

S6261—VMD+OptiX: Streaming Interactive Ray Tracing from Remote GPU Clusters to Your VR Headset

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/>

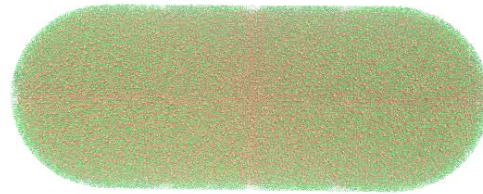
S6261, GPU Technology Conference

10:30-10:55, Room LL20C, San Jose Convention Center,
San Jose, CA, Wednesday April 6th, 2016

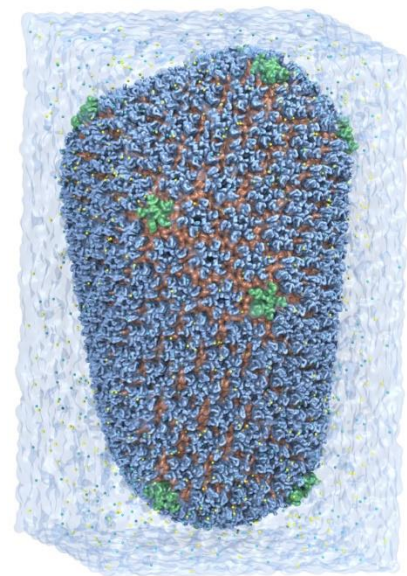


VMD – “Visual Molecular Dynamics”

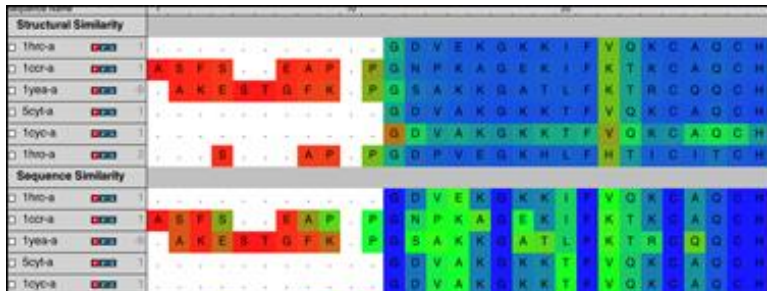
- Visualization and analysis of:
 - molecular dynamics simulations
 - particle systems and whole cells
 - cryoEM densities, volumetric data
 - quantum chemistry calculations
 - sequence information
- User extensible w/ scripting and plugins
- <http://www.ks.uiuc.edu/Research/vmd/>



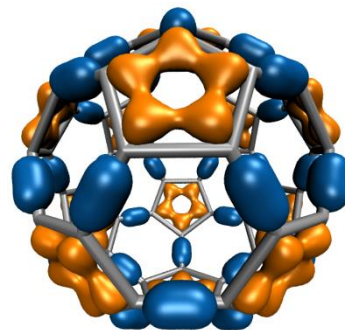
Whole Cell Simulation



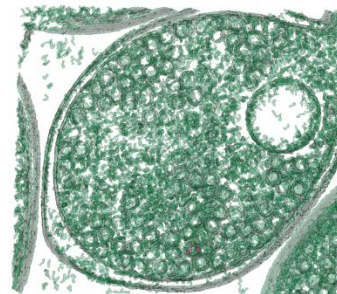
MD Simulations



Sequence Data



Quantum Chemistry

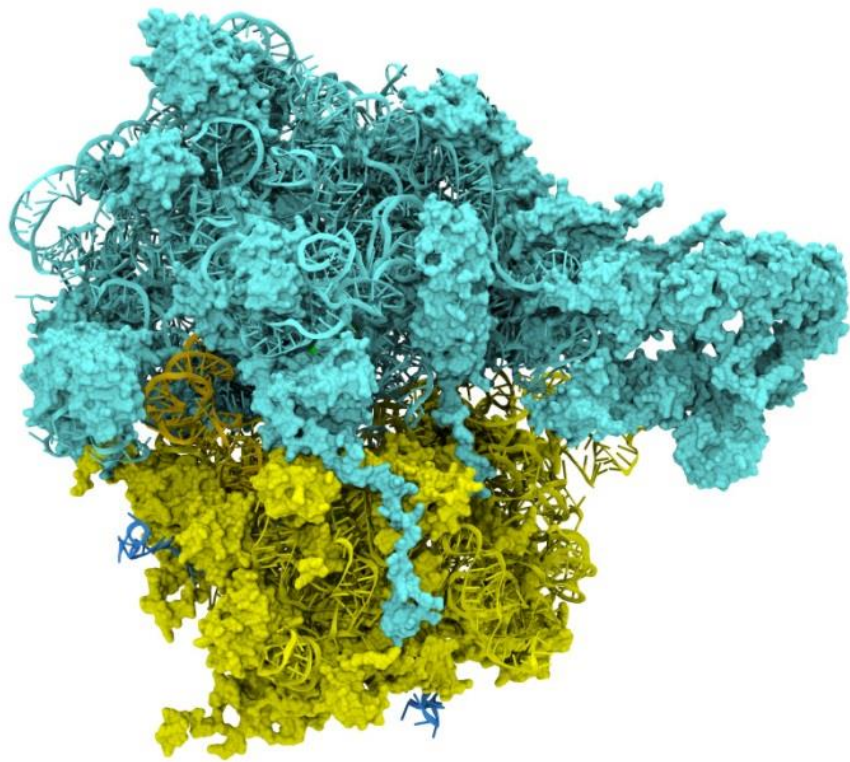


CryoEM, Cellular Tomography

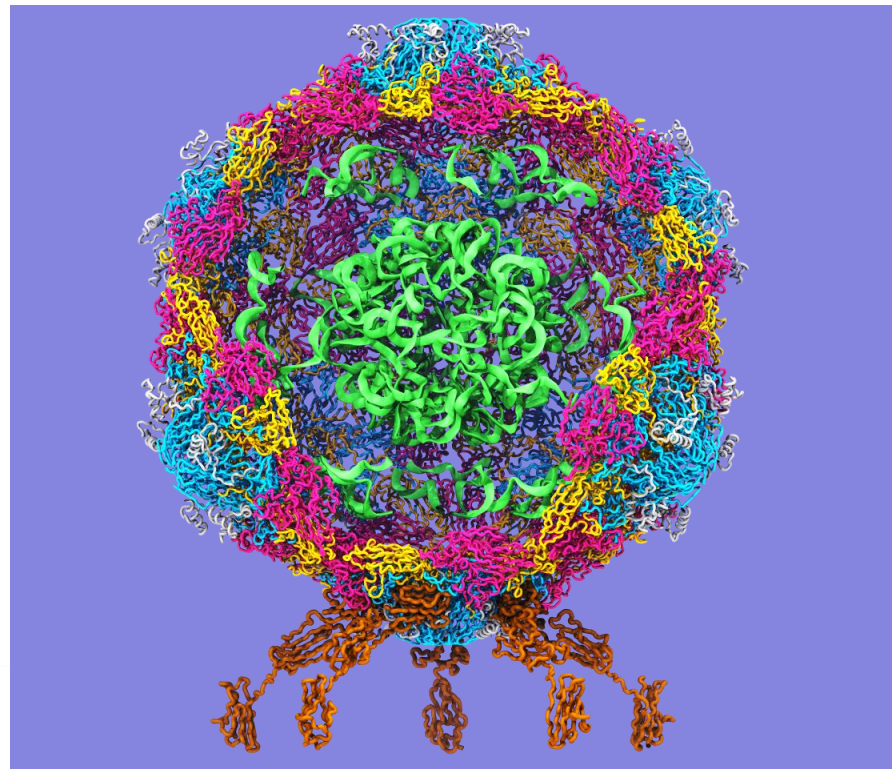
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus



Immersive Viz. w/ VMD

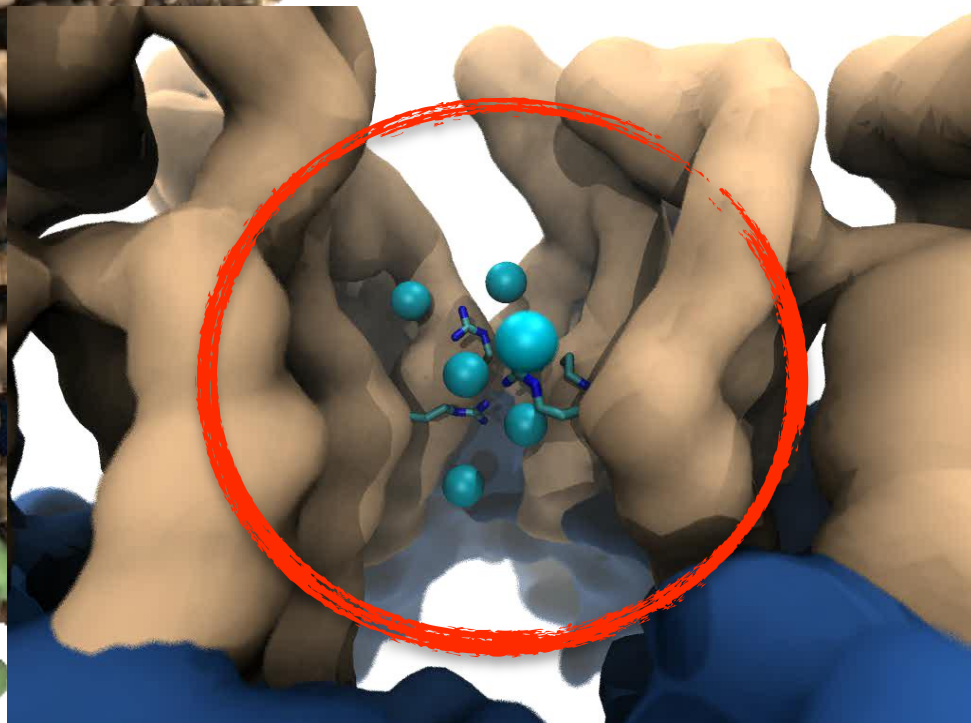
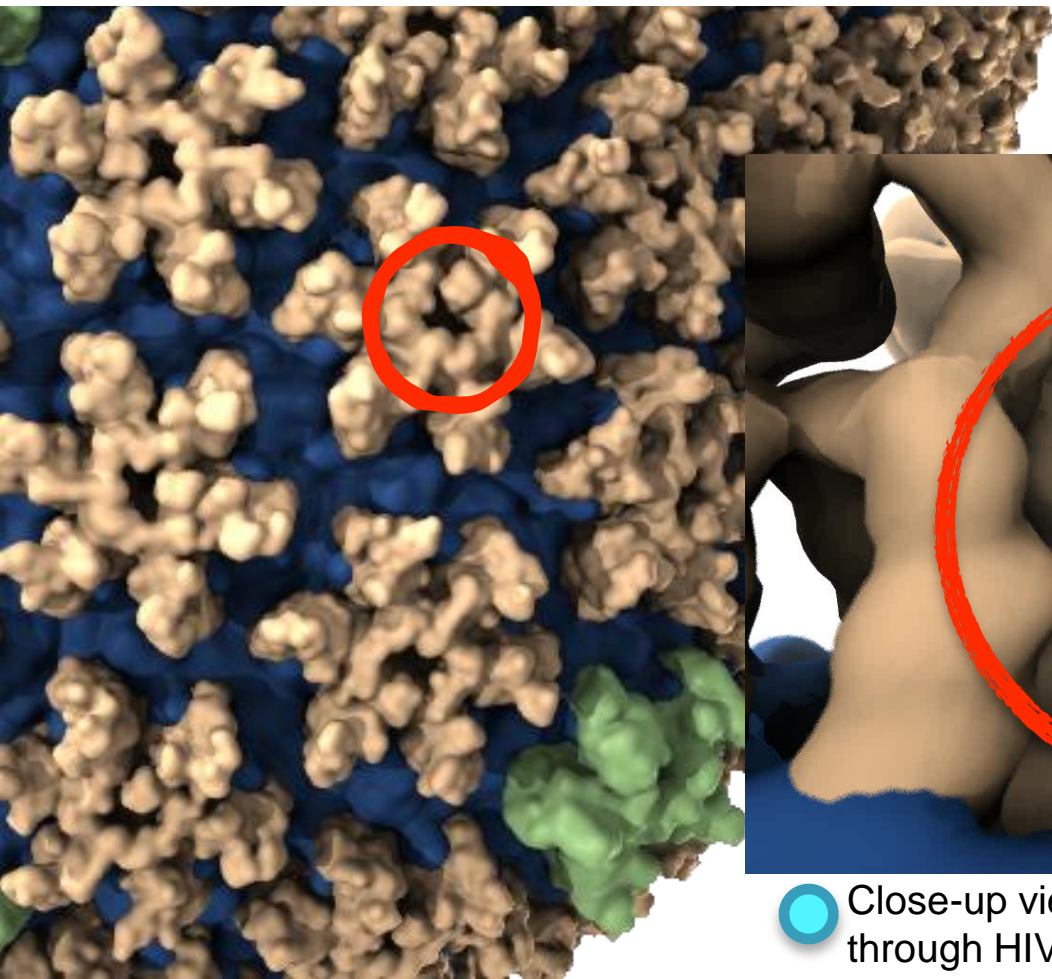
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability, convenience
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
 - Incorporate support for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




VMD running in a CAVE w/ VR Juggler

Goal: Intuitive interactive viz. in crowded molecular complexes

Results from 64 M atom, 1 μ s sim!



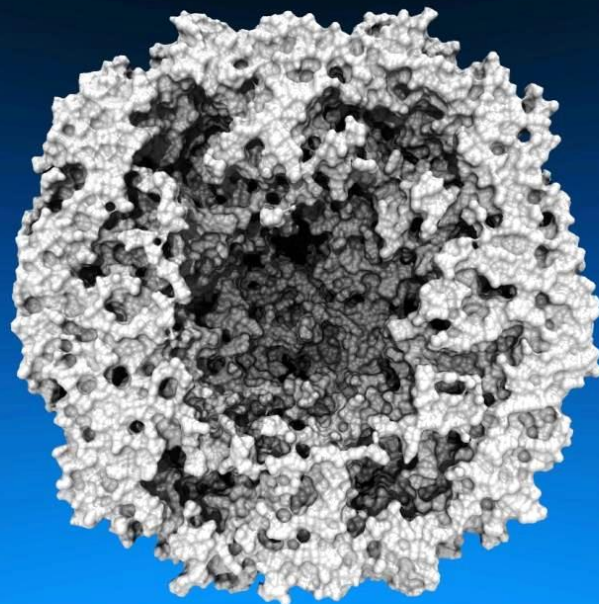
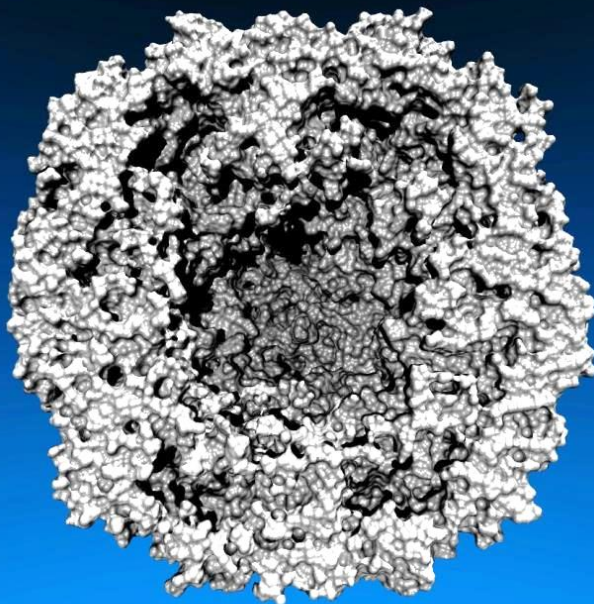
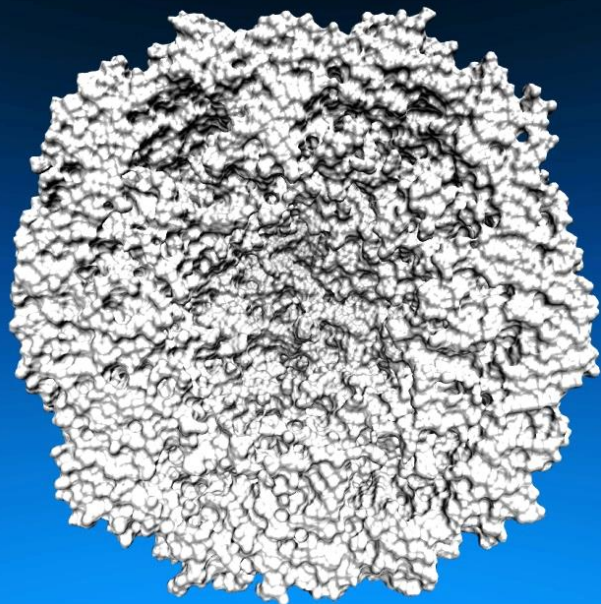
 Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers

Lighting Comparison

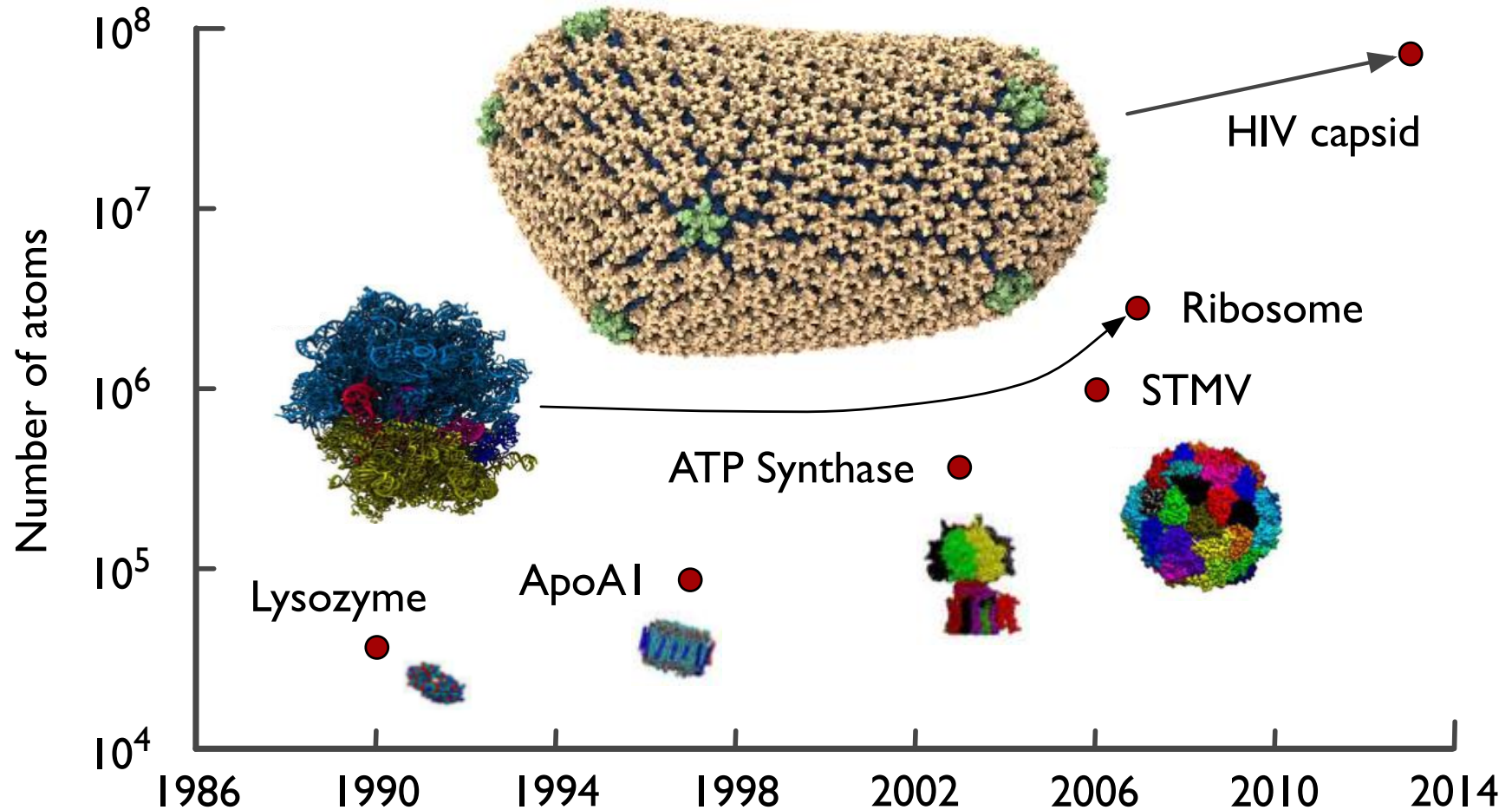
Two lights, no shadows

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



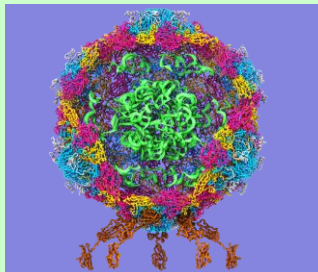
HMD Ray Tracing Challenges

- 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**



VMD Molecular Structure Data and Global State

Scene Graph



Graphical Representations

DrawMolecule

Non-Molecular
Geometry

User Interface Subsystem

Tcl/Python Scripting

Mouse + Windows

VR Input "Tools"

Display Subsystem

VMDDisplayList

DisplayDevice

OpenGLDisplayDevice

FileRenderer

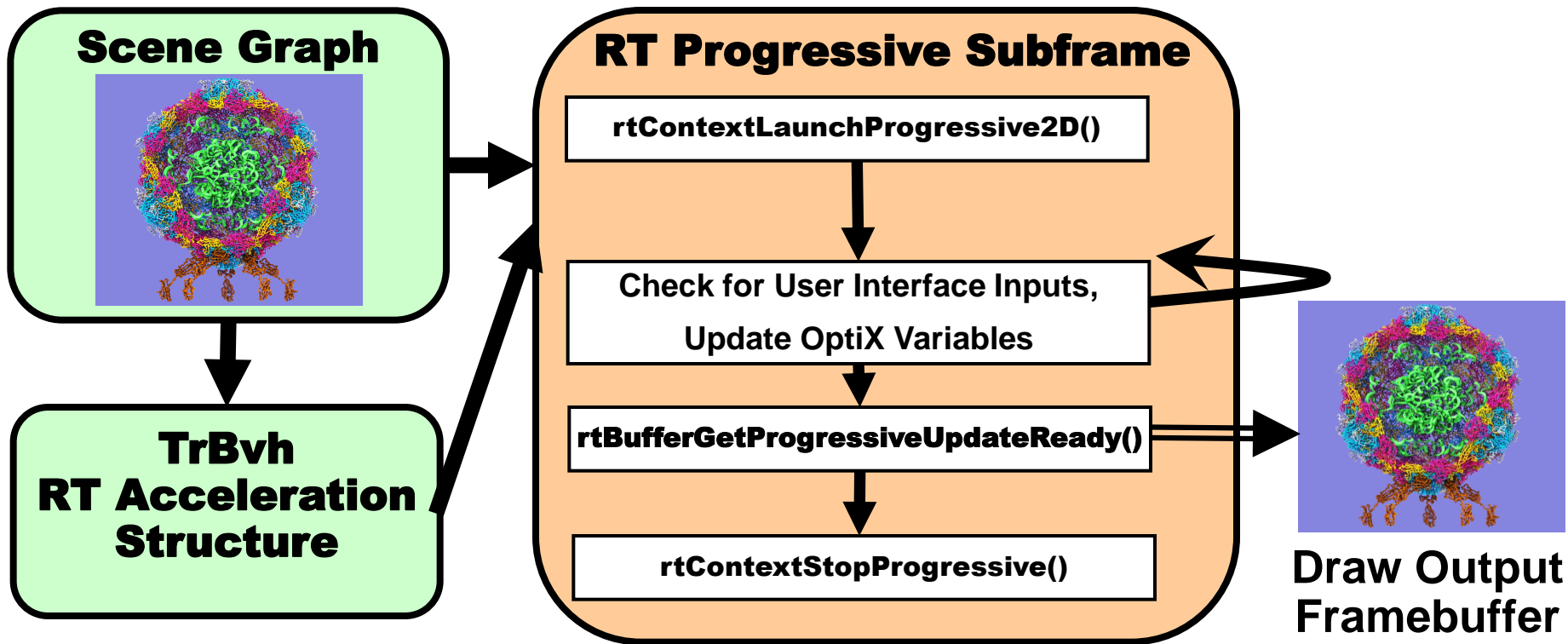
Windowed OpenGL GPU

OpenGL Pbuffer GPU

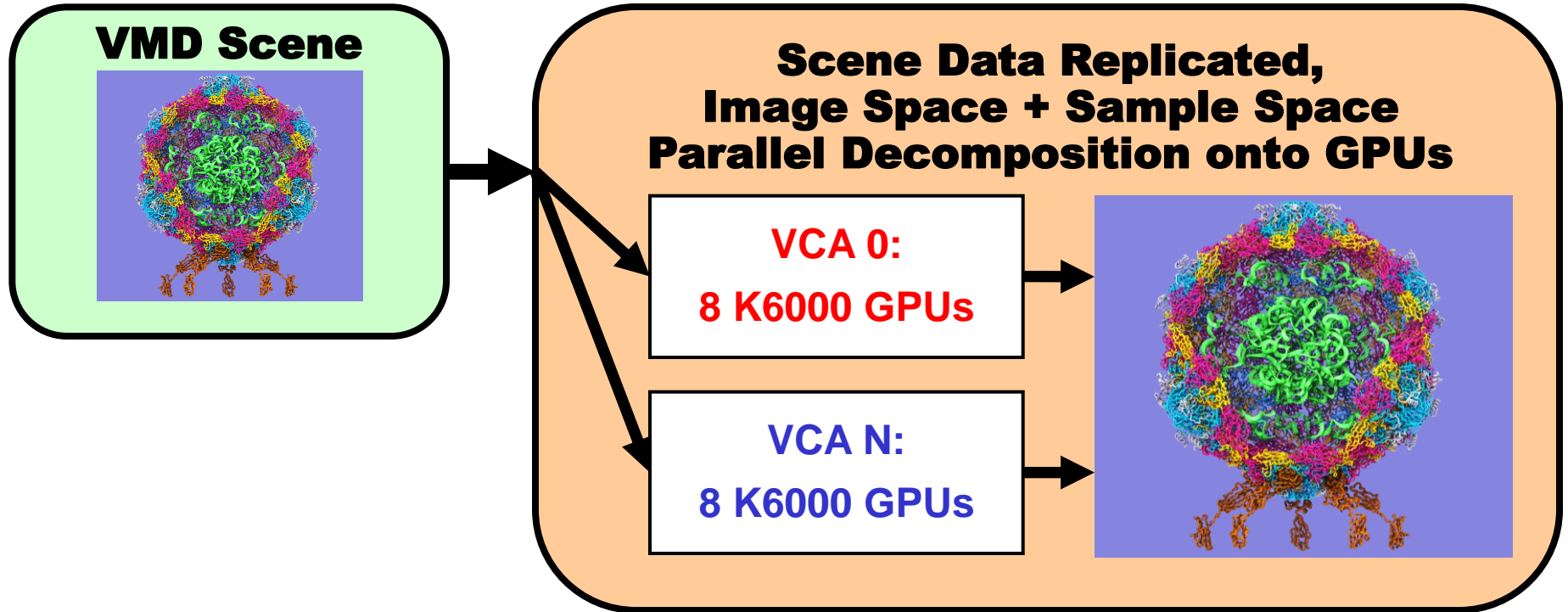
Tachyon CPU RT

TachyonL-OptiX GPU RT
Batch + Interactive

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



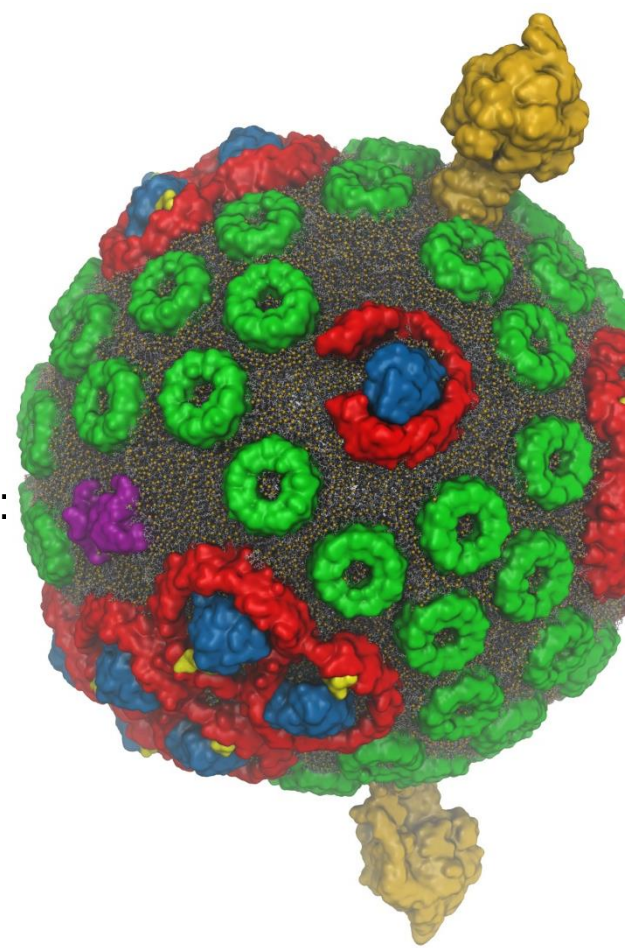
VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster



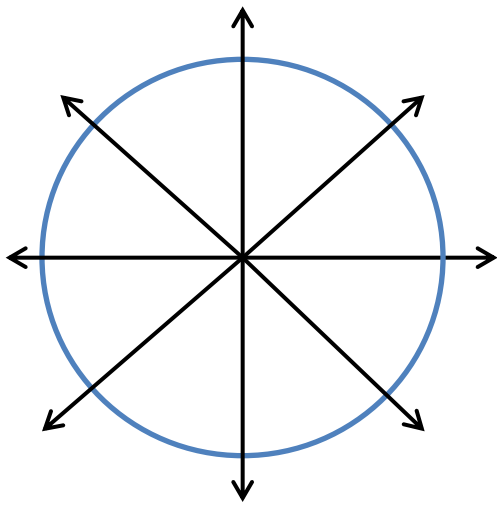
VMD 1.9.3 + OptiX 3.8 + CUDA 7.0

~1.5x Performance Increase

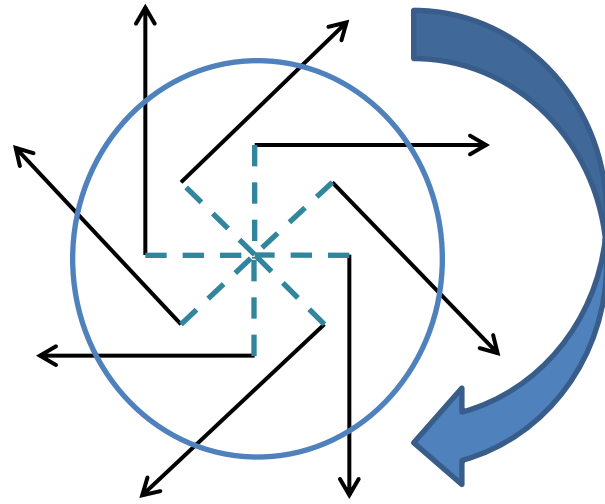
- OptiX GPU-native “**Trbv**h” **acceleration structure builder** yields substantial perf increase vs. CPU builders running on Opteron 6276 CPUs
- New optimizations in VMD TachyonL-OptiX RT engine:
 - **CUDA C++ Template specialization of RT kernels**
 - Combinatorial expansion of ray-gen and shading 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.

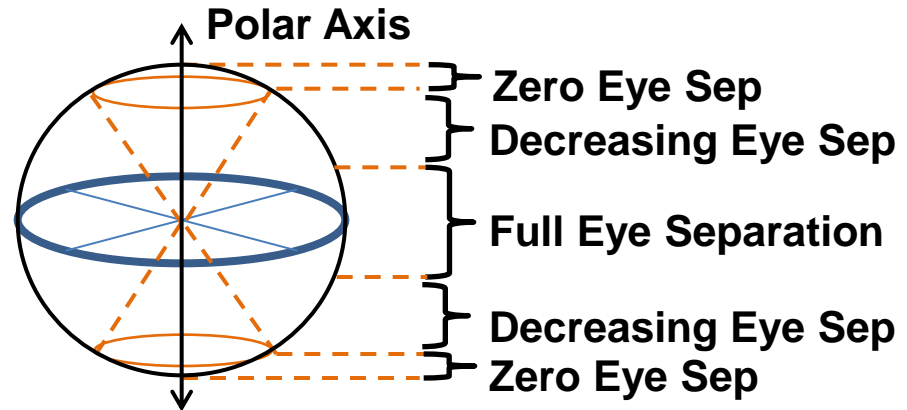


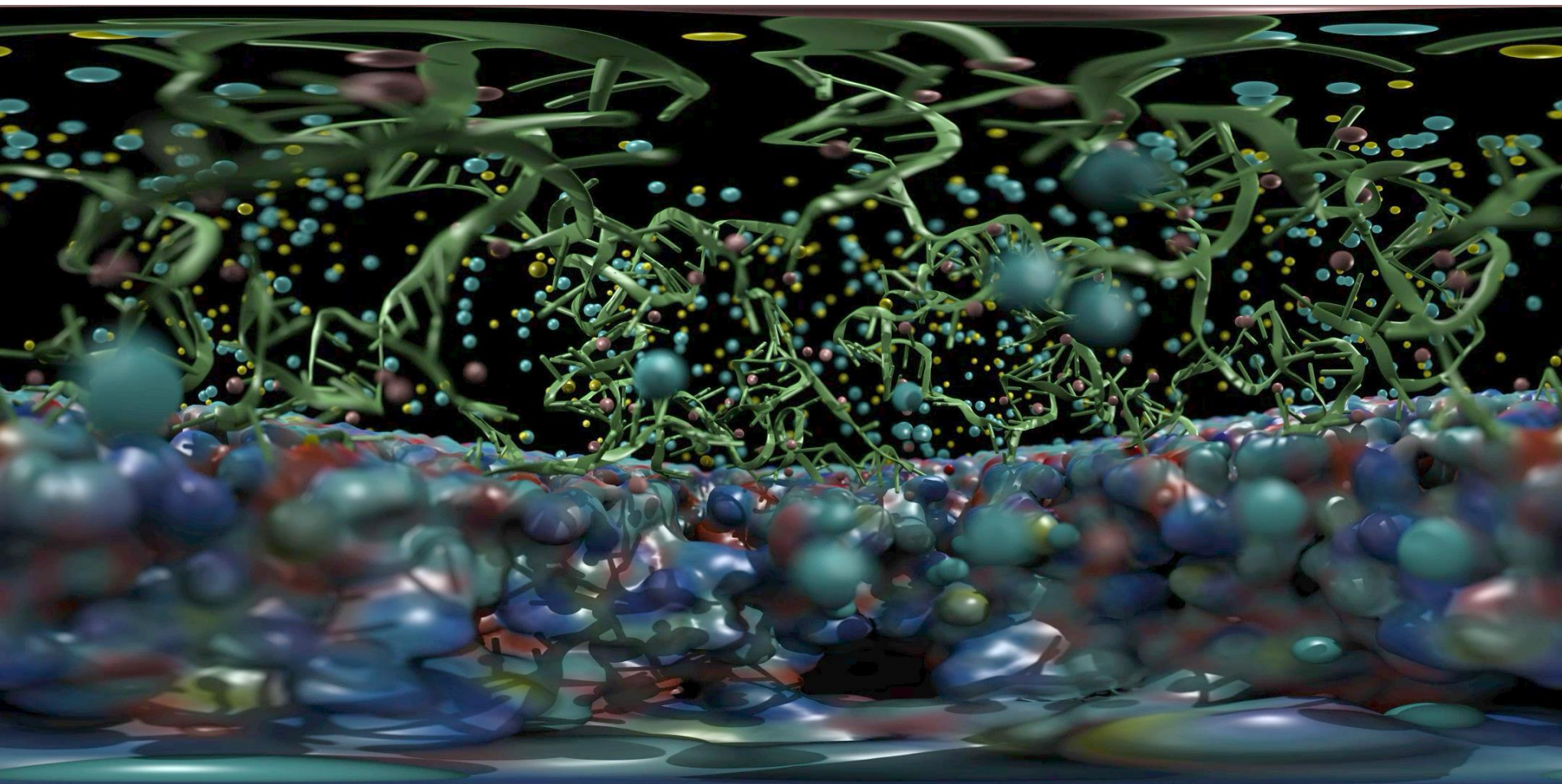
**A) Monoscopic circular projection.
Eye at center of projection (COP).**

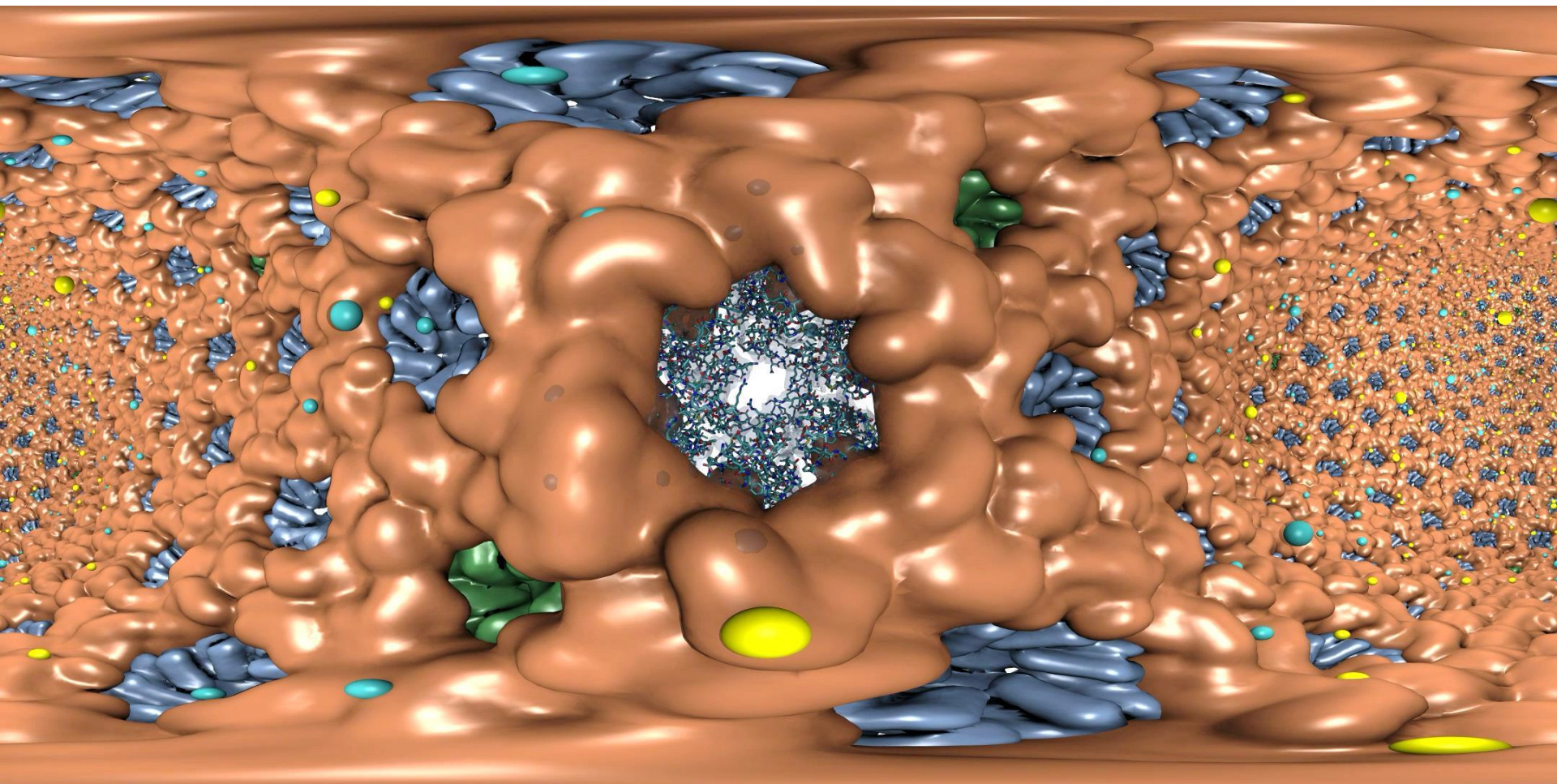


**B) Left eye stereo circular projection.
Eye offset from COP by half of interocular distance.**

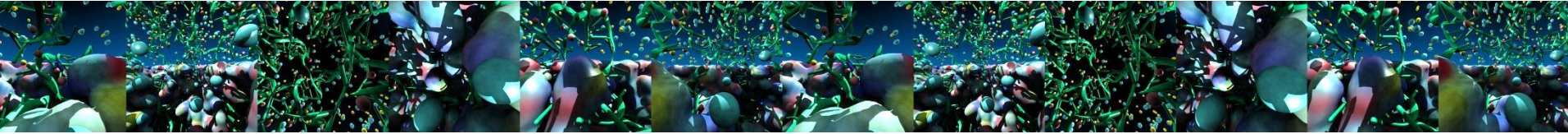
C) Stereo eye separation smoothly decreased to zero at zenith and nadir points on the polar axis to prevent incorrect stereo when HMD sees the poles.



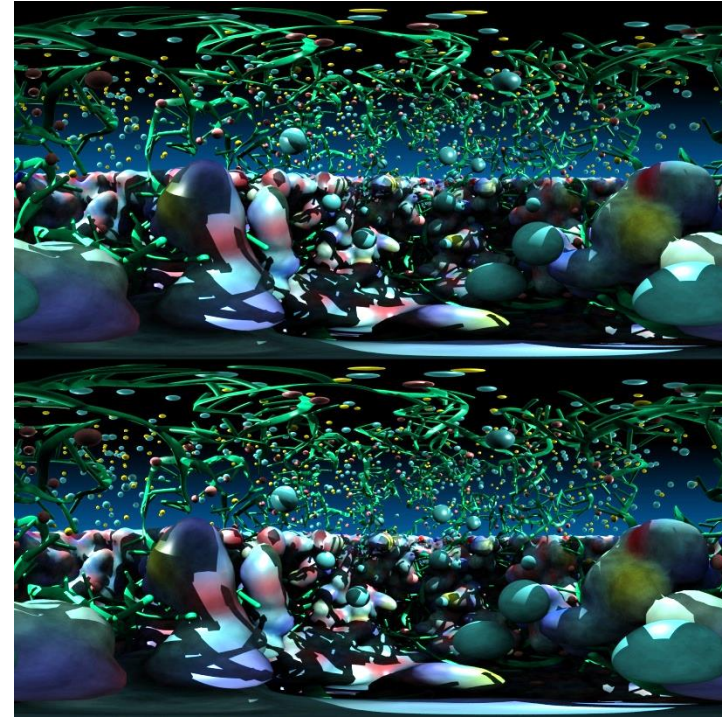


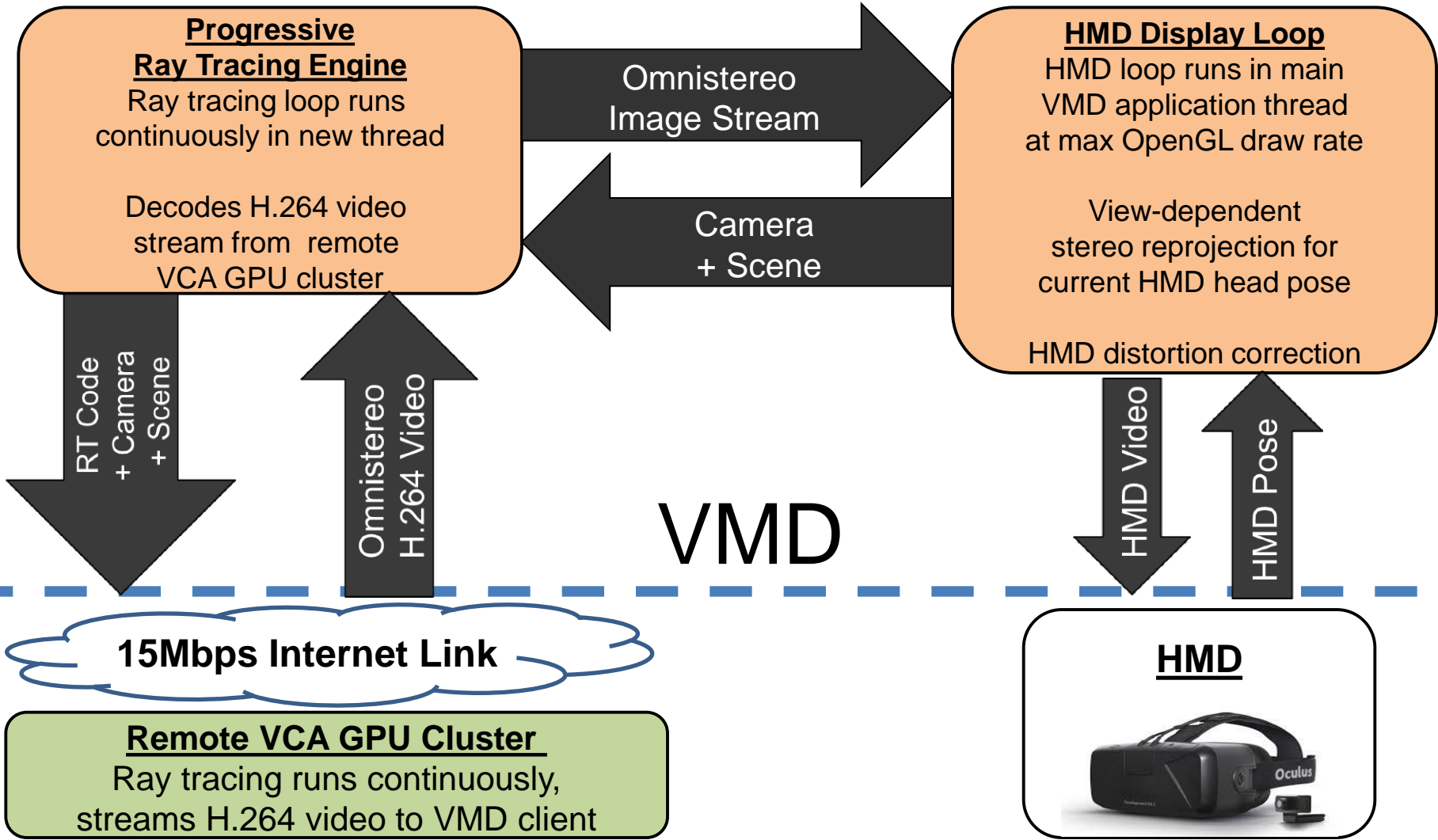


Stereoscopic Panorama Ray Tracing w/ OptiX



- **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**





Remote Omnidirectional Stereoscopic RT Performance @ 3072x1536 w/ 2-subframes

Scene	Per-subframe samples AA : AO (AO per-hit)	RT update rate (FPS)
STMV shadows	1:0	22.2
	2:0	18.1
	4:0	10.3
STMV Shadows+AO	1:1	18.2
	1:2	16.1
	1:4	12.4
STMV Shadows+AO+DoF	1:1	16.1
	2:1	11.1
	2:2	8.5
HIV-1 Shadows	1:0	20.1
	2:0	18.1
	4:0	10.2
HIV-1 Shadows+AO	1:1	17.4
	1:2	12.2
	1:4	8.1

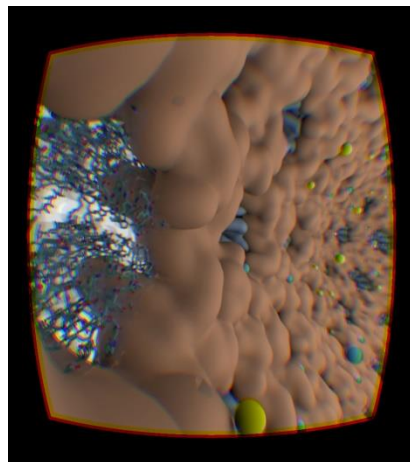
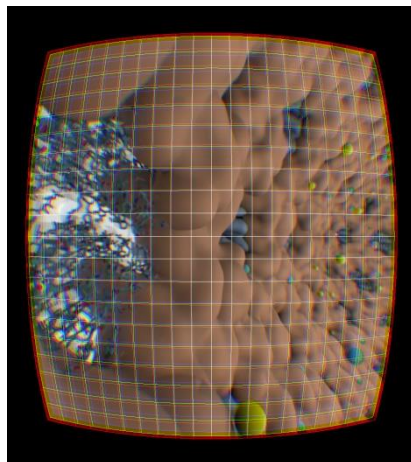
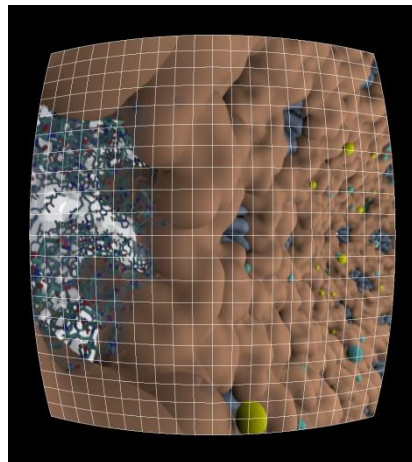
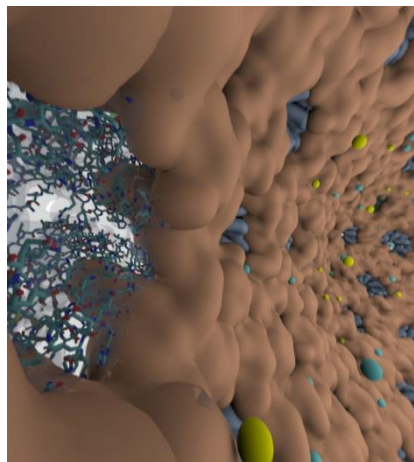
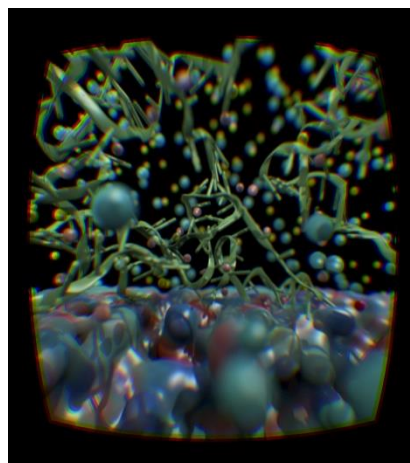
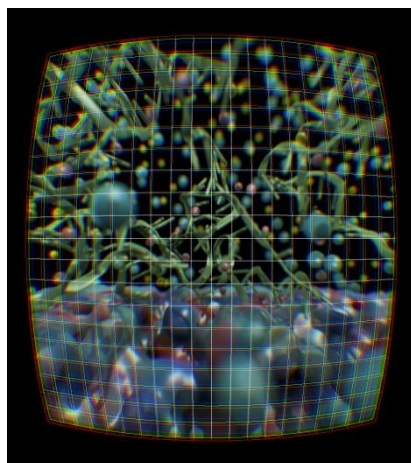
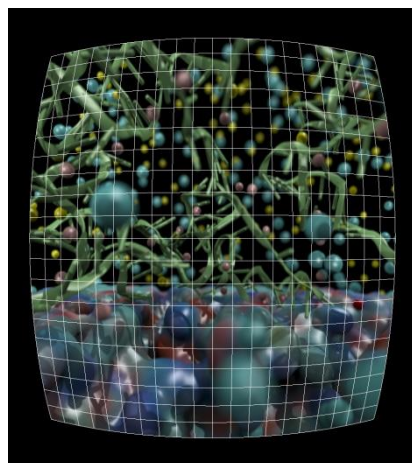
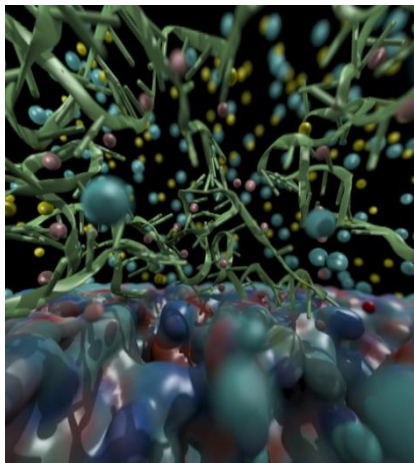
HMD View-Dependent Reprojection with OpenGL

- 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, high-frame-rate redraw** as HMD head pose changes (150Hz or more)



VMD can support a variety of HMD lens designs, e.g.
<http://research.microsoft.com/en-us/um/redmond/projects/lensfactory/oculus/>





Future Work

- Support for more commodity HMDs as they become generally available
- Support for OSes besides Linux
- Ray tracing engine and optimizations:
 - **Multi-node parallel RT and remote viz. on general clusters and supercomputers, e.g. NCSA Blue Waters, ORNL Titan**
 - Interactive RT stochastic sampling strategies to improve interactivity
 - Improved omnidirectional cubemap/spheremap sampling approaches
- Tons of work to do on VR user interfaces, multi-user collaborative visualization, ...



Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- **Bill Sherman at Indiana University**
- NVIDIA OptiX and CUDA teams
- NCSA Blue Waters, ORNL OCLF Titan teams
- NVIDIA CUDA Center of Excellence, University of Illinois at Urbana-Champaign
- Funding:
 - NSF Blue Waters:
NSF OCI 07-25070, PRAC “The Computational Microscope”,
ACI-1238993, ACI-1440026
 - DOE INCITE, ORNL Titan: DE-AC05-00OR22725
 - NIH support: 9P41GM104601, 5R01GM098243-02





NIH BTRC for Macromolecular Modeling and Bioinformatics

1990-2017

Beckman Institute
University of Illinois at
Urbana-Champaign



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)**
- **High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL.** John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
- **Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads.** John E. Stone, Michael J. Hallock, James C. Phillips, Joseph R. Peterson, Zaida Luthey-Schulten, and Klaus Schulten. 25th International Heterogeneity in Computing Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
- **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, 2016. **(In-press)**
- **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.

Related Publications

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

- **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, 2014. **(In press)**
- **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.

Related Publications

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

- **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

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

- **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. 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.