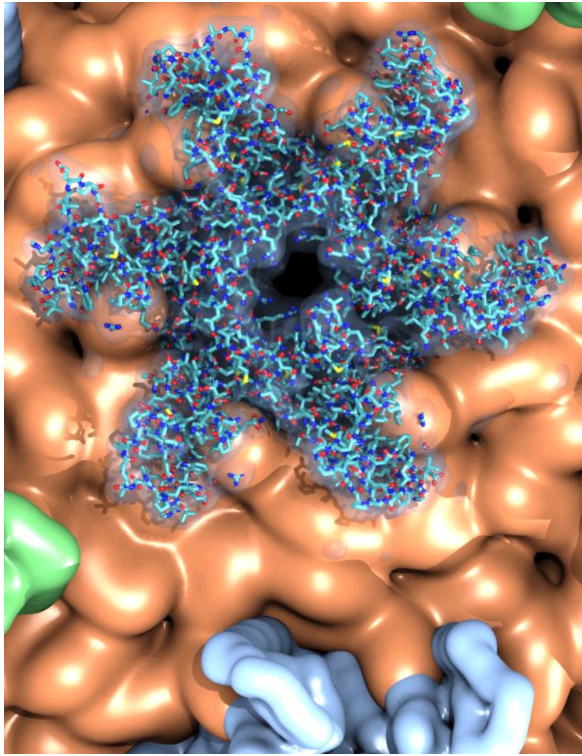
HMD View-Dependent Reprojection with OpenGL

- Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface
- HMD uses standard perspective frustum to view the textured surface
- HMD optics require software lens distortion and chromatic aberration corrections prior to display, implemented with multi-pass FBO rendering


Edmund Optics PN
47-737
Edmund Optics PN
47-717
ZEISS
FISHER LENS PAPER

Future Work

- Support for Khronos Vulkan for multi-GPU rasterization, superceding OpenGL…
- Further integration of interactive ray tracing into VMD
  - **Seamless interactive RT** in main VMD display
  - Support **trajectory playback** in interactive RT
- Improved performance / quality trade-offs in interactive RT stochastic sampling strategies
- Optimize GPU scene DMA and BVH regen speed for **time-varying geometry**, e.g. MD trajectories
- GPU-accelerated h.264 movie encoder back-end
- **Interactive RT combined with multi-node rendering and remote viz. on large HPC systems, e.g. NCSA Blue Waters, ORNL Titan, …**



GPU Ray Tracing of HIV-1 Capsid Detail

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- NVIDIA CUDA Center of Excellence, University of Illinois at Urbana-Champaign
- NVIDIA CUDA+OptiX development teams
- Intel SDVIS team
- Bill Sherman, Indiana University
- NCSA Blue Waters Team
- 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

Visualization Publications

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

- **Chemical Visualization of Human Pathogens: the Retroviral Capsids.** Juan R. Perilla, Boon Chong Goh, John E. Stone, and Klaus Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.
- **Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.** J. E. Stone, M. Sener, K. L. Vandivort, A. Barragan, A. Singharoy, I. Teo, J. V. Ribeiro, B. Isralewitz, B. Liu, B. Goh, J. C. Phillips, C. MacGregor-Chatwin, M. Johnson, L. F. Kourkoutis, C. N. Hunter, and K. Schulten. (submitted)
- **Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.** M. Sener, J. E. Stone, A. Barragan, A. Singharoy, I. Teo, K. L. Vandivort, B. Isralewitz, B. Liu, B. Goh, J. C. Phillips, L. F. Kourkoutis, C. N. Hunter, and K. Schulten. SC'14 Visualization and Data Analytics Showcase, 2014.
***Winner of the SC'14 Visualization and Data Analytics Showcase**
- **Unlocking the Full Potential of the Cray XK7 Accelerator.** M. D. Klein and J. E. Stone. Cray Users Group, Lugano Switzerland, May 2014.
- **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.

Visualization Publications

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

- **Stable Small Quantum Dots for Synaptic Receptor Tracking on Live Neurons.** E. Cai, P. Ge, S. Lee, O. Jeyifous, Y. Wang, Y. Liu, K. M. Wilson, S. Lim, M. A. Baird, J. E. Stone, K. Y. Lee, D. G. Fernig, M. W. Davidson, H. J. Chung, K. Schulten, A. M. Smith, W. N. Green, and P. R. Selvin. Angewandte Chemie - International Edition in English, 53(46):12484-12488, 2014.
- **Methodologies for the Analysis of Instantaneous Lipid Diffusion in MD Simulations of Large Membrane Systems.** Matthieu Chavent, Tyler Reddy, Joseph Goose, Anna Caroline E. Dahl, John E. Stone, Bruno Jobard, and Mark S.P. Sansom.Faraday Discussions, 169:455-475, 2014.
- **GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.** J. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13: Proceedings of the 8th International Workshop on Ultrascale Visualization, pp. 6:1-6:8, 2013.
- **Early Experiences Scaling VMD Molecular Visualization and Analysis Jobs on Blue Waters.** J. Stone, B. Isralewitz, and K. Schulten. In proceedings, Extreme Scaling Workshop, 2013.

Visualization Publications

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

- **Lattice Microbes: High-performance stochastic simulation method for the reaction-diffusion master equation.** E. Roberts, J. Stone, and Z. Luthey-Schulten. J. Computational Chemistry 34 (3), 245-255, 2013**.**
- **Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.** M. Krone, J. Stone, T. Ertl, and K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012.
- **Immersive Out-of-Core Visualization of Large-Size and Long-Timescale Molecular Dynamics Trajectories.** J. Stone, K. L. Vandivort, and K. Schulten. G. Bebis et al. (Eds.): *7th International Symposium on Visual Computing (ISVC 2011)*, LNCS 6939, pp. 1-12, 2011.
- **High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs**. J. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Pricessing Units (GPGPU-2), ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.
- **Visualization of Cyclic and Multi-branched Molecules with VMD.** Simon Cross, Michelle M. Kuttell, John E. Stone, and James E. Gain. Journal of Molecular Graphics and Modelling. 28:131-139, 2009.
- **A System for Interactive Molecular Dynamics Simulation.** John E. Stone, Justin Gullingsrud, Klaus Schulten, and Paul Grayson.In *2001 ACM Symposium on Interactive 3D Graphics*,John F. Hughes and Carlo H. Sequin, editors, pages 191-194, New York, 2001, ACM SIGGRAPH
- **An Efficient Library for Parallel Ray Tracing and Animation.** John E. Stone, Master's Thesis, University of Missouri-Rolla, Department of Computer Science, April 1998
- **Rendering of Numerical Flow Simulations Using MPI**. John Stone and Mark Underwood.Second MPI Developers Conference, pages 138-141, 1996.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