

S7452—Cutting Edge OptiX Ray Tracing Techniques for Visualization of Biomolecular and Cellular Simulations in VMD

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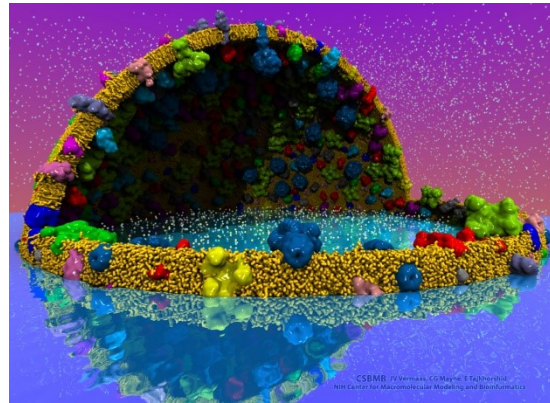
S7452, GPU Technology Conference

15:30-15:55, Room 230C, San Jose Convention Center,
San Jose, CA, Tuesday May 9th, 2017

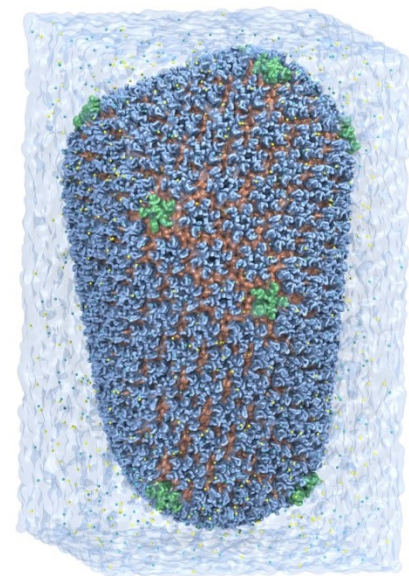


VMD – “Visual Molecular Dynamics”

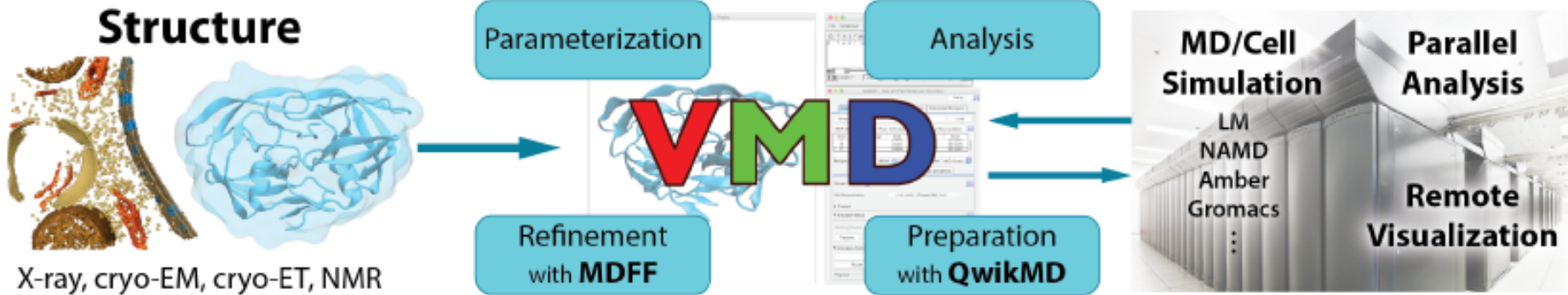
- Visualization and analysis of:
 - Molecular dynamics simulations
 - Lattice cell simulations
 - Quantum chemistry calculations
 - Cryo-EM densities, volumetric data
 - Sequence information
- User extensible scripting and plugins
- <http://www.ks.uiuc.edu/Research/vmd/>



Cell-Scale Modeling



MD Simulation



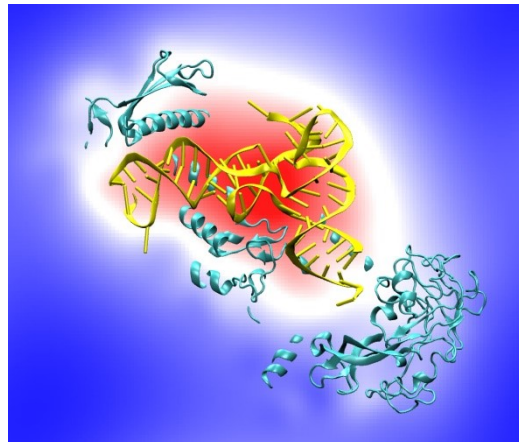
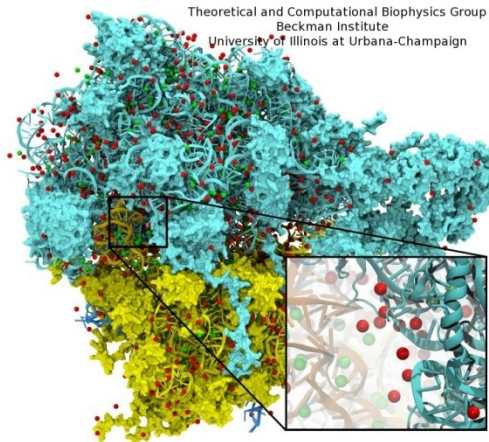
10 Years of GPU Computing in VMD, 5 Years of OptiX

- Has stood the test of time
- Modeling, Visualization, Rendering, and Analysis

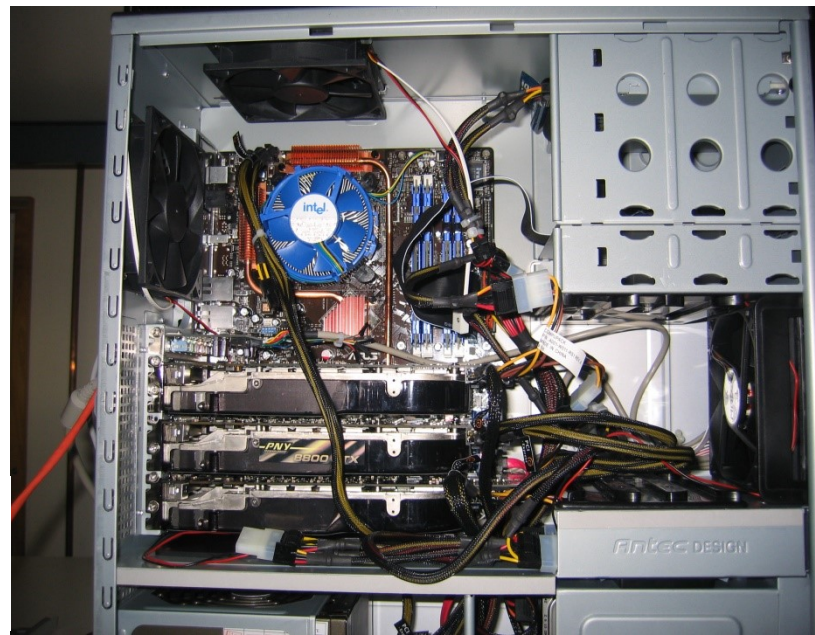
Blast from the past:

CUDA starting with version 0.7 !!!

Quad core Intel QX6700, three NVIDIA GeForce 8800GTX GPUs, RHEL4 Linux



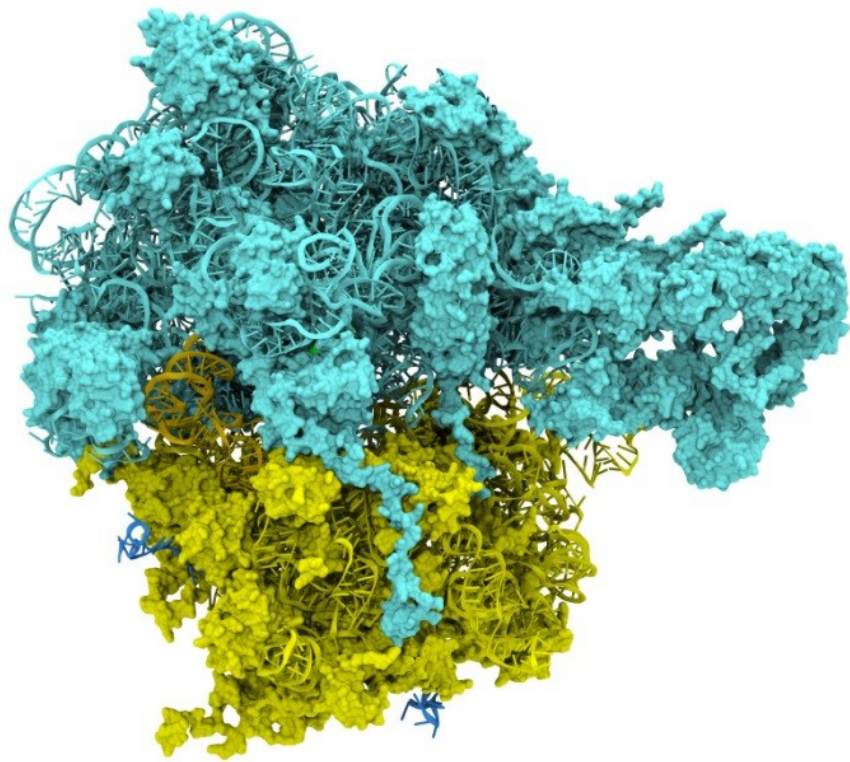
Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.



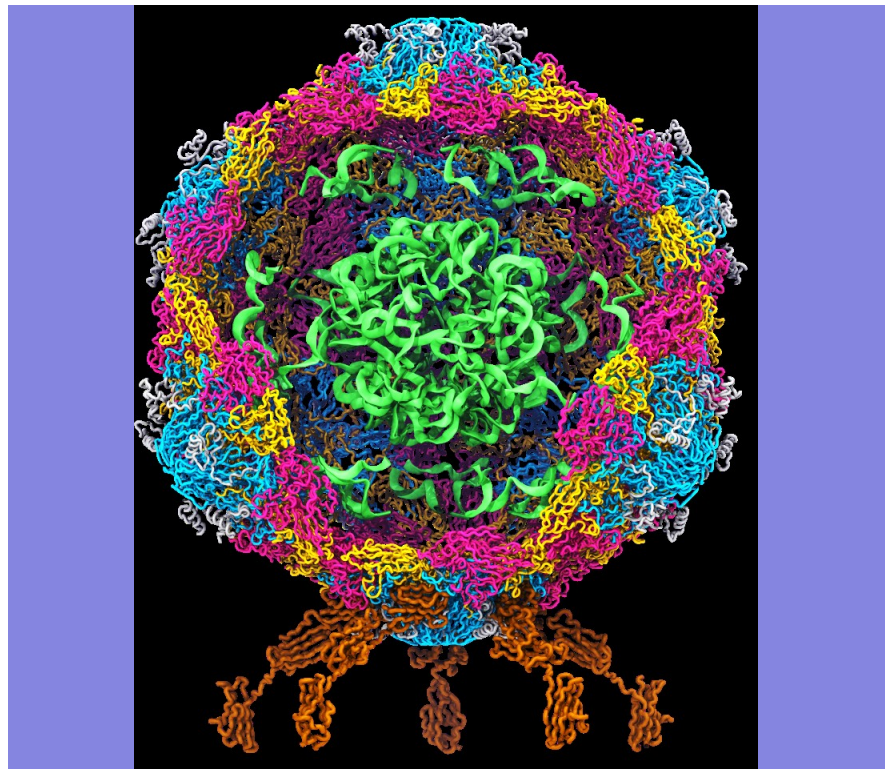
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

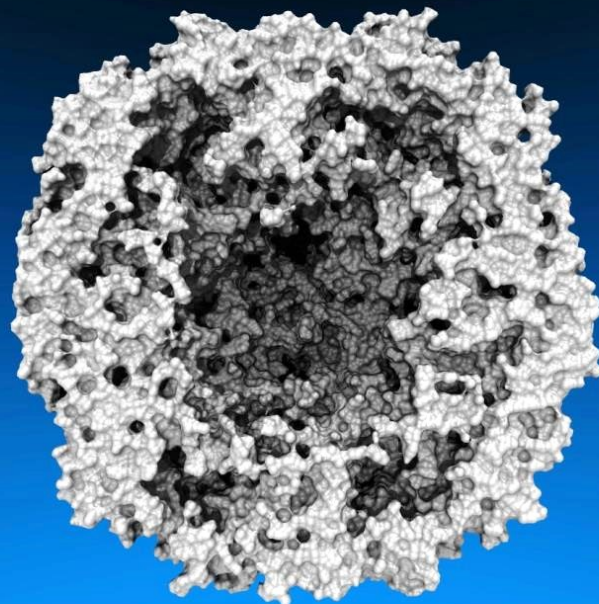
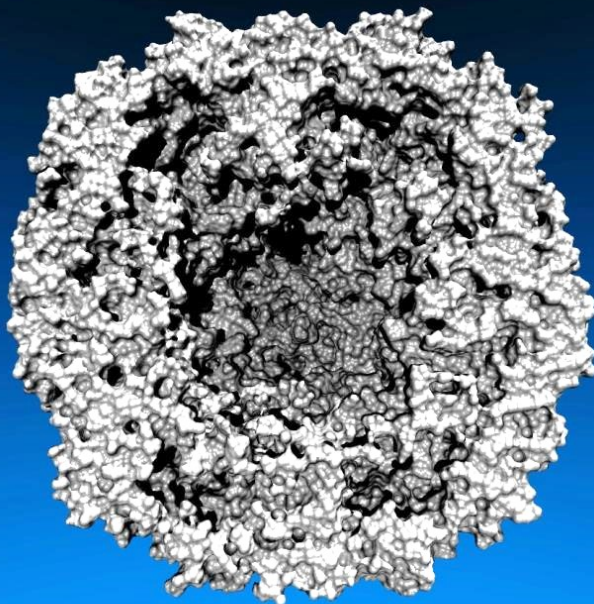
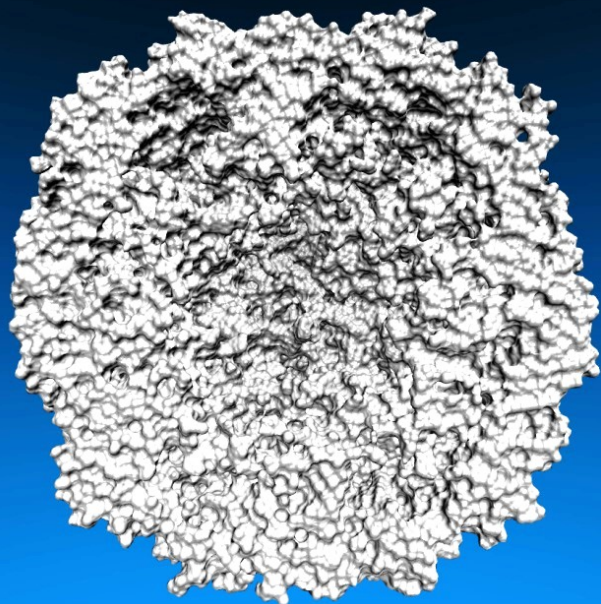


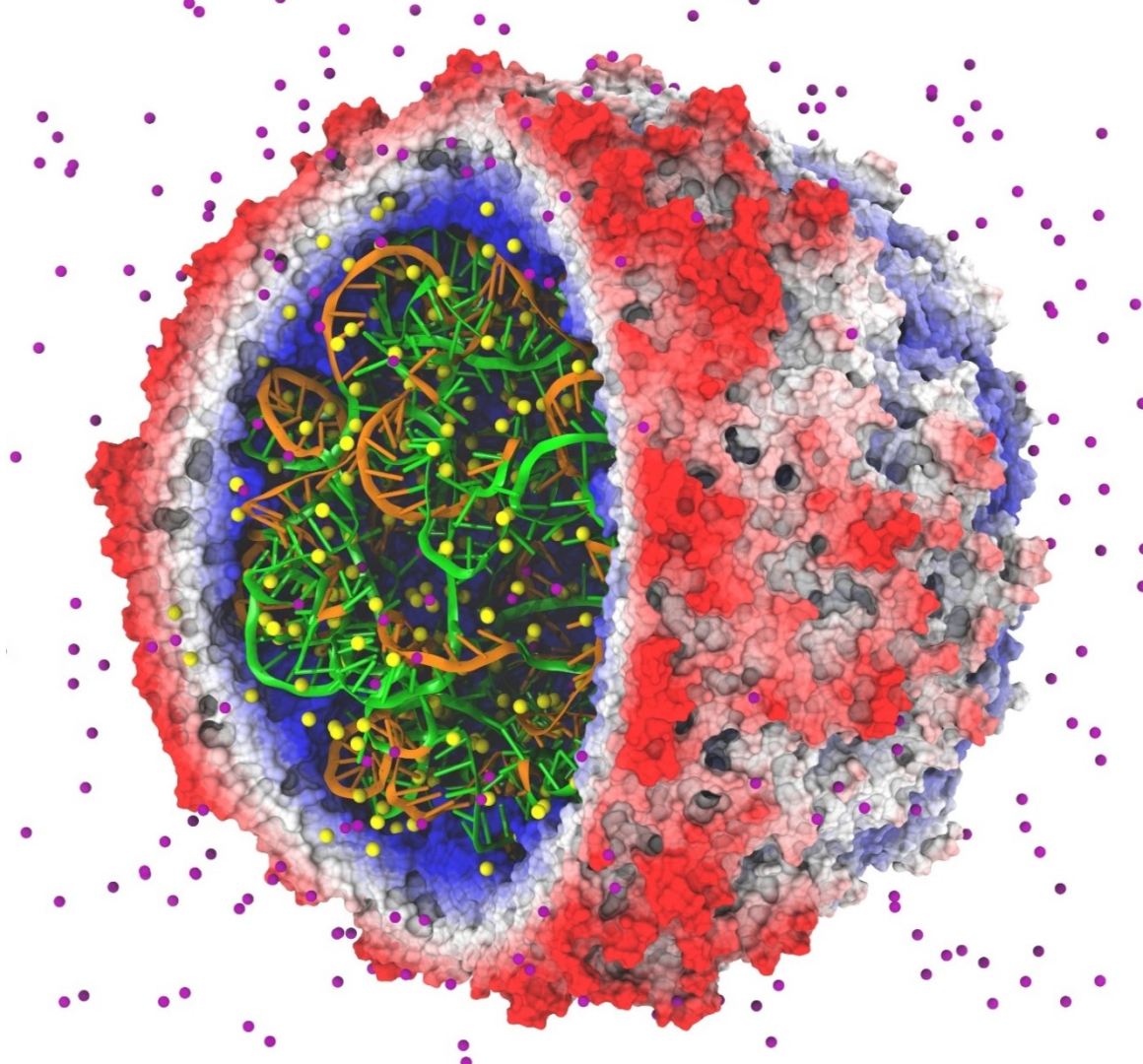
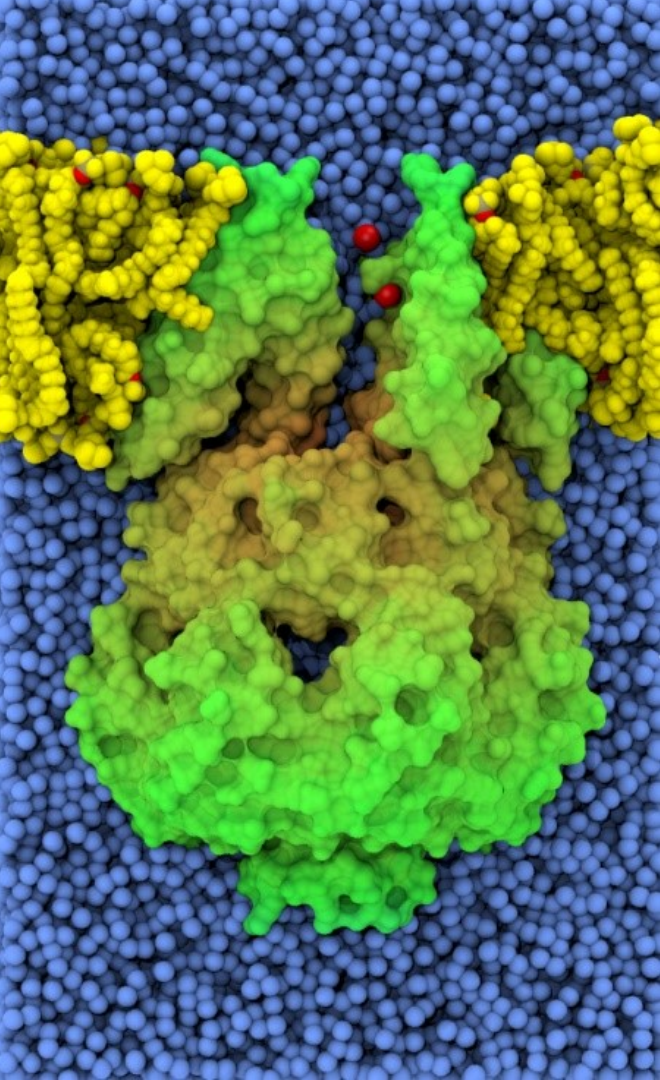
Lighting Comparison

Two lights, no shadows

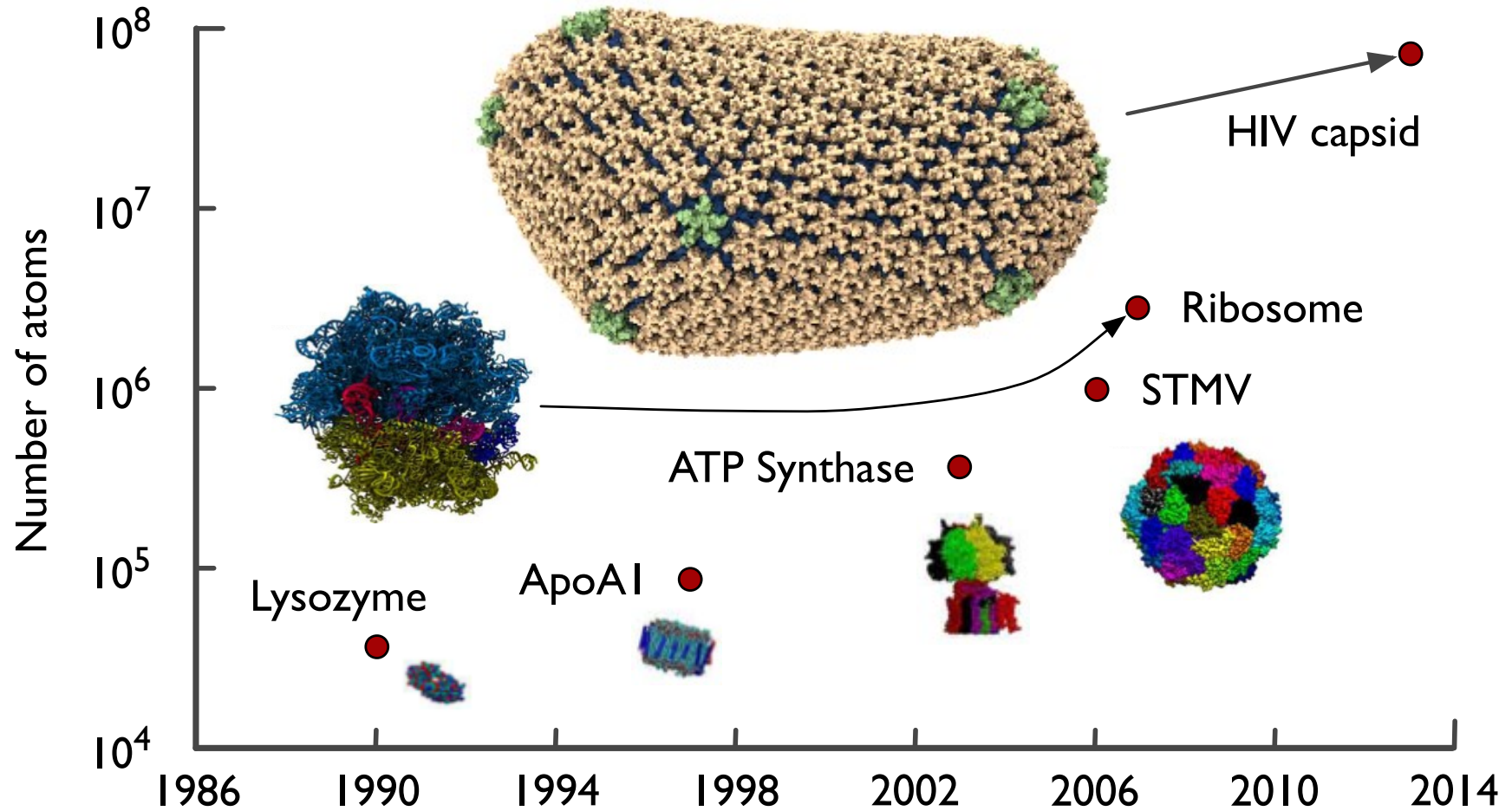
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit





Computational Biology's Insatiable Demand for Processing Power



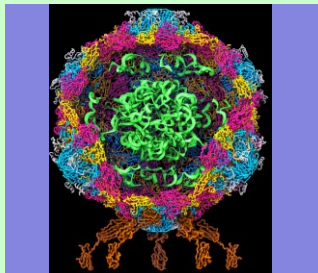
Why Built-In VMD Ray Tracing Engines?

- **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 geometry and texture data**
- Implement all **curved surface primitives**, volume rendering, texturing, special cameras, 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

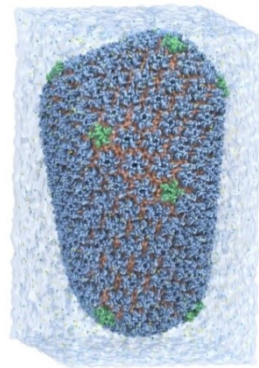
Windowed OpenGL GPU

OpenGL Pbuffer GPU

Tachyon CPU RT

TachyonL-OptiX GPU RT
Batch + Interactive

VMD 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

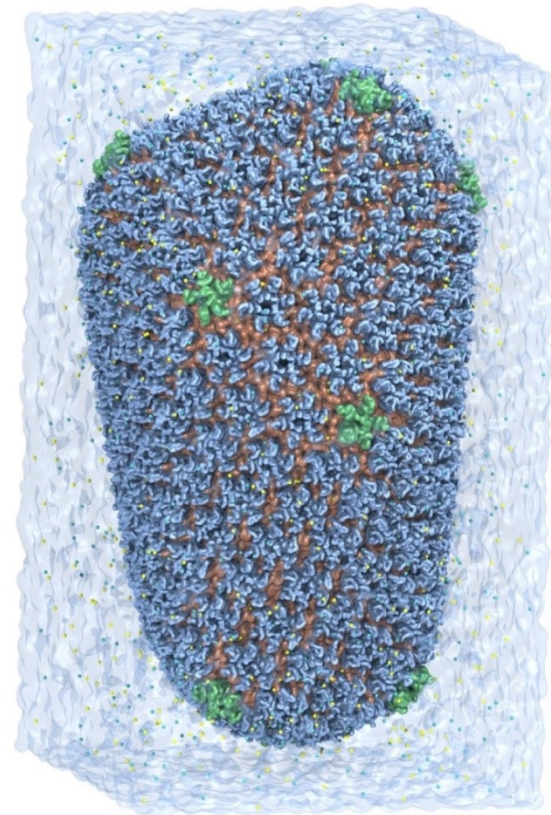
Ray Tracer Version	Node Type and Count	Script Load	State Load	Geometry + Ray Tracing	Total Time
New TachyonL-OptiX [2]	64 XK7 Tesla K20X GPUs	2 s	39 s	435 s	476 s
New TachyonL-OptiX [2]	128 XK7 Tesla K20X GPUs	3 s	62 s	230 s	295 s
TachyonL-OptiX [1]	64 XK7 Tesla K20X GPUs	2 s	38 s	655 s	695 s
TachyonL-OptiX [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.

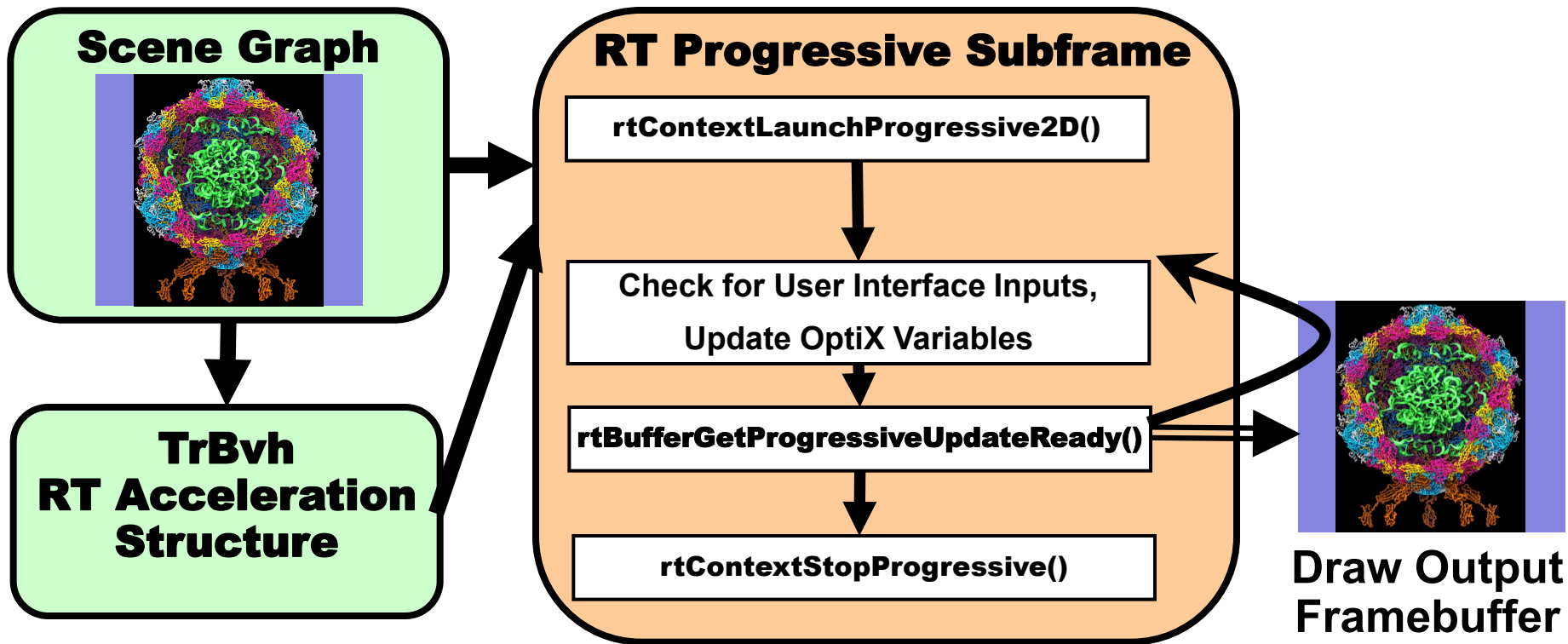
[2] **Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.** J. E. Stone et al., J. Parallel Computing, 2016 (in-press)

VMD 1.9.x Interactive GPU Ray Tracing

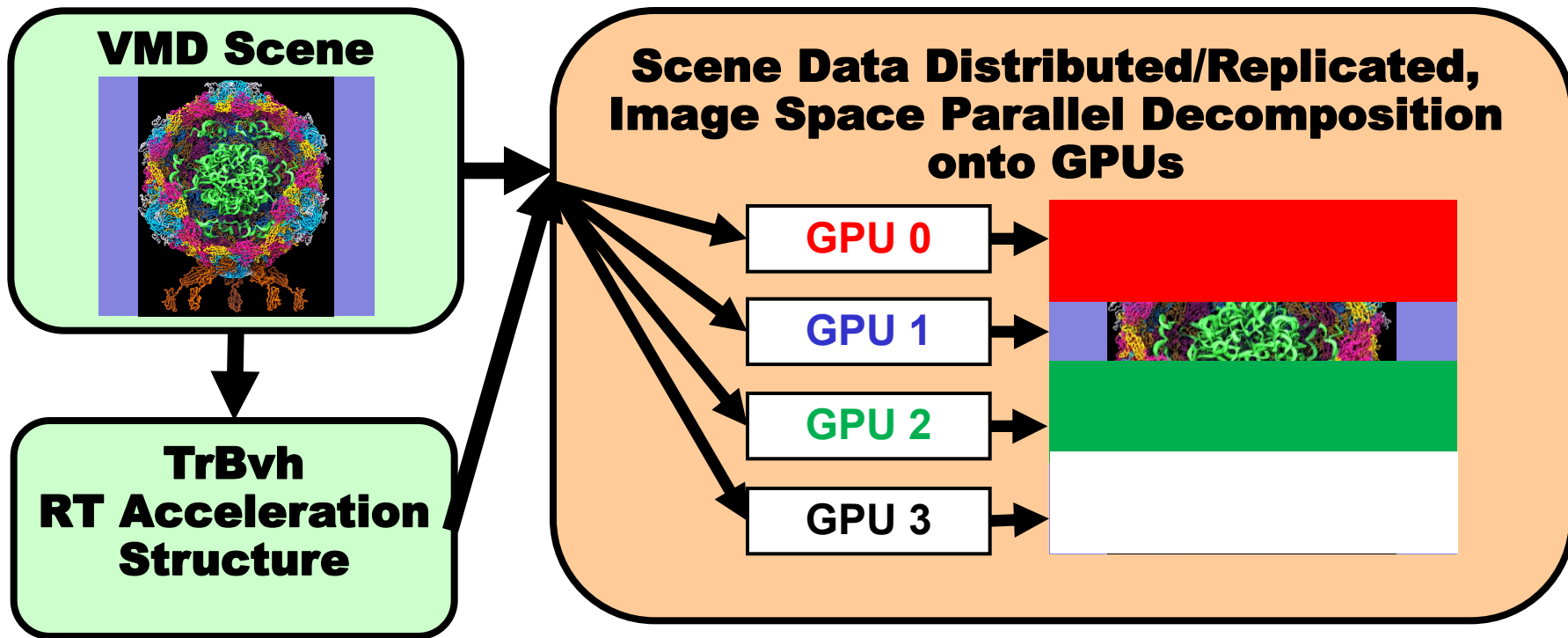
- Ray tracing heavily used for VMD publication-quality images/movies
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD provides **–interactive–** ray tracing on laptops, desktops, **remote** clouds, supercomputers



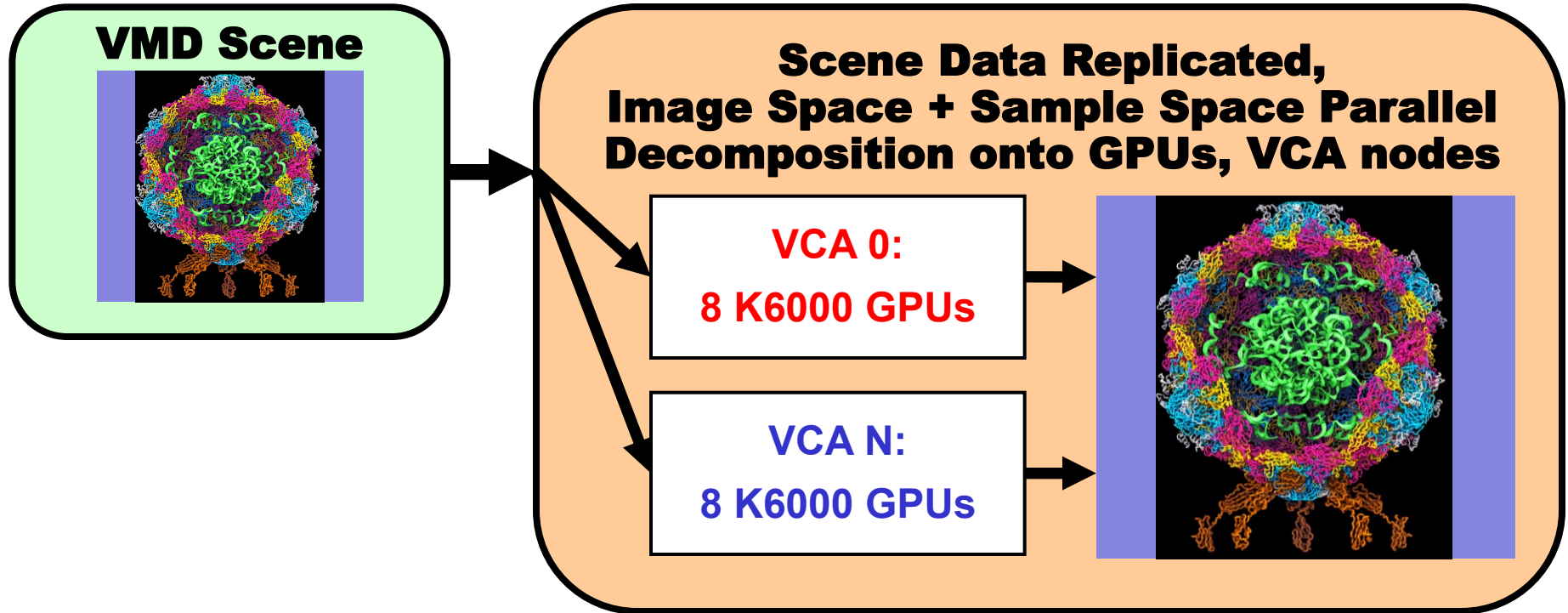
VMD TachyonL-OptiX Interactive RT w/ OptiX Progressive RT API



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



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



VMD w/ OptiX 4.1

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization tasks
- Remote RT on NVIDIA VCA clusters
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- **Top-end Pascal Tesla GPUs roughly 2x faster than Kepler, based on early tests on CSCS Piz Daint Cray XC50**
- **GPU memory sharing via NVLink on Quadro GP100, Tesla P100**

GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.

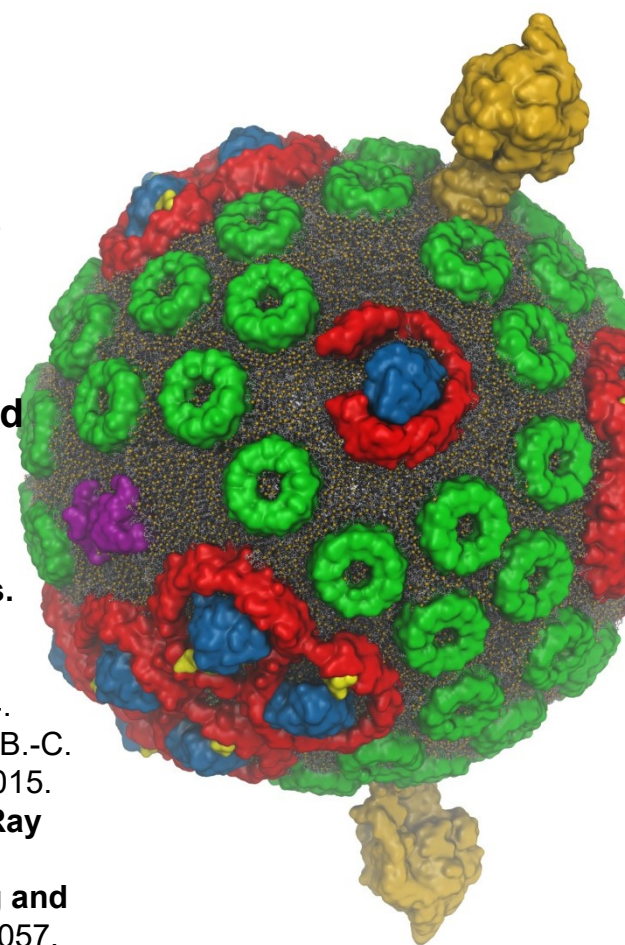
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, pp. 6:1-6:8, 2013.

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.

Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

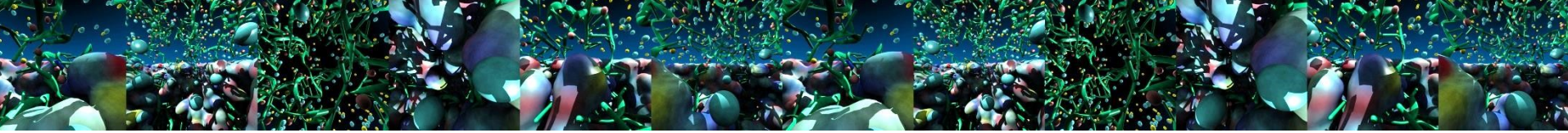
Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone et al., J. Parallel Computing, 55:17-27, 2016.

Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering J. E. Stone, W. R. Sherman, and K. HPDAV, IPDPSW, pp. 1048-1057, 2016.

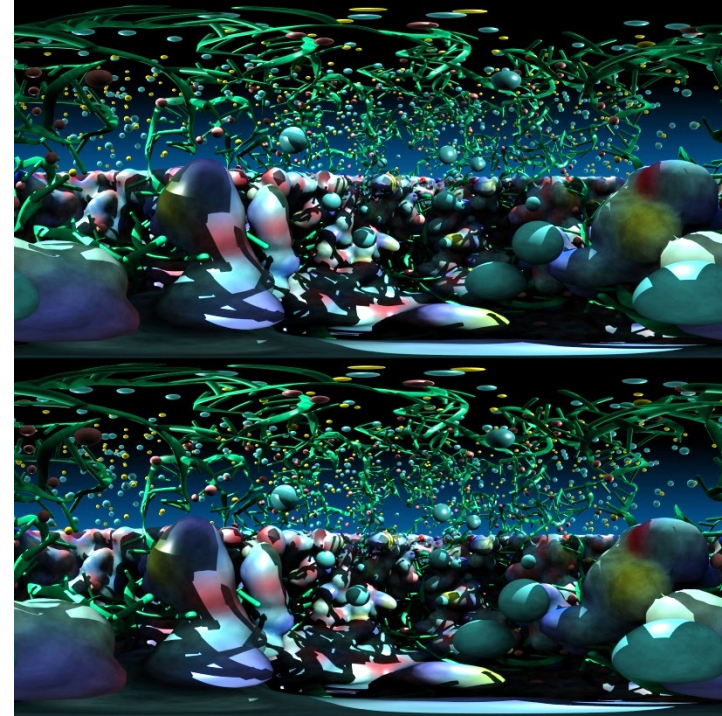


VMD/OptiX GPU Ray Tracing of
all-atom Chromatophore w/ lipids.

Stereoscopic Panorama Ray Tracing w/ OptiX

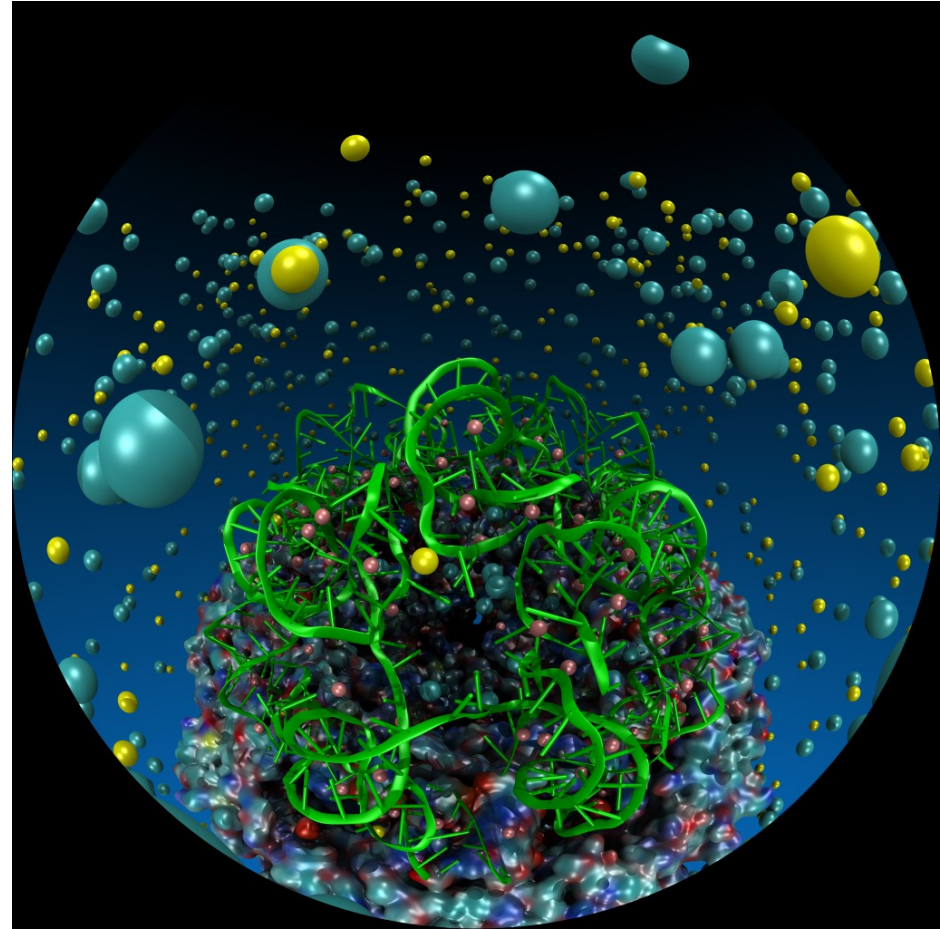


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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

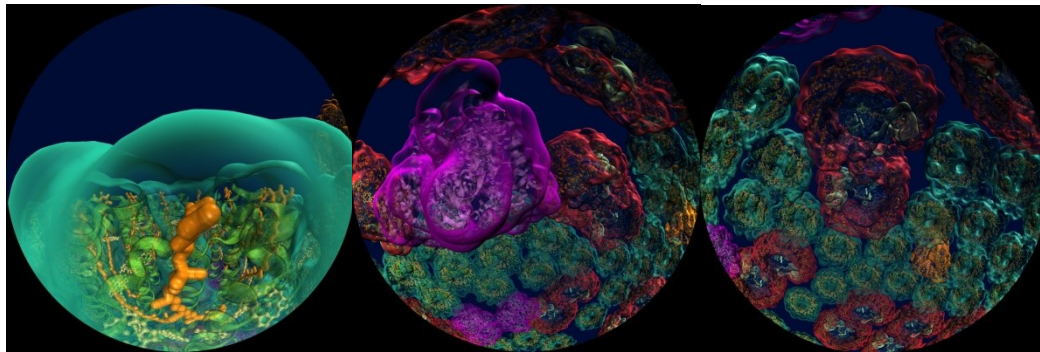
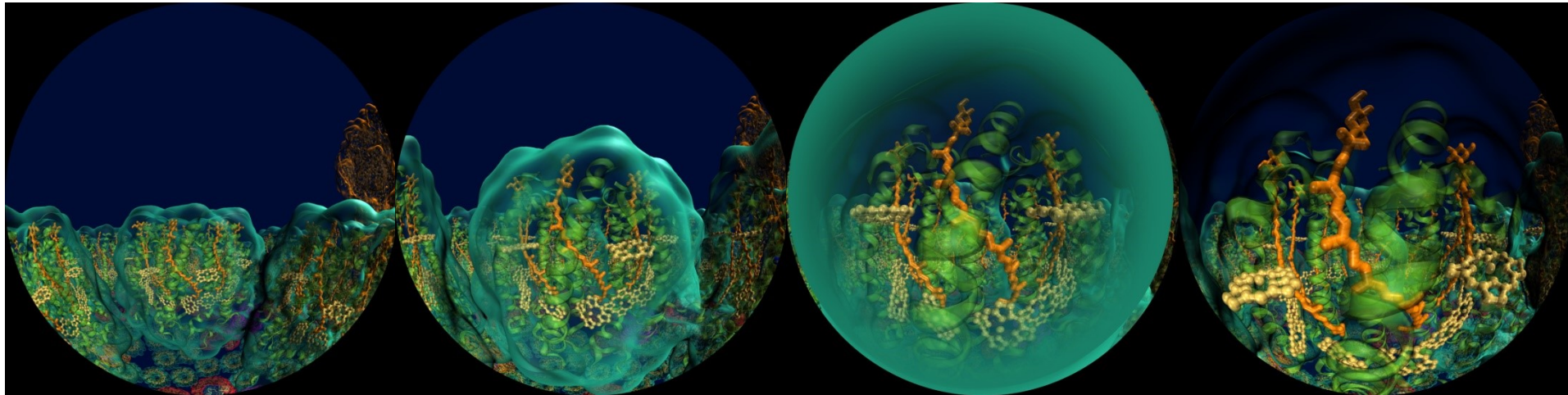


VMD Planetarium Dome Master Camera

- Trivial to implement in OptiX
- 40 lines of CUDA code including antialiasing and handling corner cases for transcendental fctns
- Try implementing this in OpenGL . . . (yuck)
- Stereoscopic cameras and other special purpose projections are similarly easy



CADENS “Birth of Planet Earth” Planetarium Dome Master Test Frames

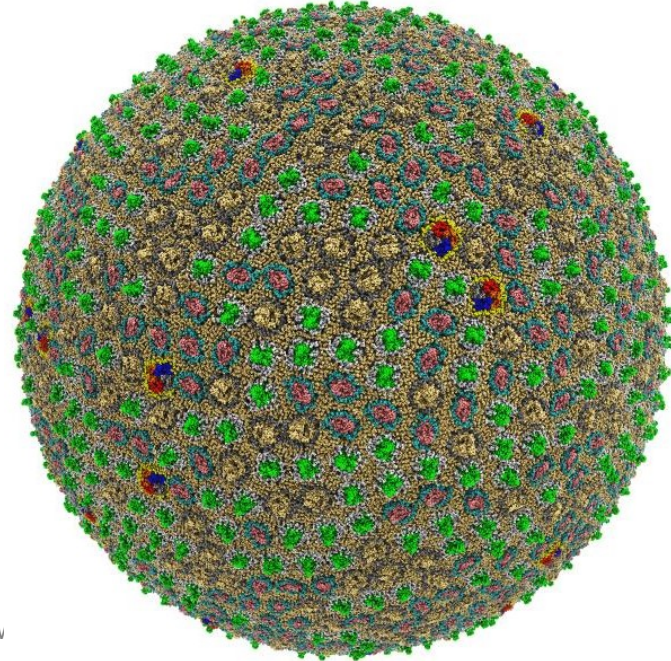


Preparation, Visualization, Analysis of All-Atom Cell-Scale Simulations

- Interactive rasterization w/ OpenGL/EGL now, Vulkan in future releases of VMD
 - **Interactive ray tracing on CPUs and GPUs**
 - Support for large host memory (TB), up to **2 billion atoms per “molecule” now**
 - Parallel analysis, visualization w/ MPI
- 200 nm spherical envelope
 - Membrane with ~50% occupancy by proteins
 - 63M atoms in envelope model

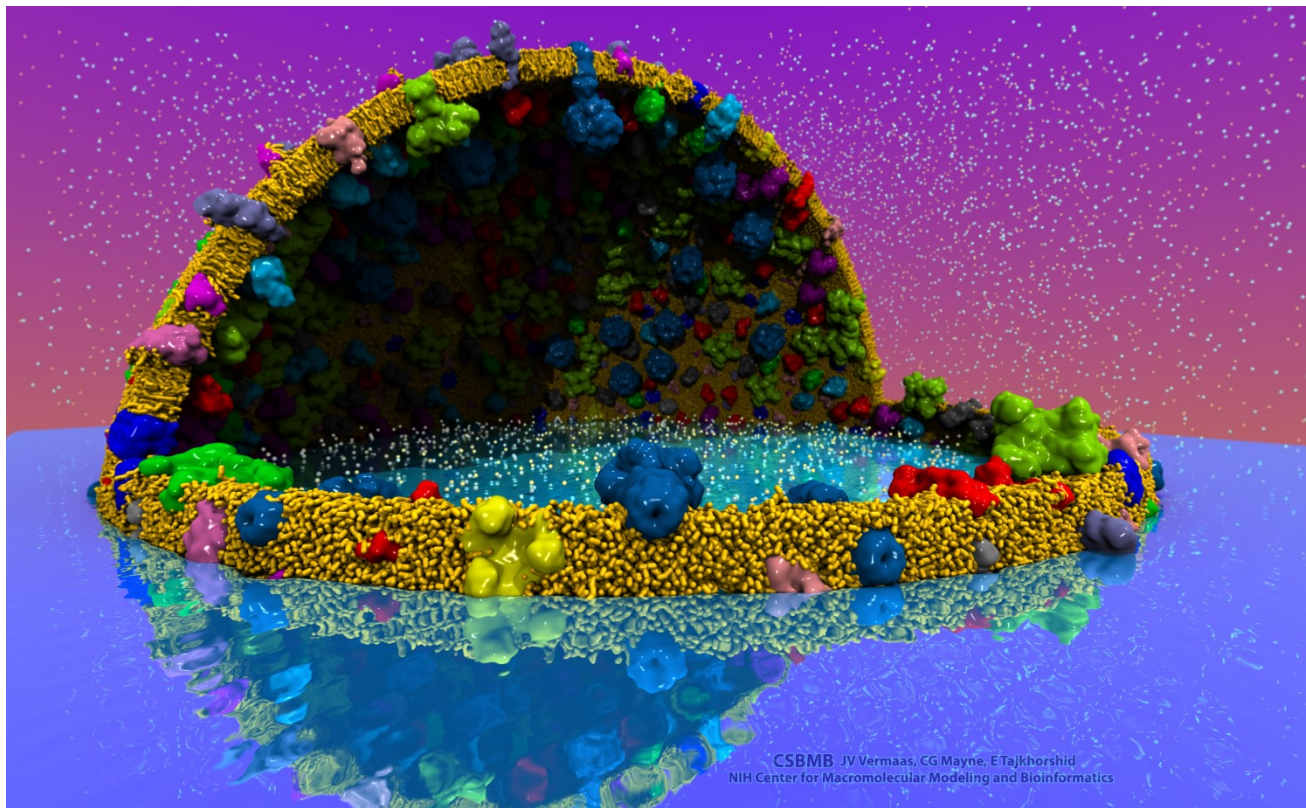
Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J.E. Stone, ..., K. Schulten, J. Parallel Computing, 55:17-27, 2016.

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.



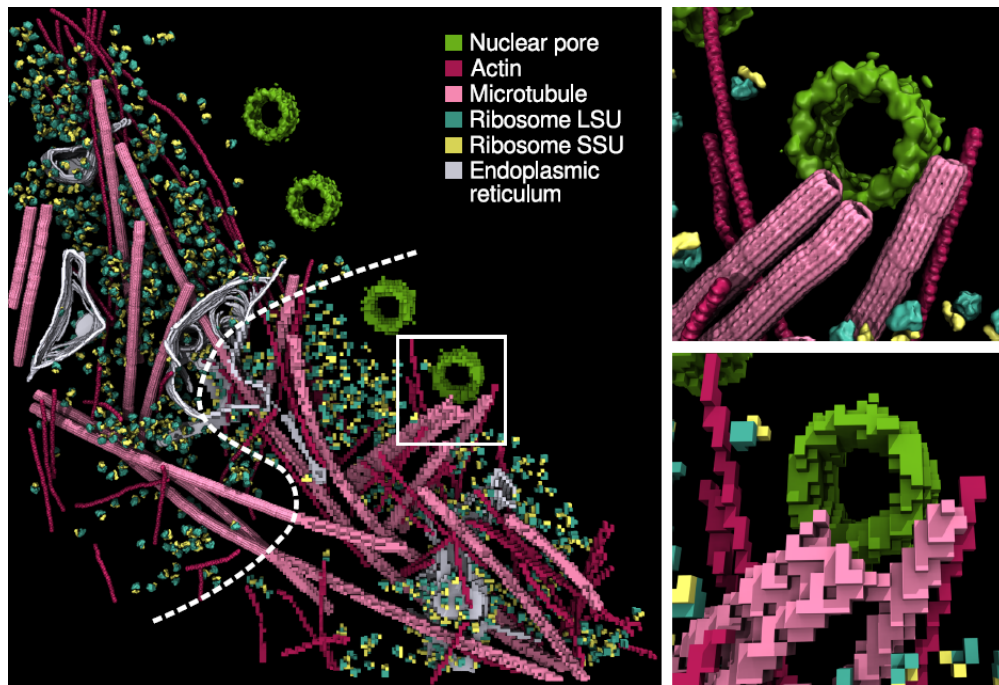
Proto-Cell Rendered with VMD+OptiX

- 113M particles
- 1,397 copies of 14 different membrane proteins
- Preparing for simulations on pre-exascale computers



Interactive Ray Tracing of Cells

- High resolution cellular tomograms
- Multi-billion voxels
- Even isosurface or lattice site graphical representations involve ~100M geometric primitives
- 24GB Quadro M6000s used for interactive RT of cellular tomograms of this size
- **Latest Quadro GP100 GPUs benefit from OptiX 4.1 support for NVLink and distribution of scene data across multiple GPUs**



Earnest, et al. J. Physical Chemistry B, 121(15): 3871-3881, 2017.

VMD Molecule Instancing: In-Progress Development

- VMD 1.9.4 supports instancing of graphical representations associated with molecules
- Will exploit VBO caching in OpenGL to eliminate host-GPU geometry transfers
- OptiX instancing of geometry buffers to eliminate GPU memory consumption for instances

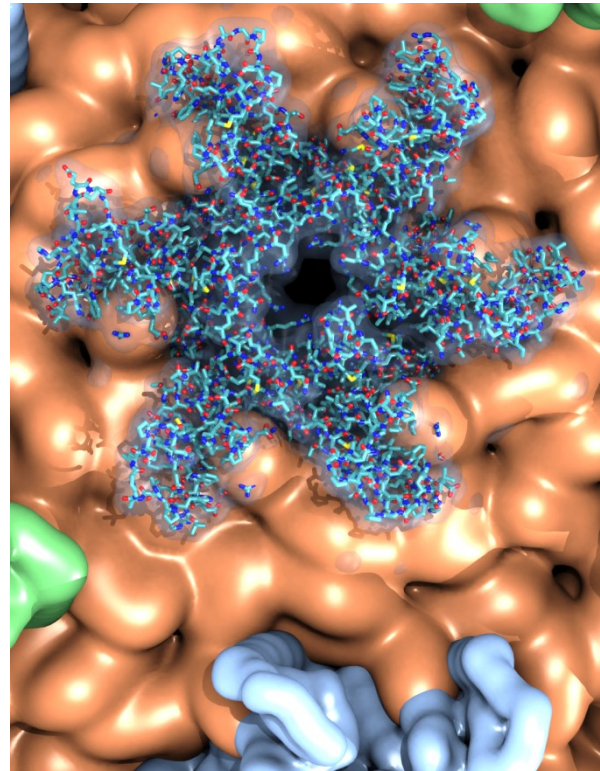




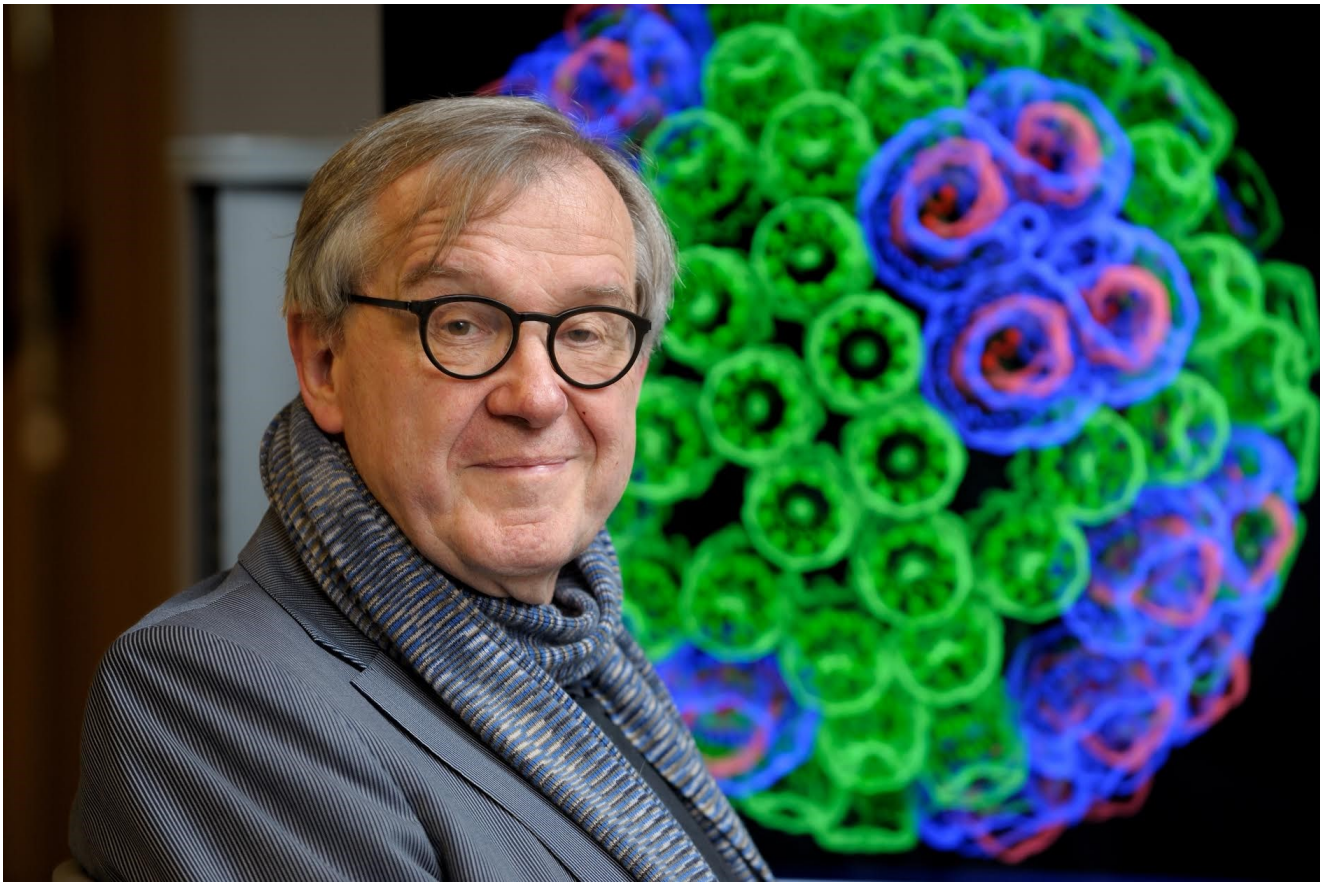
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing

VMD-Next: Coming Soon

- Further integration of interactive ray tracing into VMD
 - Seamless interactive RT in main VMD display window
 - Much larger scene sizes, complexity, enhanced stochastic sampling techniques
 - Continue tuning of GPU-specific RT intersection routines, memory layout
 - Support trajectory playback in interactive RT
 - Optimize GPU scene DMA and BVH regen speed for time-varying geometry, e.g. MD trajectories
 - Enable multi-node interactive RT on HPC systems
- Improved movie making tools, parallel movie rendering, GPU-accelerated movie encoder back-end
- Built-in (basic) interactive remote visualization on HPC clusters and supercomputers



GPU Ray Tracing of
HIV-1 Capsid Detail



“When I was a young man, my goal was to look with mathematical and computational means at the inside of cells, one atom at a time, to decipher how living systems work. That is what I strived for and I never deflected from this goal.” – Klaus Schulten

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- CUDA Center of Excellence, University of Illinois at Urbana-Champaign
- NVIDIA CUDA and OptiX teams
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 - 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

Related Publications

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

- **Challenges of Integrating Stochastic Dynamics and Cryo-electron Tomograms in Whole-cell Simulations.** T. M. Earnest, R. Watanabe, J. E. Stone, J. Mahamid, W. Baumeister, E. Villa, and Z. Luthey-Schulten. J. Physical Chemistry B, 121(15): 3871-3881, 2017.
- **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, and K. Schulten. International Workshop on OpenPOWER for HPC (IWOPH'16), LNCS 9945, pp. 188-206, 2016.
- **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 Symposium Workshop (IPDPSW), pp. 1048-1057, 2016.
- **High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL.** J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), pp. 1014-1023, 2016.
- **Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads.** J. E. Stone, M. J. Hallock, J. C. Phillips, J. R. Peterson, Z. Luthey-Schulten, and K. Schulten. 25th International Heterogeneity in Computing Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), pp. 89-100, 2016.
- **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.-C. Goh, J. C. Phillips, C. MacGregor-Chatwin, M. P. Johnson, L. F. Kourkoutis, C. Neil Hunter, and K. Schulten. J. Parallel Computing, 55:17-27, 2016.

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- **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
- **Runtime and Architecture Support for Efficient Data Exchange in Multi-Accelerator Applications.** J. Cabezas, I. Gelado, J. E. Stone, N. Navarro, D. B. Kirk, and W. Hwu. IEEE Transactions on Parallel and Distributed Systems, 26(5):1405-1418, 2015.
- **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.
- **Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations.** M. J. Hallock, J. E. Stone, E. Roberts, C. Fry, and Z. Luthey-Schulten. Journal of Parallel Computing, 40:86-99, 2014.

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- **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.
- **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.
- **Fast Analysis of Molecular Dynamics Trajectories with Graphics Processing Units – Radial Distribution Functions.** B. Levine, J. Stone, and A. Kohlmeyer. *J. Comp. Physics*, 230(9):3556-3569, 2011.

Related Publications

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

- **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.
- **GPU-accelerated molecular modeling coming of age.** J. Stone, D. Hardy, I. Ufimtsev, K. Schulten. *J. Molecular Graphics and Modeling*, 29:116-125, 2010.
- **OpenCL: A Parallel Programming Standard for Heterogeneous Computing.** J. Stone, D. Gohara, G. Shi. *Computing in Science and Engineering*, 12(3):66-73, 2010.
- **An Asymmetric Distributed Shared Memory Model for Heterogeneous Computing Systems.** I. Gelado, J. Stone, J. Cabezas, S. Patel, N. Navarro, W. Hwu. *ASPLOS '10: Proceedings of the 15th International Conference on Architectural Support for Programming Languages and Operating Systems*, pp. 347-358, 2010.

Related Publications

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- **GPU Clusters for High Performance Computing.** V. Kindratenko, J. Enos, G. Shi, M. Showerman, G. Arnold, J. Stone, J. Phillips, W. Hwu. *Workshop on Parallel Programming on Accelerator Clusters (PPAC)*, In Proceedings IEEE Cluster 2009, pp. 1-8, Aug. 2009.
- **Long time-scale simulations of in vivo diffusion using GPU hardware.** E. Roberts, J. Stone, L. Sepulveda, W. Hwu, Z. Luthey-Schulten. In *IPDPS'09: Proceedings of the 2009 IEEE International Symposium on Parallel & Distributed Computing*, pp. 1-8, 2009.
- **High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs.** J. E. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Processing Units (GPGPU-2)*, *ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.
- **Probing Biomolecular Machines with Graphics Processors.** J. Phillips, J. Stone. *Communications of the ACM*, 52(10):34-41, 2009.
- **Multilevel summation of electrostatic potentials using graphics processing units.** D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

Related Publications

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

- **Adapting a message-driven parallel application to GPU-accelerated clusters.**
J. Phillips, J. Stone, K. Schulten. *Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, IEEE Press, 2008.
- **GPU acceleration of cutoff pair potentials for molecular modeling applications.**
C. Rodrigues, D. Hardy, J. Stone, K. Schulten, and W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.
- **GPU computing.** J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.
- **Accelerating molecular modeling applications with graphics processors.** J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.
- **Continuous fluorescence microphotolysis and correlation spectroscopy.** A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.