VMD: Interactive Publication-Quality Molecular Ray Tracing with OptiX

John E. Stone

Theoretical and Computational Biophysics Group

Beckman Institute for Advanced Science and Technology

University of Illinois at Urbana-Champaign

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

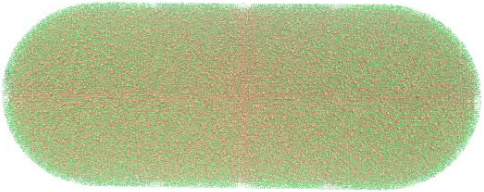
12:00pm, Wednesday August 12, 2015

Best of GTC Theater, NVIDIA Booth #500,

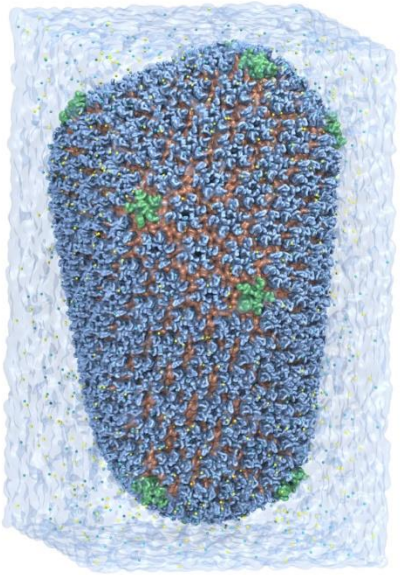
Siggraph 2015, Los Angeles, CA

VMD – “Visual Molecular Dynamics”

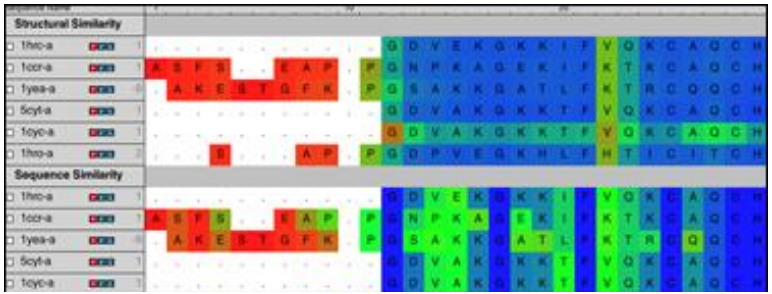
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



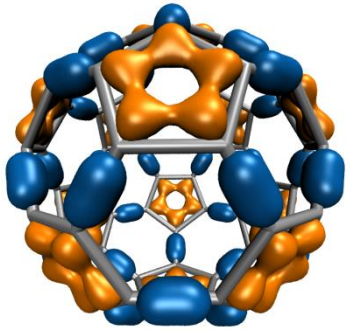
Whole Cell Simulation



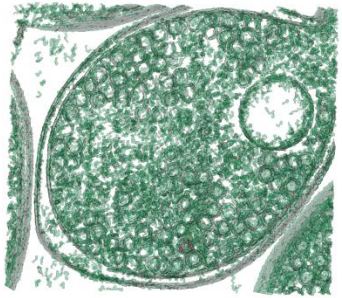
MD Simulations



Sequence Data



Quantum Chemistry

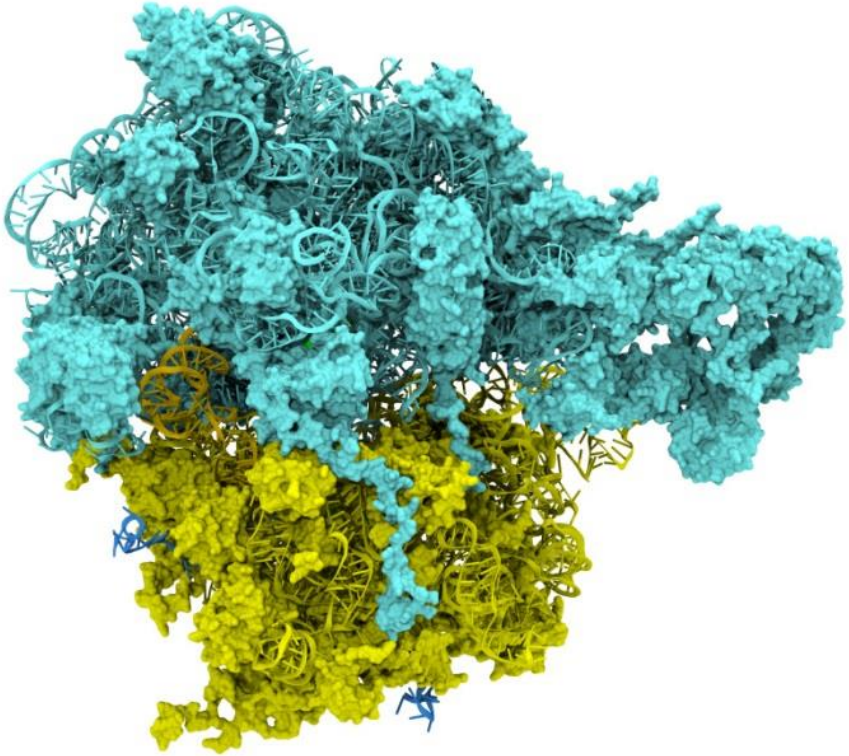


CryoEM, Cellular Tomography

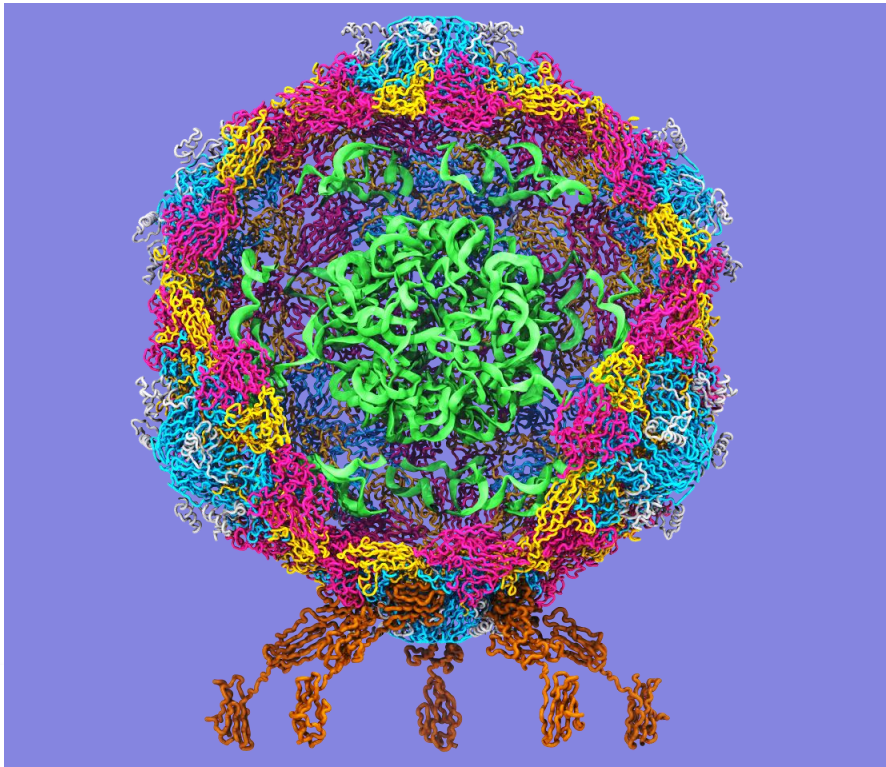
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

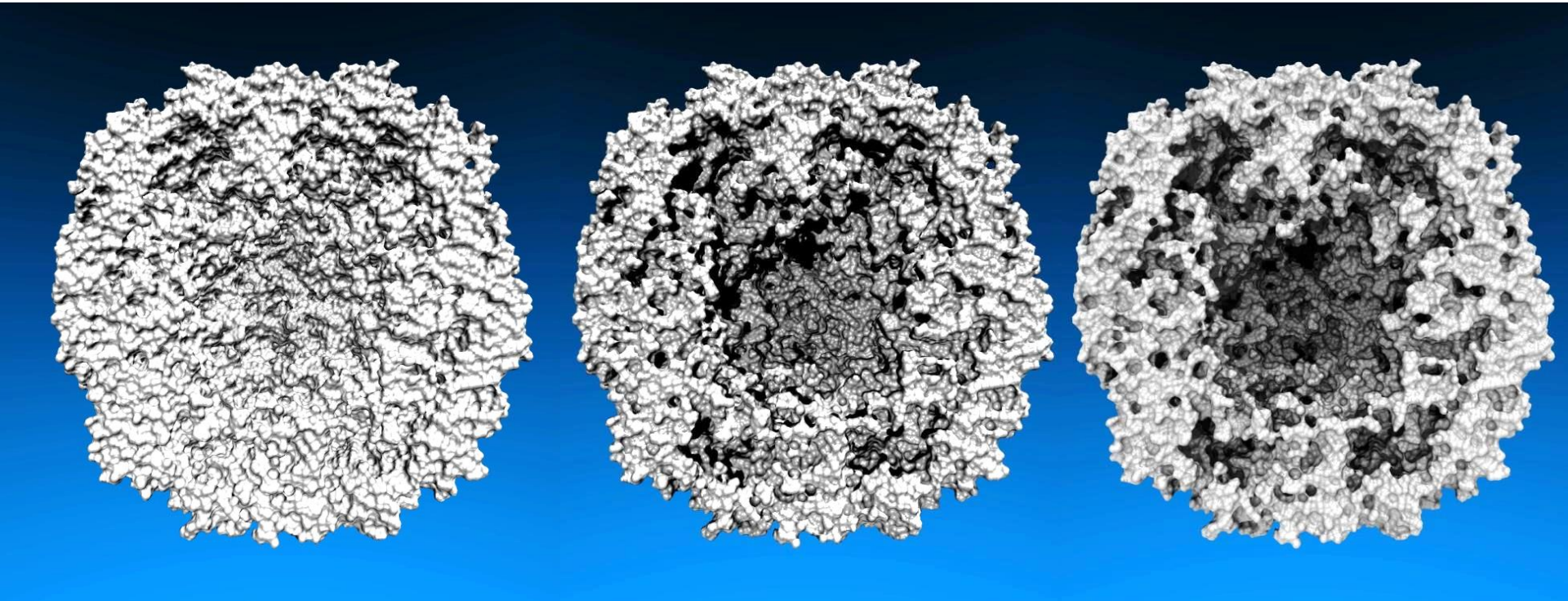


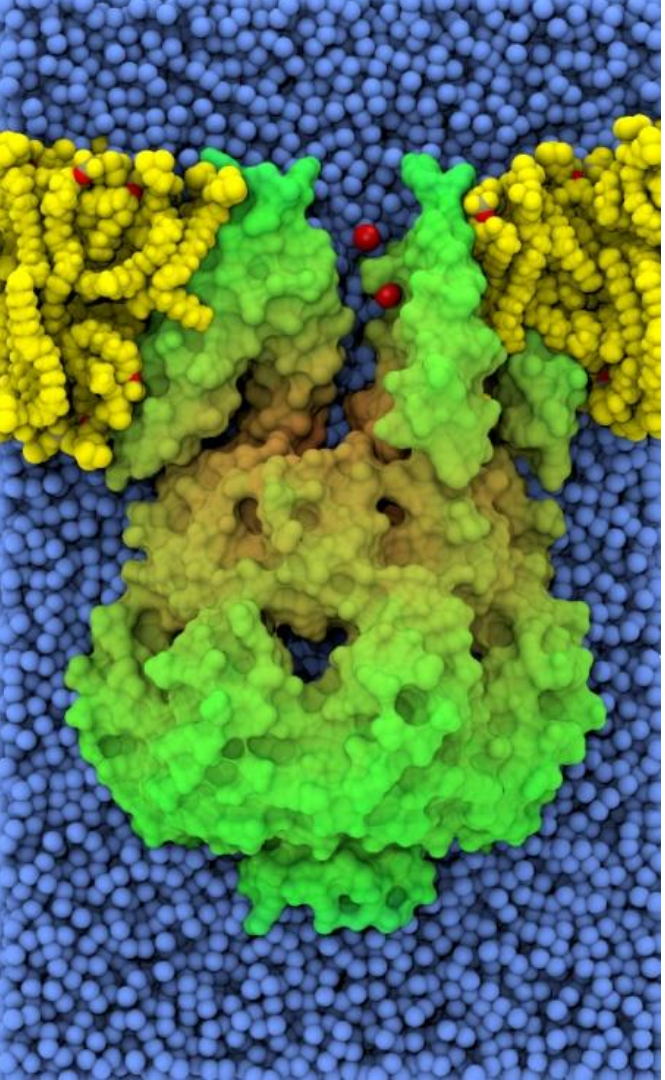
Lighting Comparison

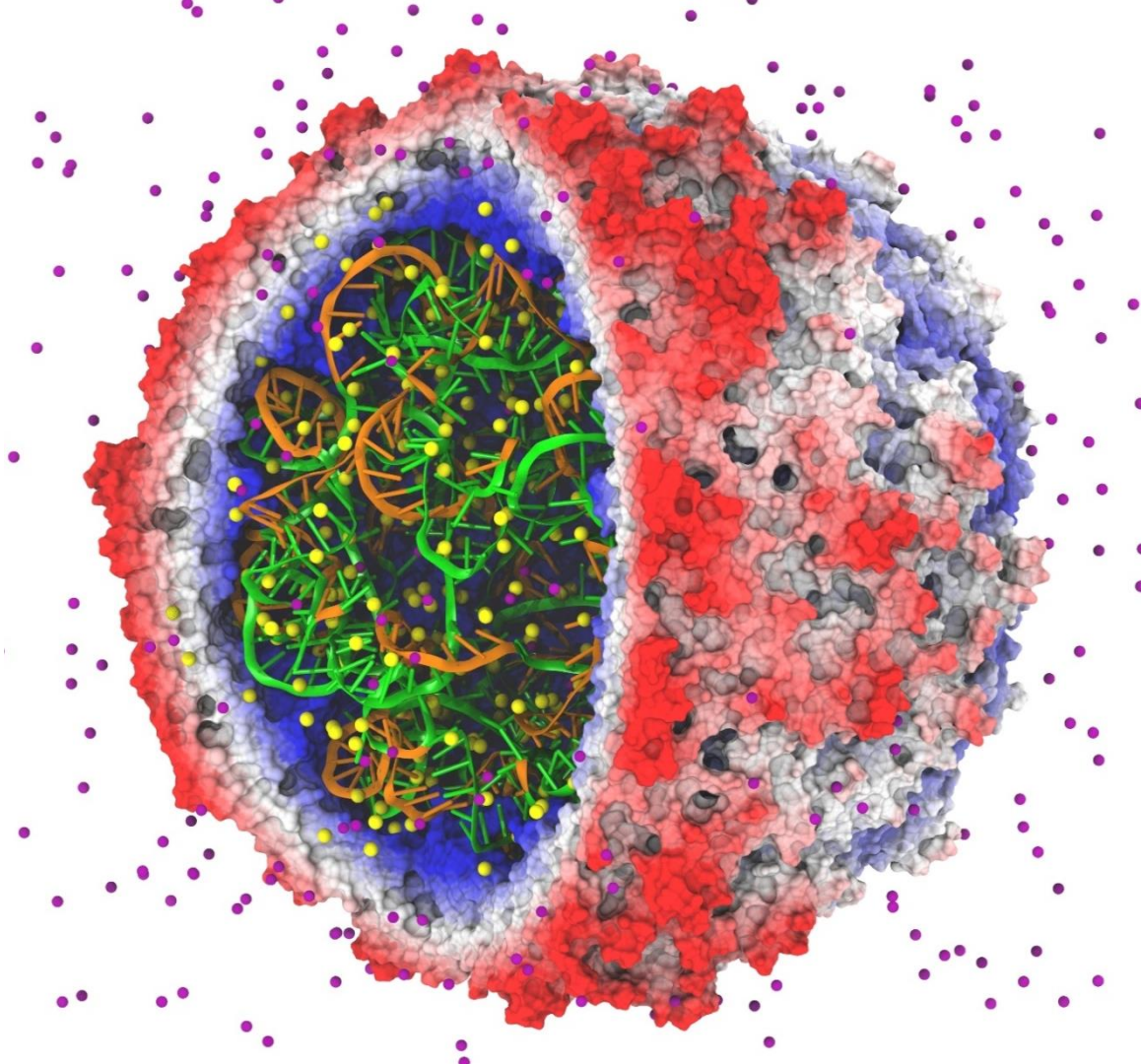
Two lights, no shadows

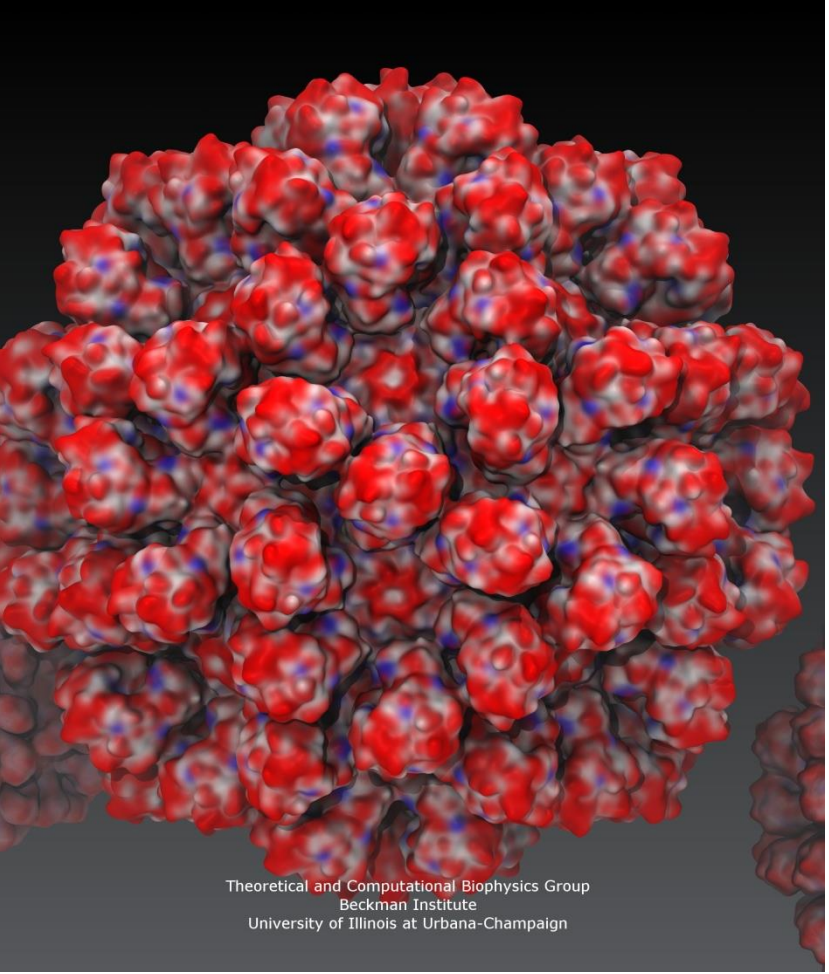
Two lights, hard shadows, 1 shadow ray per light

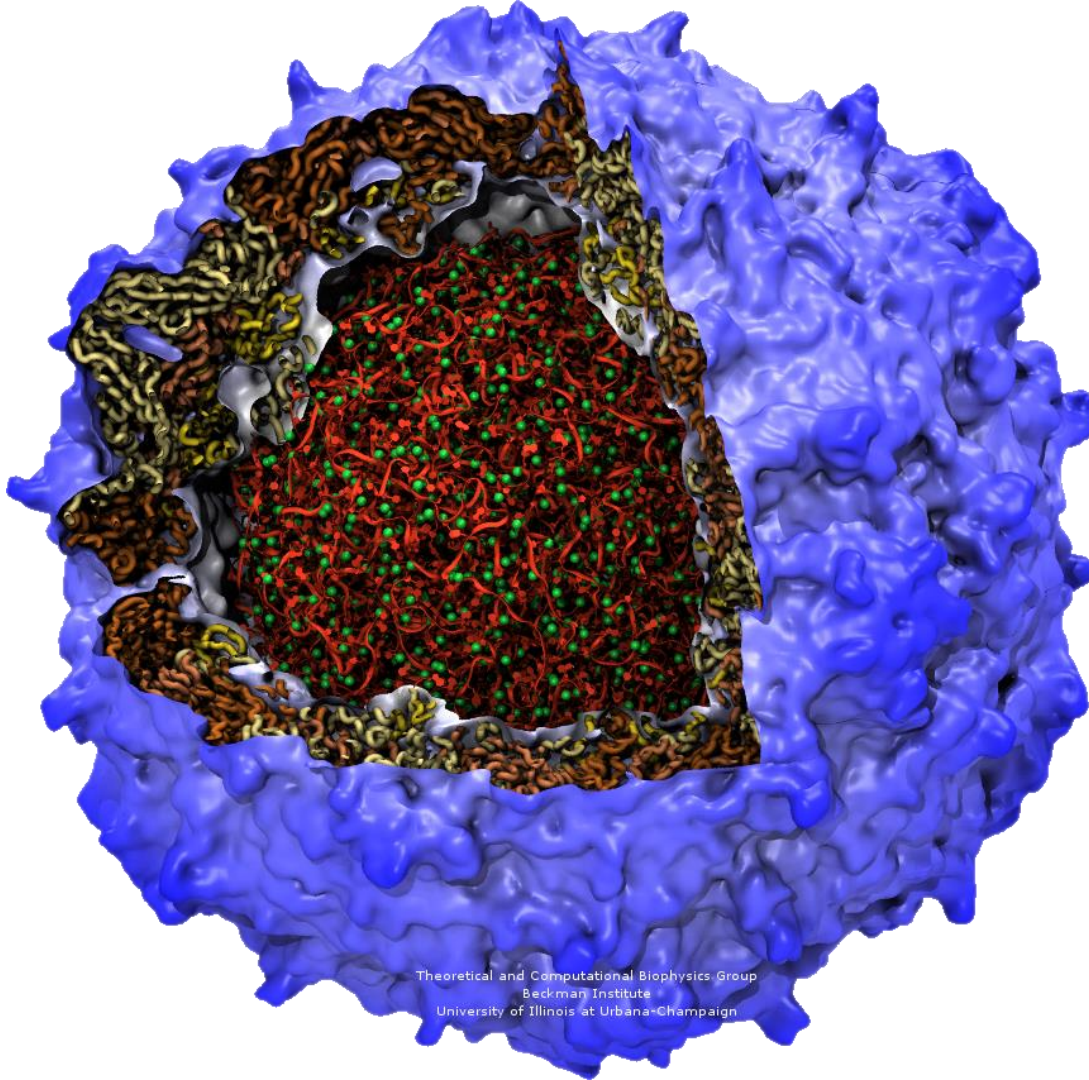
Ambient occlusion + two lights, 144 AO rays/hit



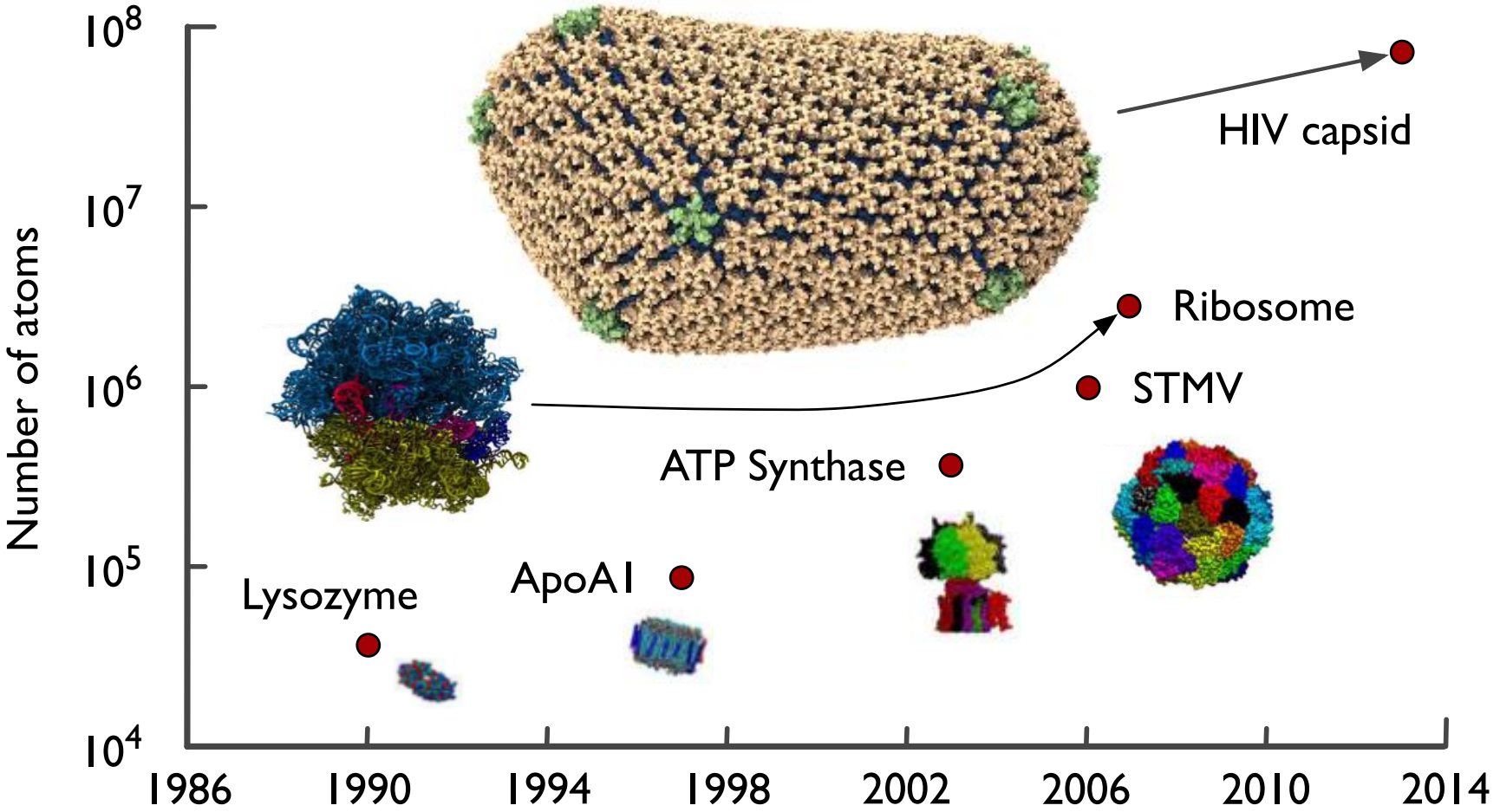





Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign


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

Computational Biology's Insatiable Demand for Processing Power



Visualization Goals, Challenges

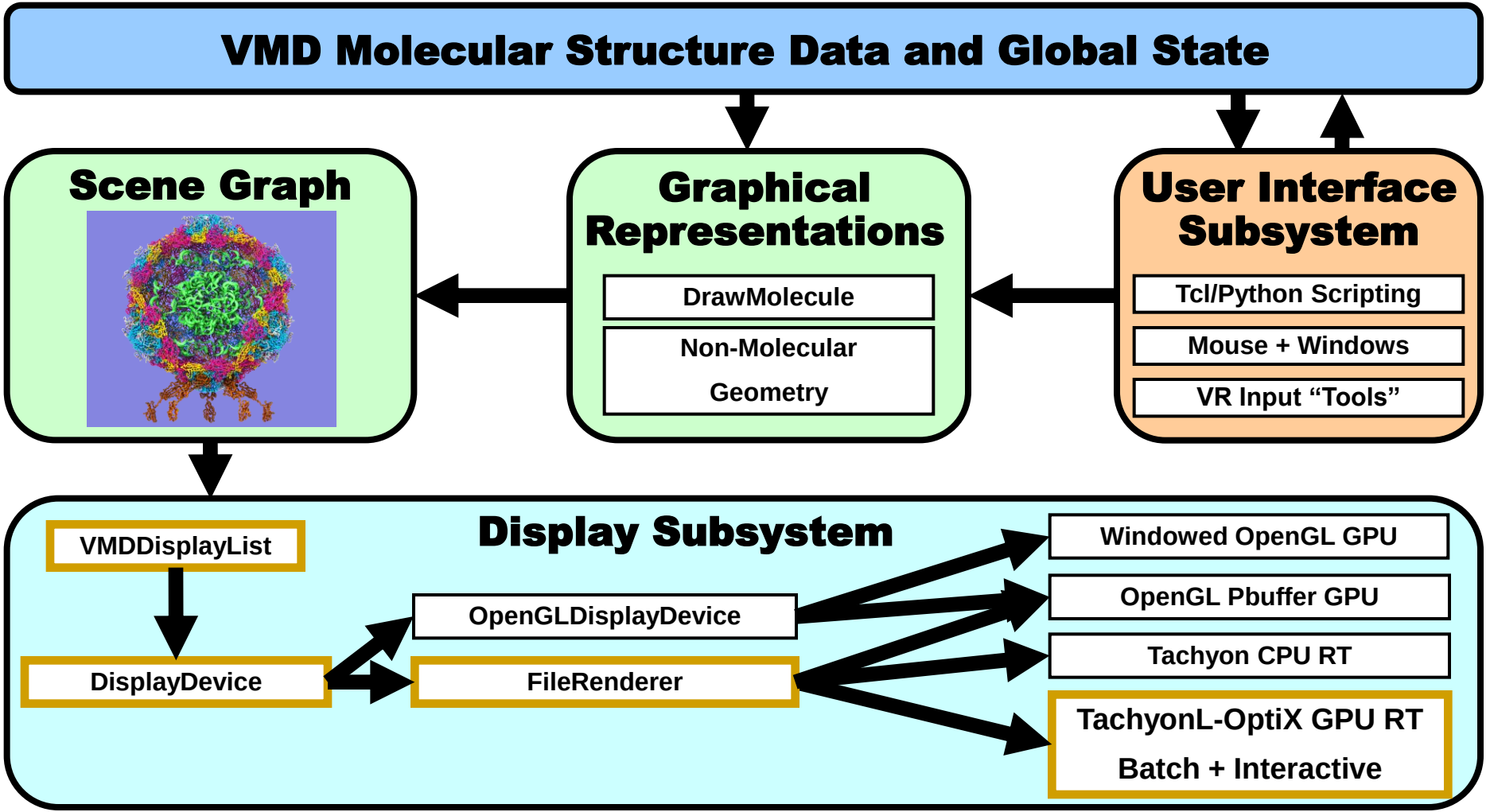
- Increased GPU acceleration for visualization of **petascale molecular dynamics trajectories**
- **Overcome GPU memory capacity limits**, enable high quality visualization of >100M atom systems
- Use GPU to accelerate not only interactive-rate visualizations, but also photorealistic ray tracing with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

VMD GPU-Accelerated Ray Tracing Engine

- Complementary to VMD OpenGL GLSL renderer
- Key ray tracing benefits:
  - Ambient occlusion lighting and shadows
  - High quality transparent surfaces
  - Depth of field focal blur and similar optical effects
  - Mirror reflection
  - Single-pass stereoscopic rendering
  - Special panoramic and 360° cameras:
    - Planetarium dome master format
    - Equirectangular spheremap projections
    - Cubemap projections

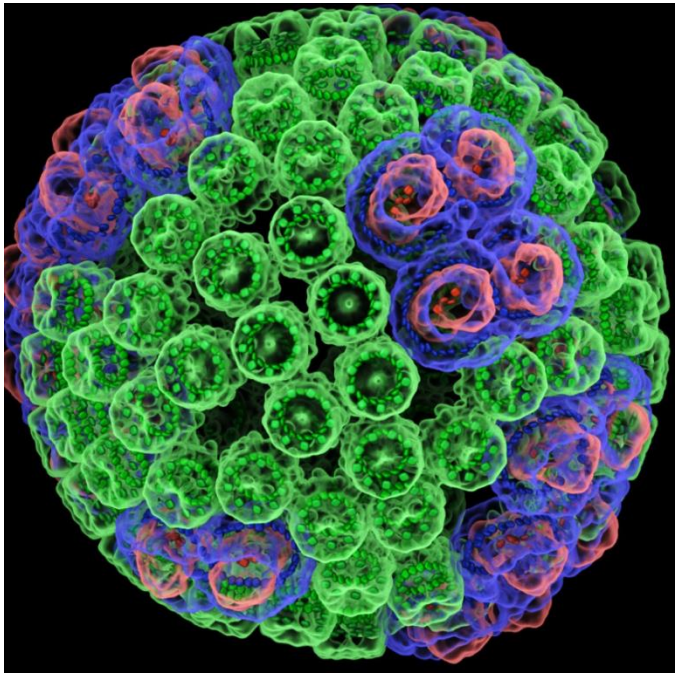
Why Built-In VMD Ray Tracing Engines?

- **No disk I/O** or communication to outboard renderers
- **Eliminate unnecessary data replication and host-GPU memory transfers**
- Directly operate on VMD internal molecular scene, **quantized/compressed data formats**
- Implement all **curved surface primitives**, volume rendering, texturing, shading features required by VMD
- **Same scripting, analysis, atom selection**, and rendering features are available on all platforms, **graceful CPU fallback**


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 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

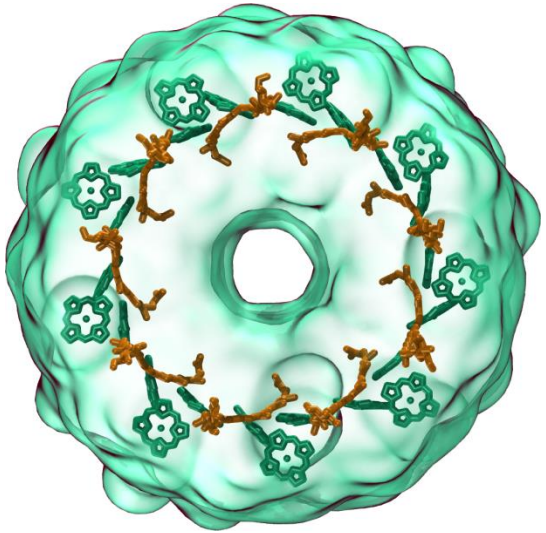


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

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**

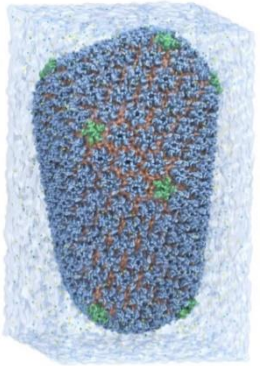
VMD 1.9.3+OptiX 3.8 – ~1.5x Performance Increase on Blue Waters Supercomputer

- OptiX GPU-native **"Trbvh" acceleration structure builder** yields substantial overall performance 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**



GPU Ray Tracing of LHII Light Harvesting Complex Showing Clorophylls (green) and Carotenoids (orange)

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



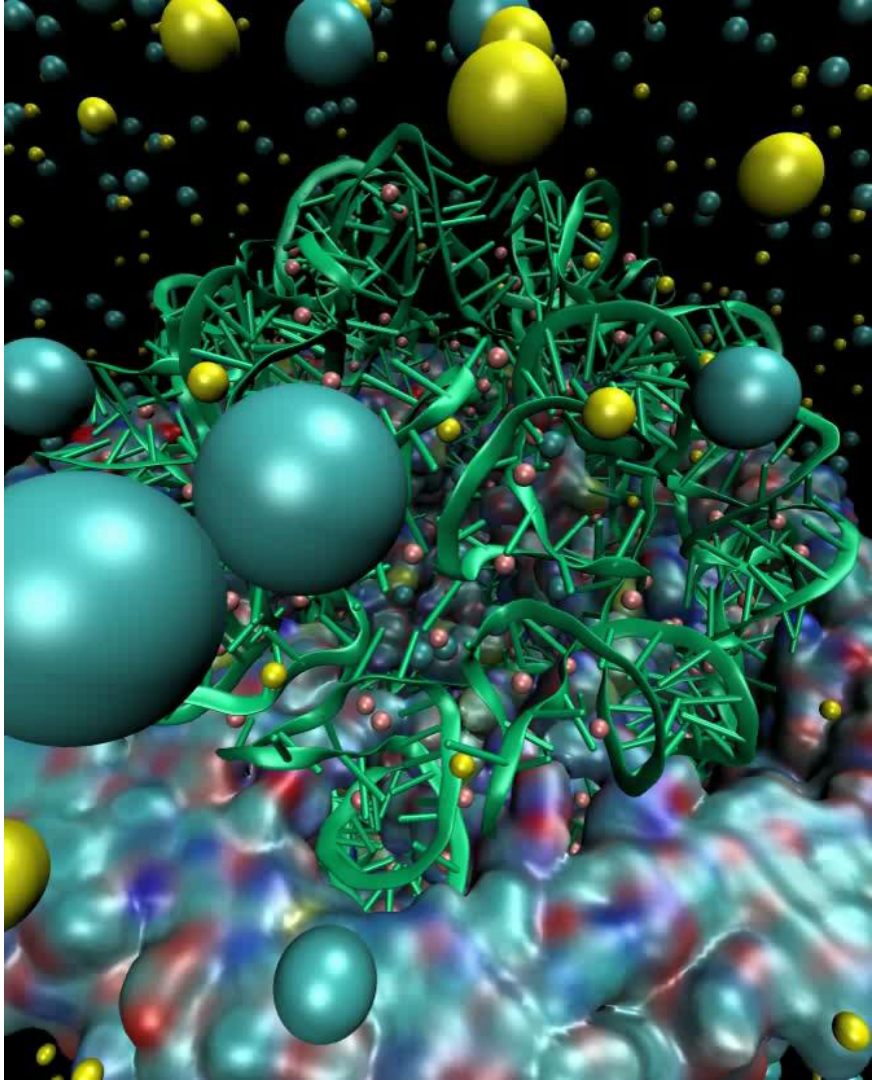
New VMD TachyonL-OptiX on XK7 vs. Tachyon on XE6:
K20X GPUs yield **up to twelve times** geom+ray tracing speedup

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

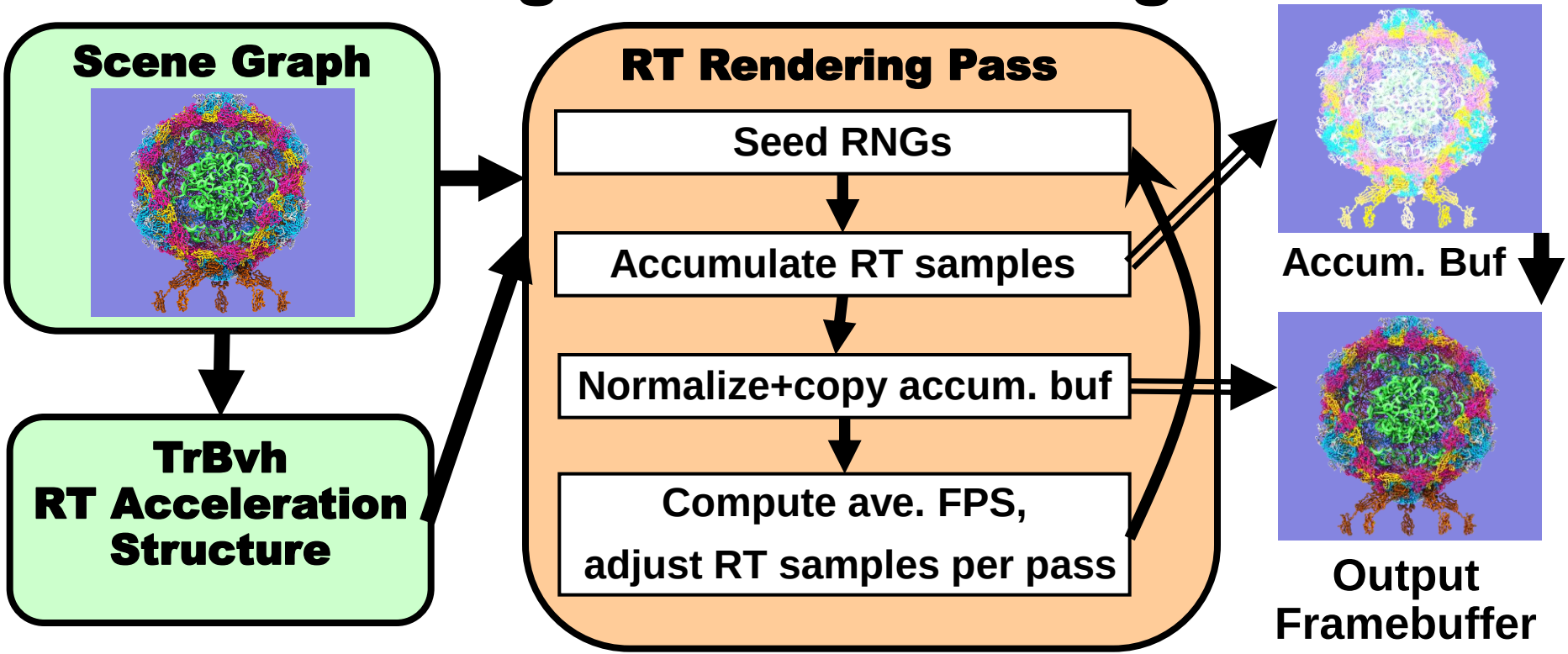
[1] GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms. J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13: Proceedings of the 8th International Workshop on Ultrascale Visualization, pp. 6:1-6:8, 2013.

VMD Interactive GPU Ray Tracing

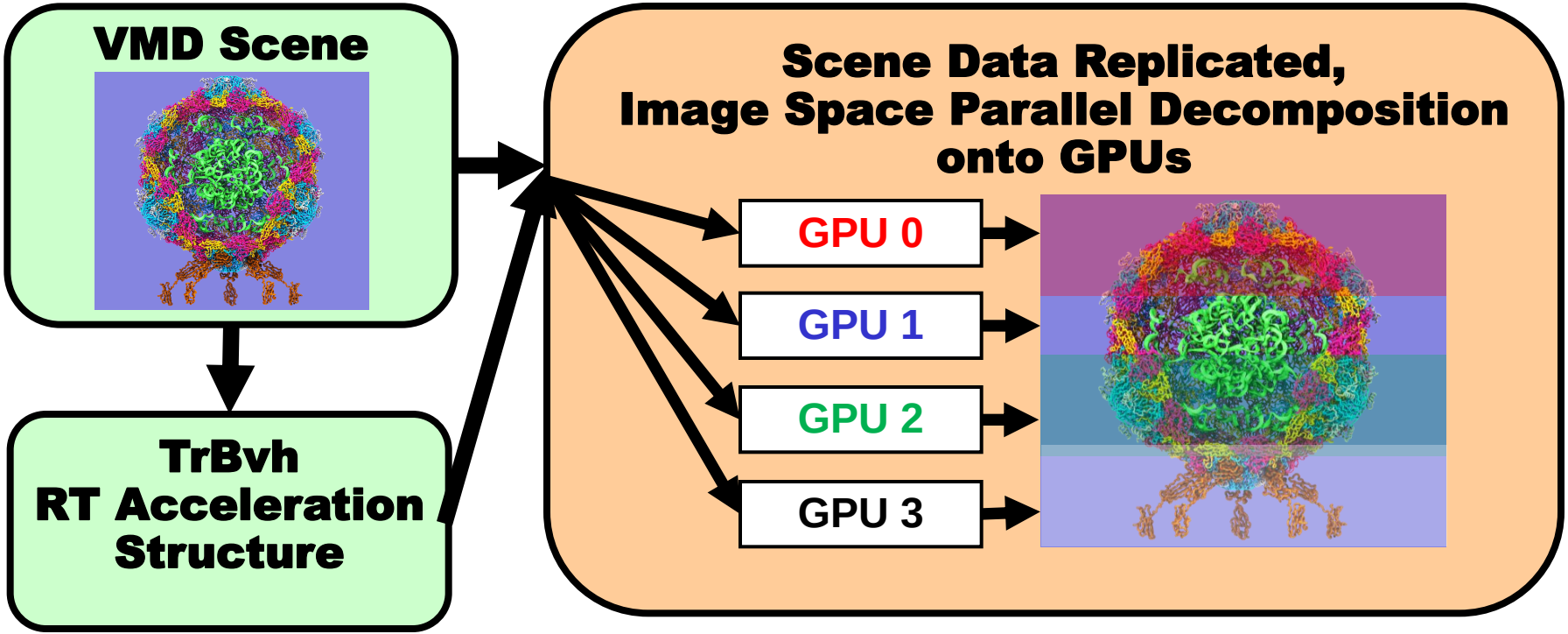
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides – ***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers
- **Movie was recorded live while using remote visualization**



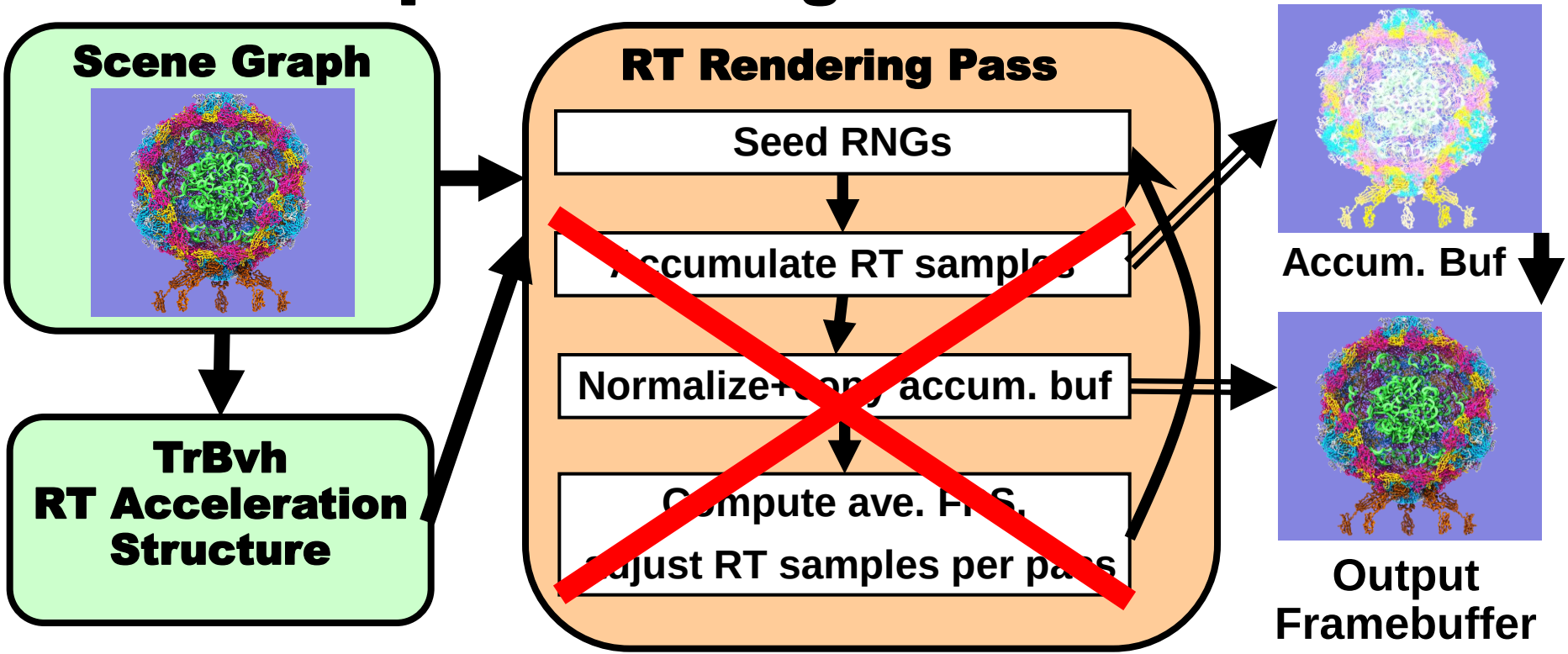
VMD TachyonL-OptiX Interactive RT w/ Progressive Rendering



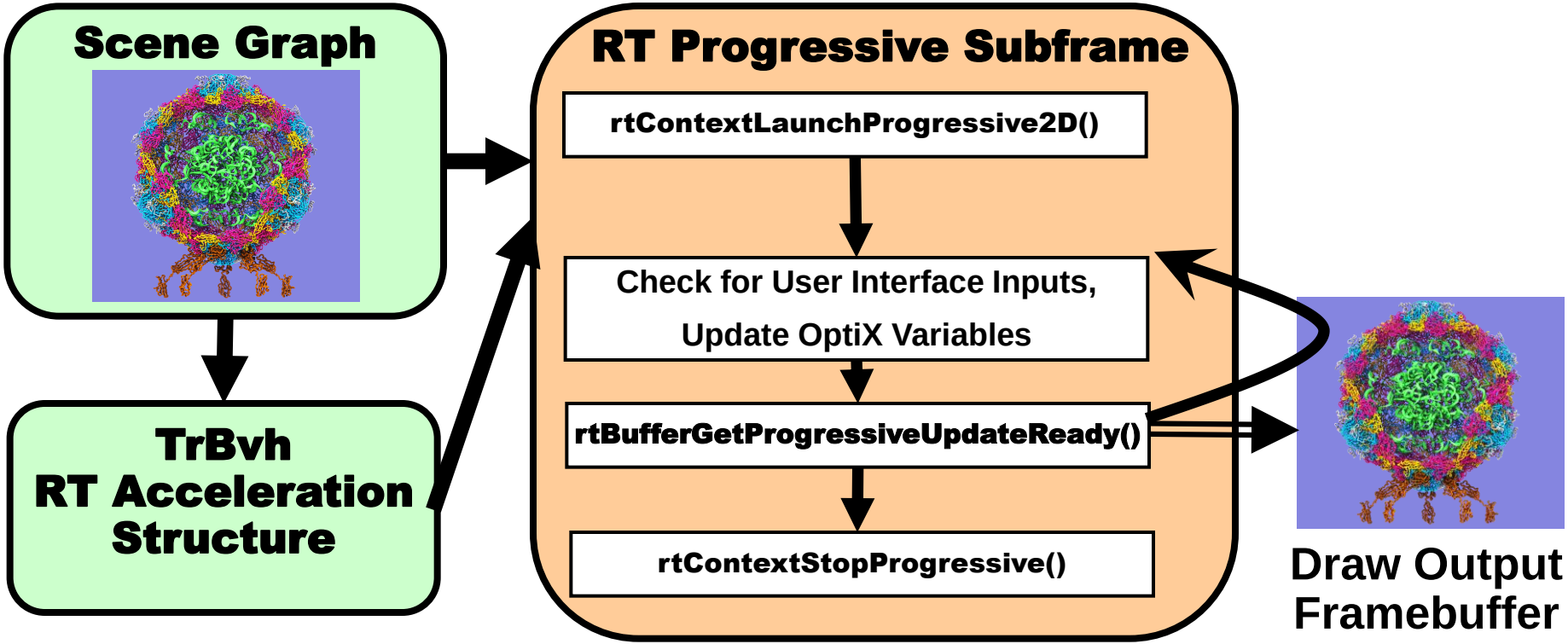
VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node



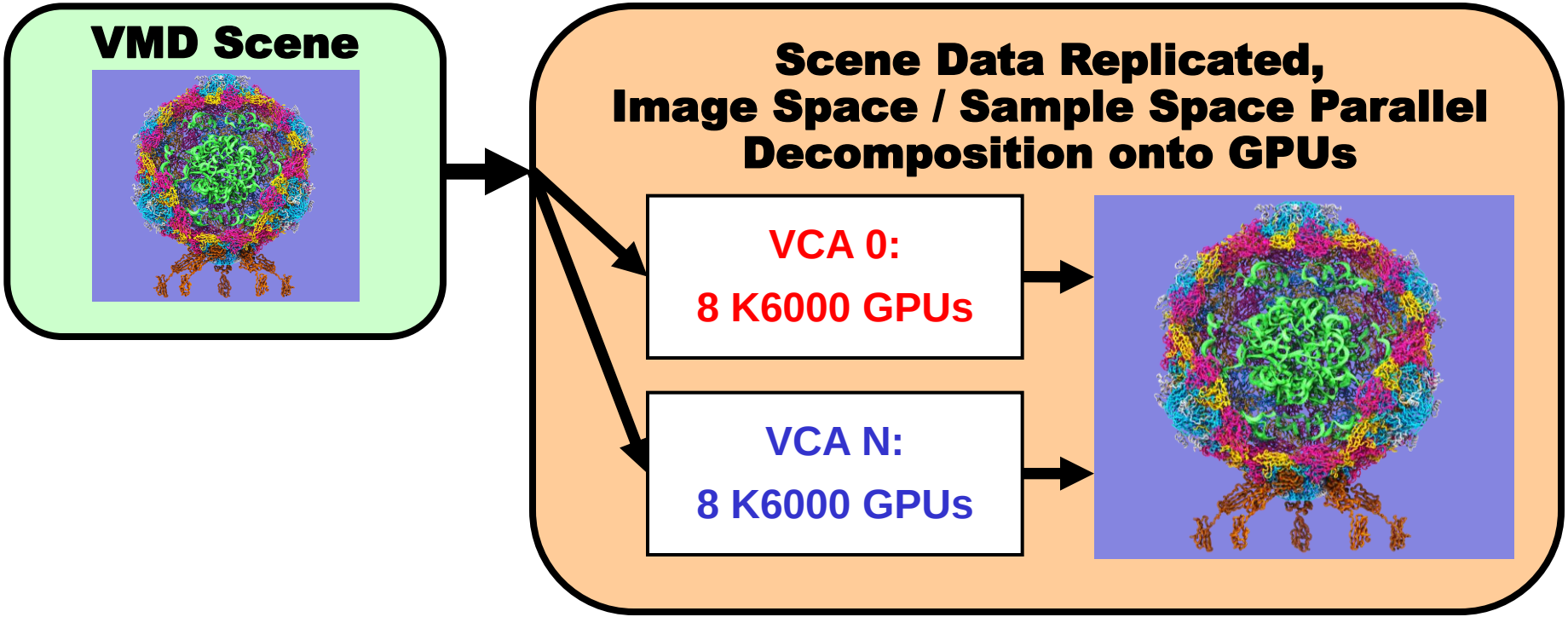
VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



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

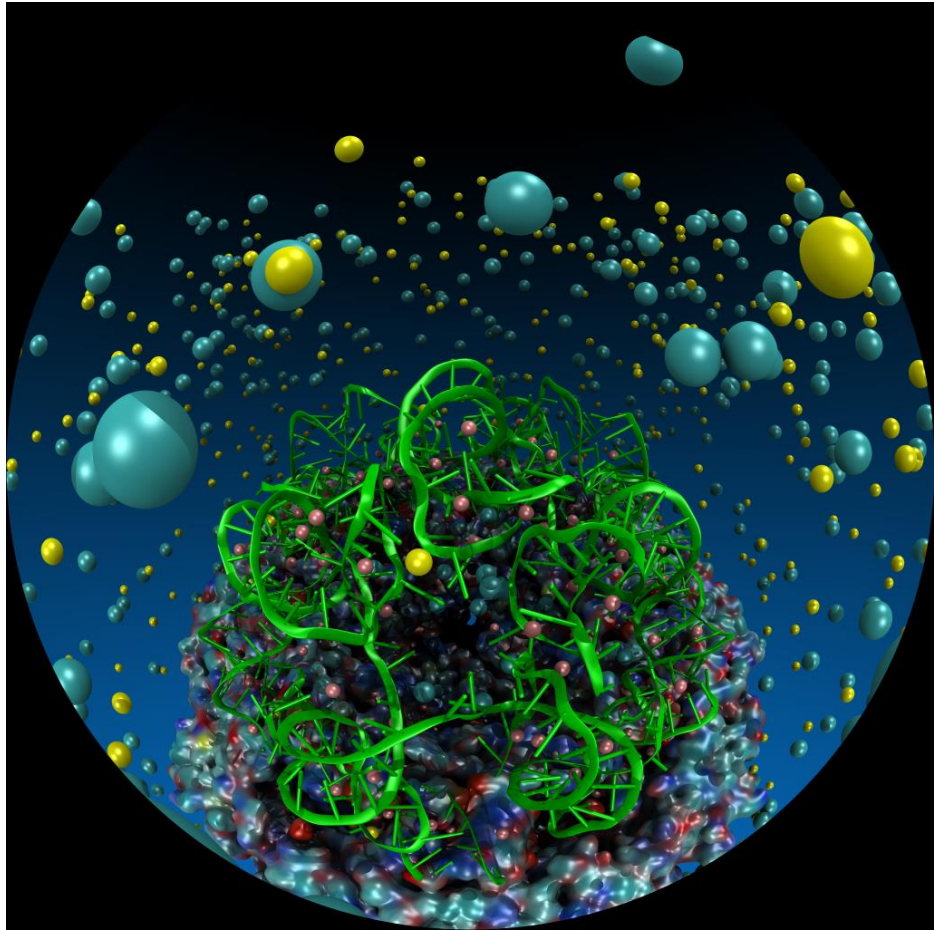


VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster

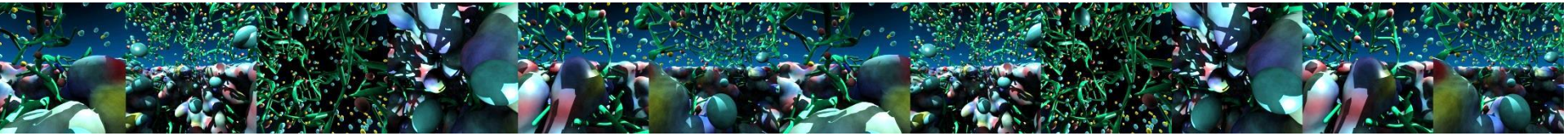


VMD Planetarium Dome Master Camera

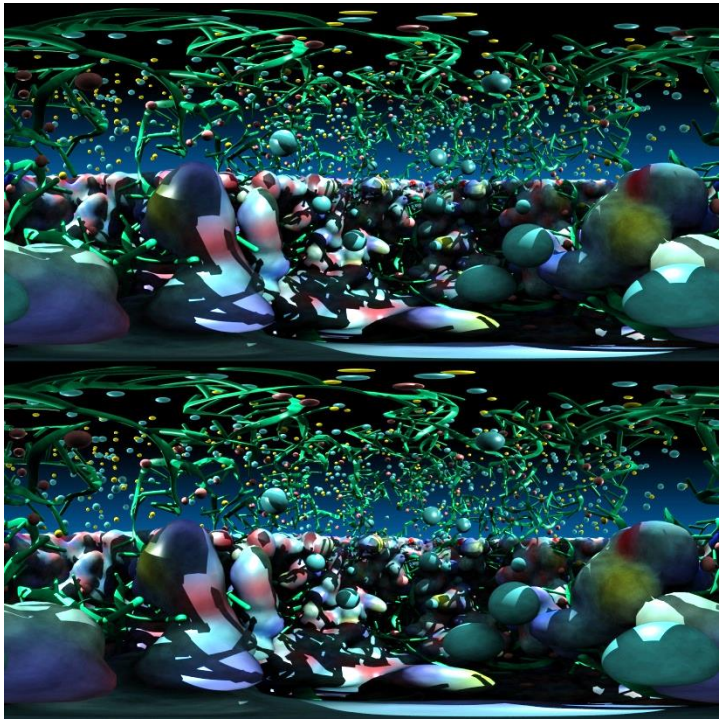
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, …
- Both mono and stereoscopic
- Single pass rendering
- No further warping or post-processing required



Stereoscopic Panorama Ray Tracing w/ OptiX

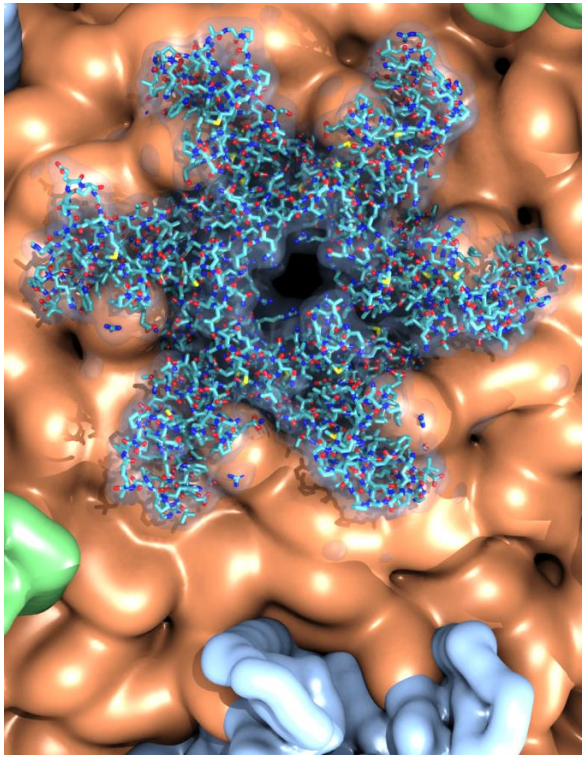


- **Render 360° images and movies** for VR headsets such as Oculus Rift, Google Cardboard
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto trivial geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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



Future Work

- 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
- Optimization of GPU-specific RT intersection routines, memory layout
- GPU-accelerated h.264 movie encoder back-end
- **Interactive RT combined with multi-node rendering and remote viz. on HPC systems, larger data sizes**



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 team
- NVIDIA OptiX team
- 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/

- **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.
- **Stable Small Quantum Dots for Synaptic Receptor Tracking on Live Neurons.** En Cai, Pinghua Ge, Sang Hak Lee, Okunola Jeyifous, Yong Wang, Yanxin Liu, Katie M. Wilson, Sung Jun Lim, Michele A. Baird, John E. Stone, Kwan Young Lee, David G. Fernig, Michael W. Davidson, Hee Jung Chung, Klaus Schulten, Andrew M. Smith, William N. Green, and Paul 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.


NIH BTRC for Macromolecular Modeling and Bioinformatics
1990-2017
Beckman Institute
University of Illinois at
Urbana-Champaign