VMD+OptiX: Bringing Interactive Molecular Ray Tracing from Remote GPU Clusters to your VR Headset

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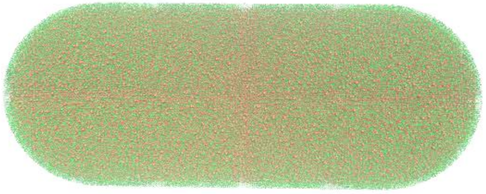
3:30pm, Wednesday Nov 18, 2015

NVIDIA GTC Theater, NVIDIA Booth #1021,

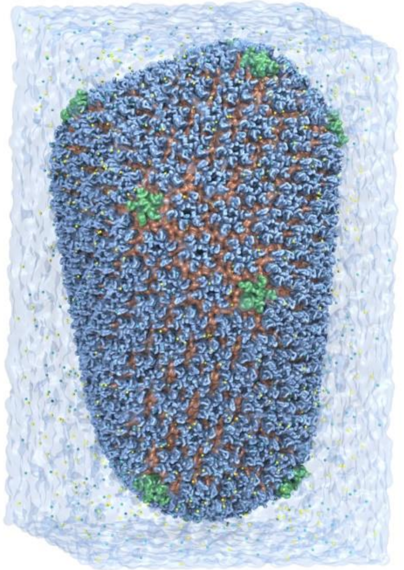
Supercomputing 2015, Austin, TX

VMD – “Visual Molecular Dynamics”

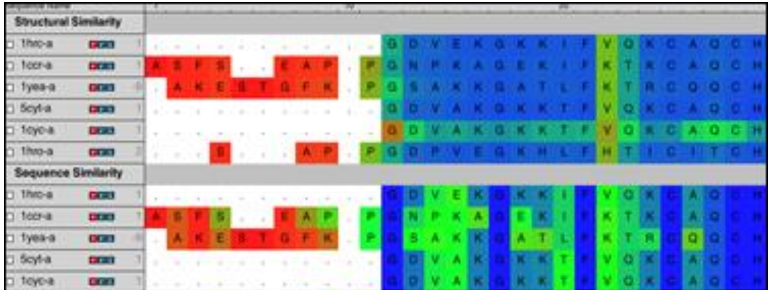
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



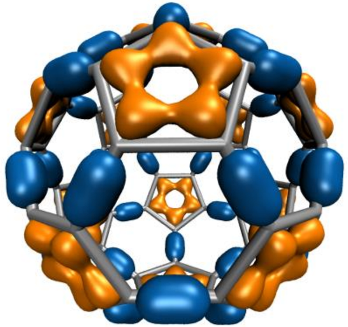
Whole Cell Simulation



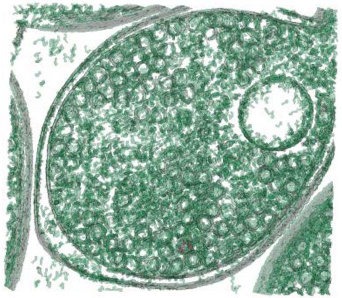
MD Simulations



Sequence Data



Quantum Chemistry

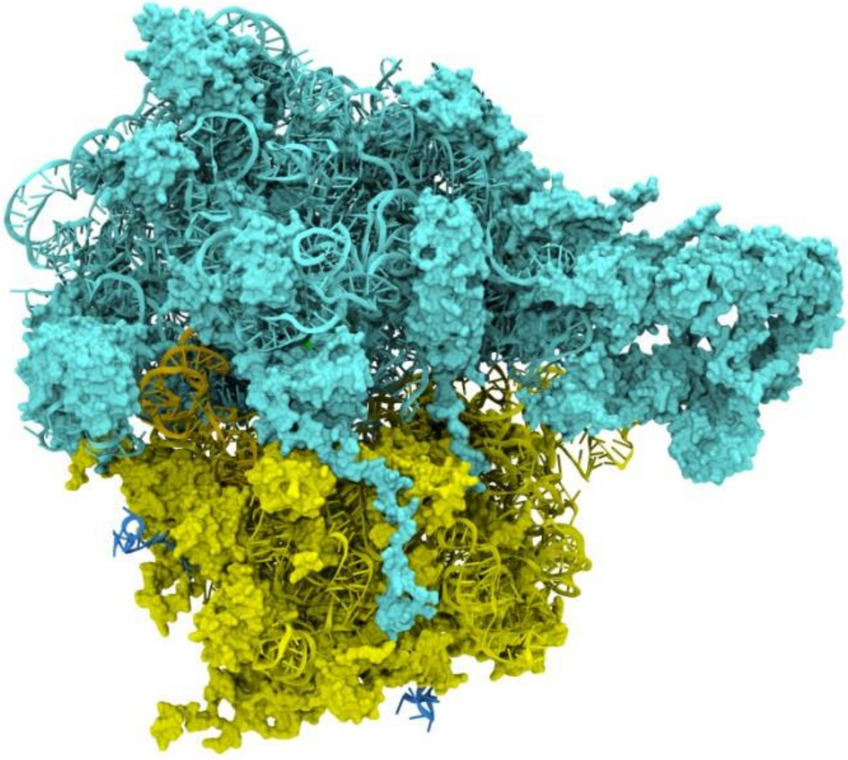


CryoEM, Cellular Tomography

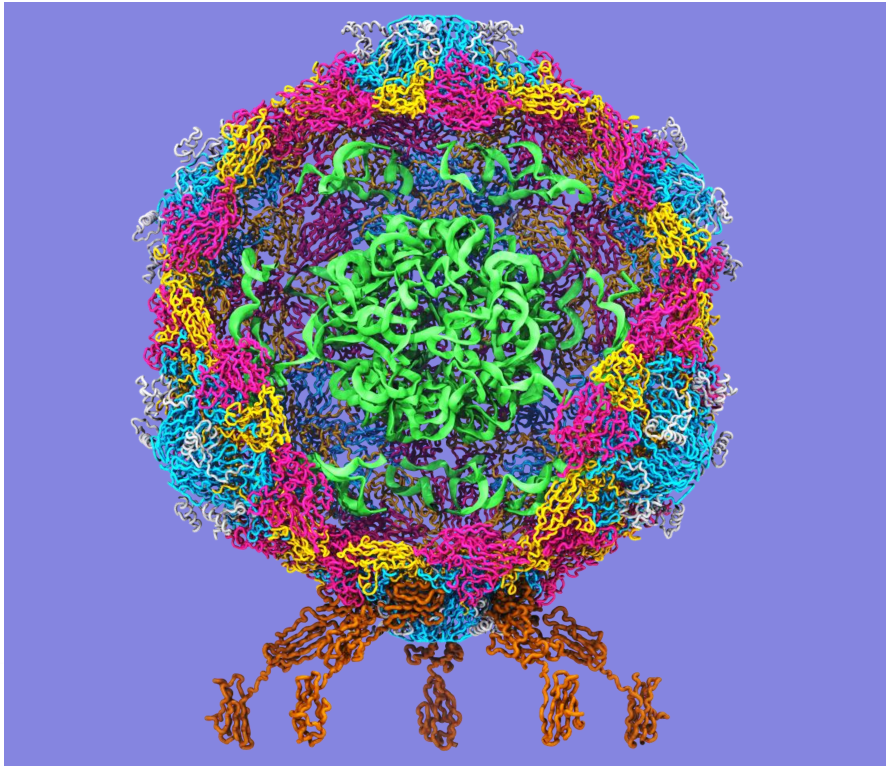
Goal: A Computational Microscope

Study the molecular machines in living cells

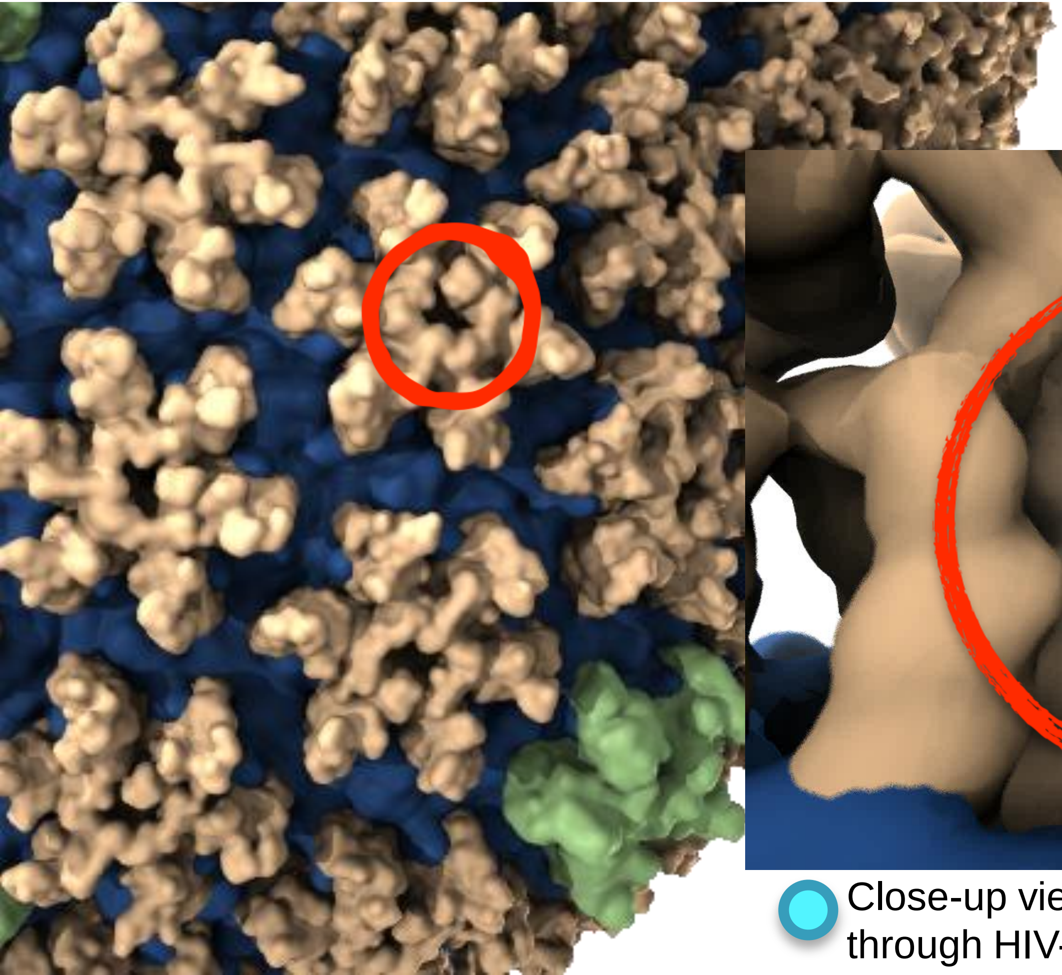
Ribosome: target for antibiotics



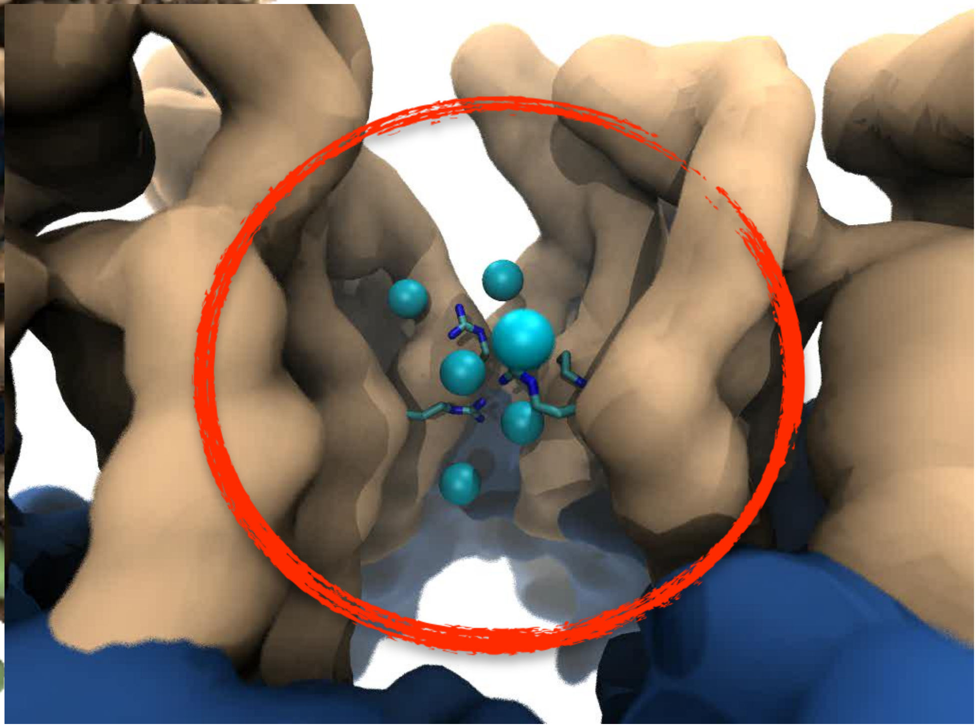
Poliovirus



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

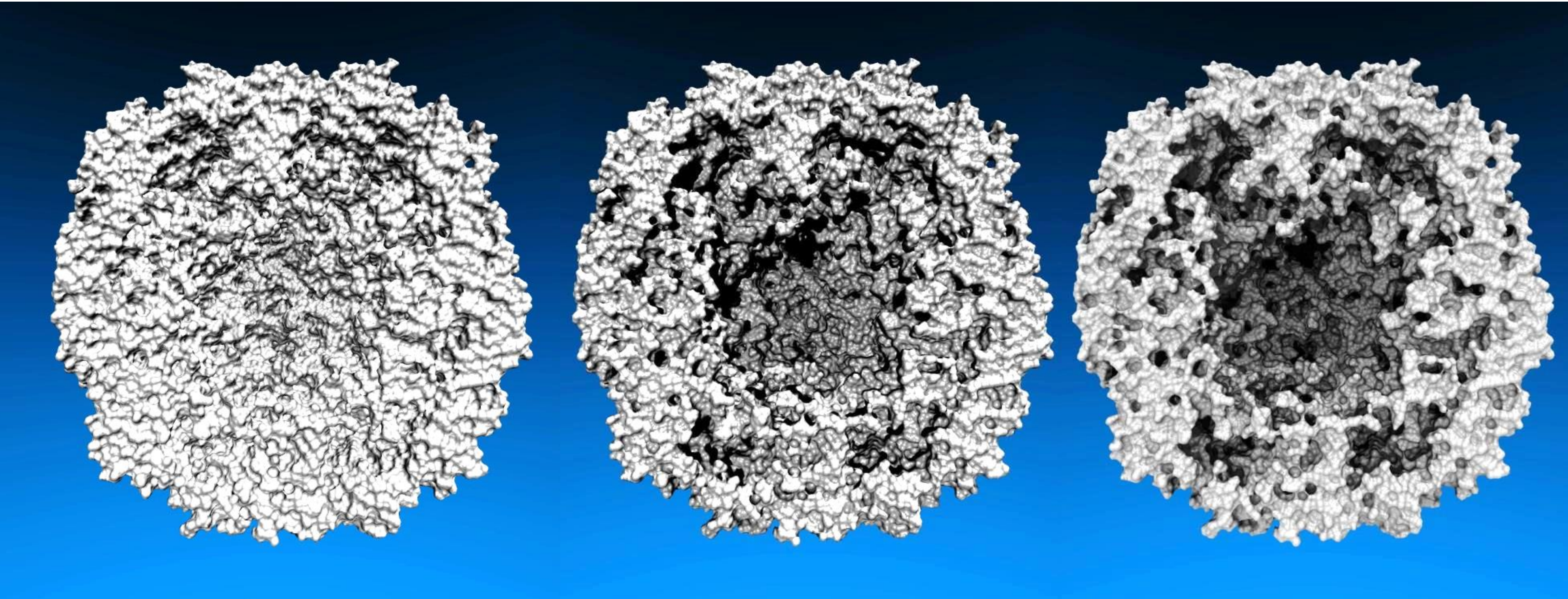
Immersive Viz. w/ VMD

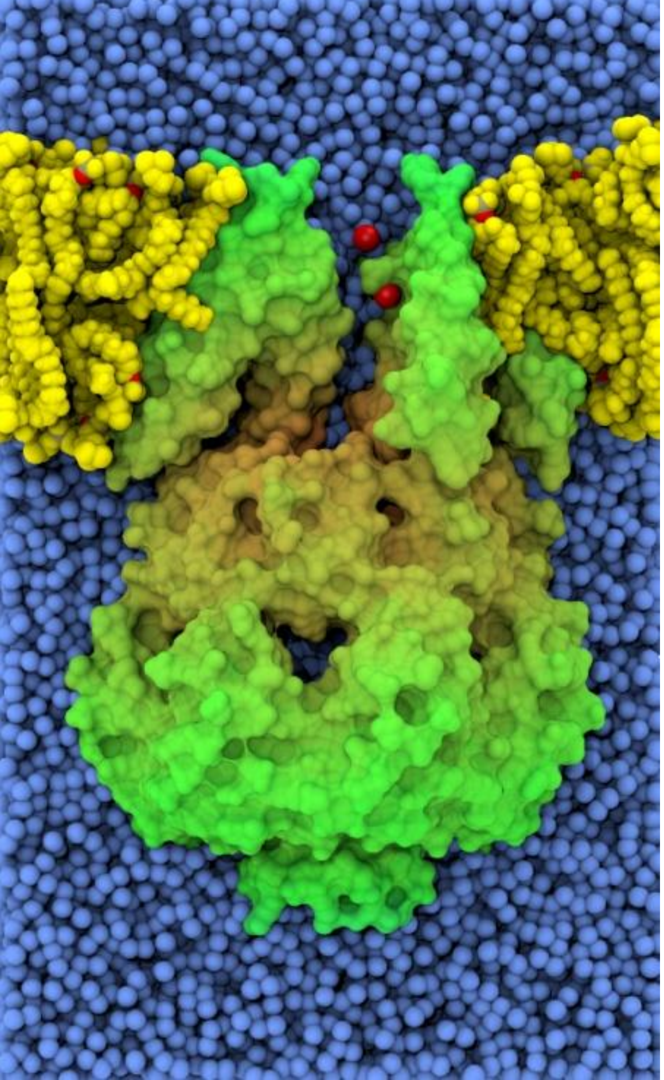
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability, convenience
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support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

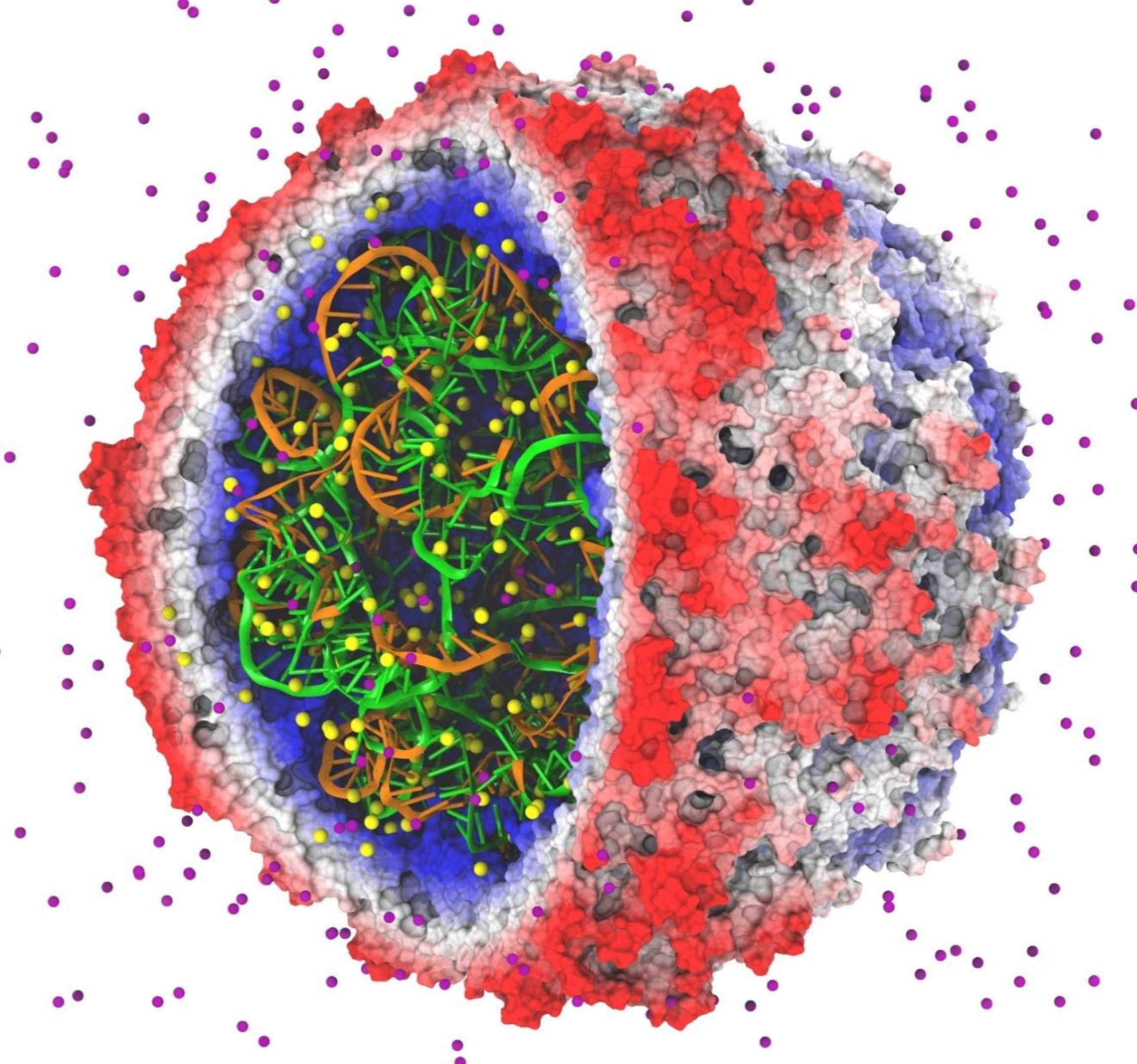
VMD running in a CAVE w/ VR Juggler

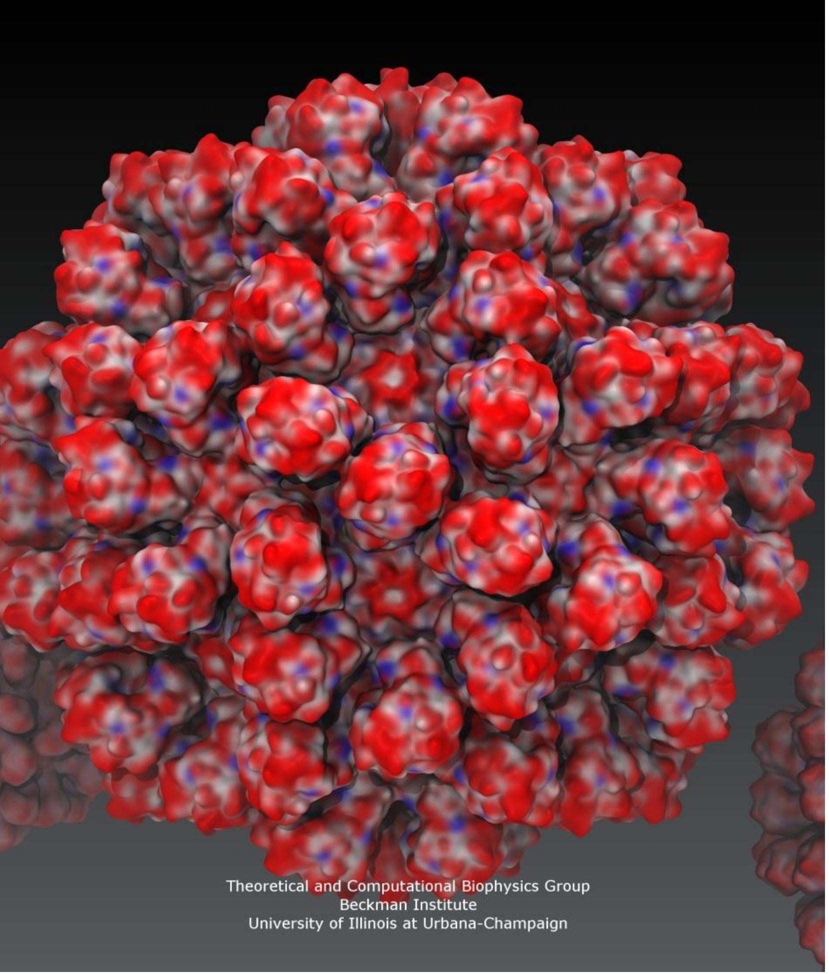
Lighting Comparison

Two lights, no shadows	Two lights, hard shadows, 1 shadow ray per light	Ambient occlusion + two lights, 144 AO rays/hit





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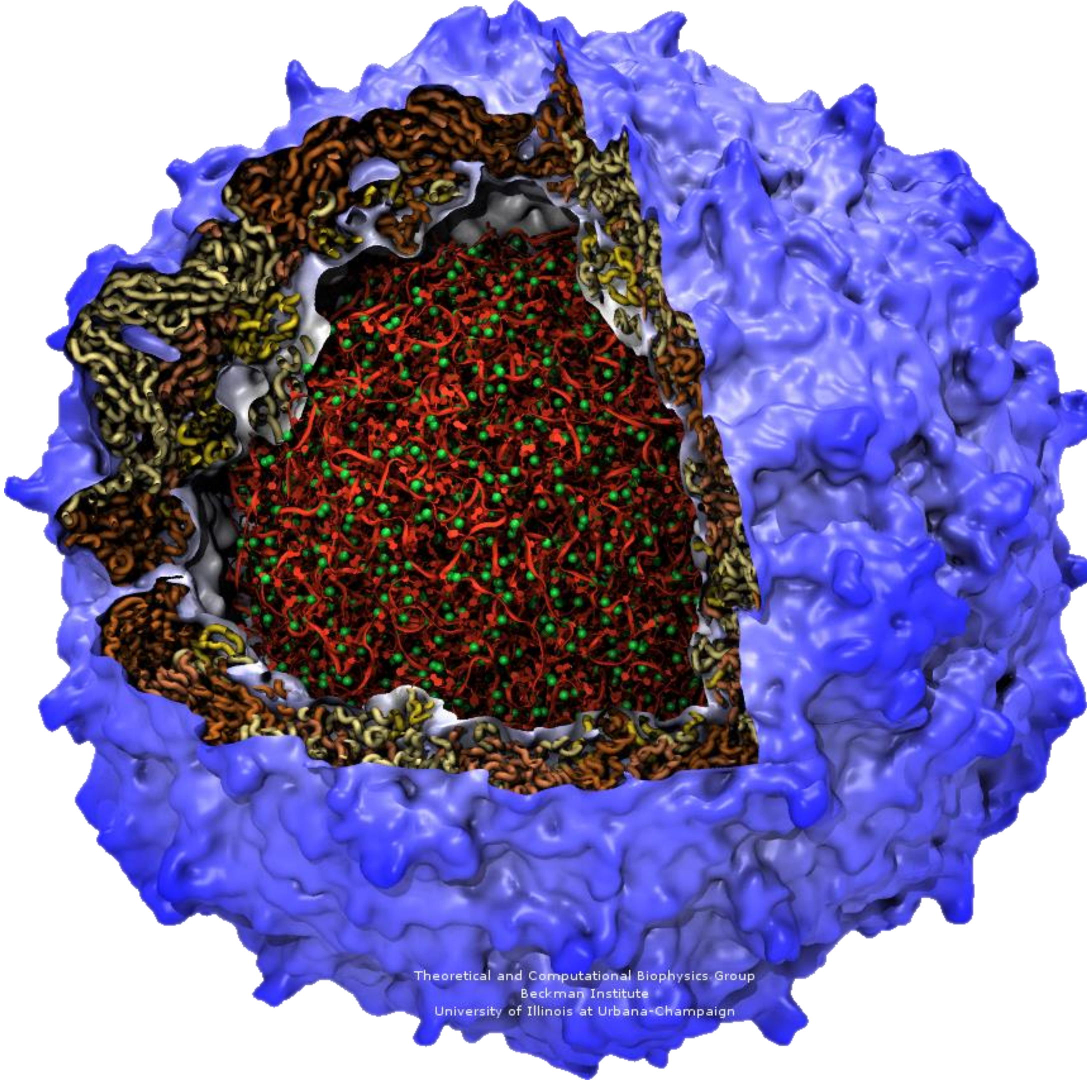
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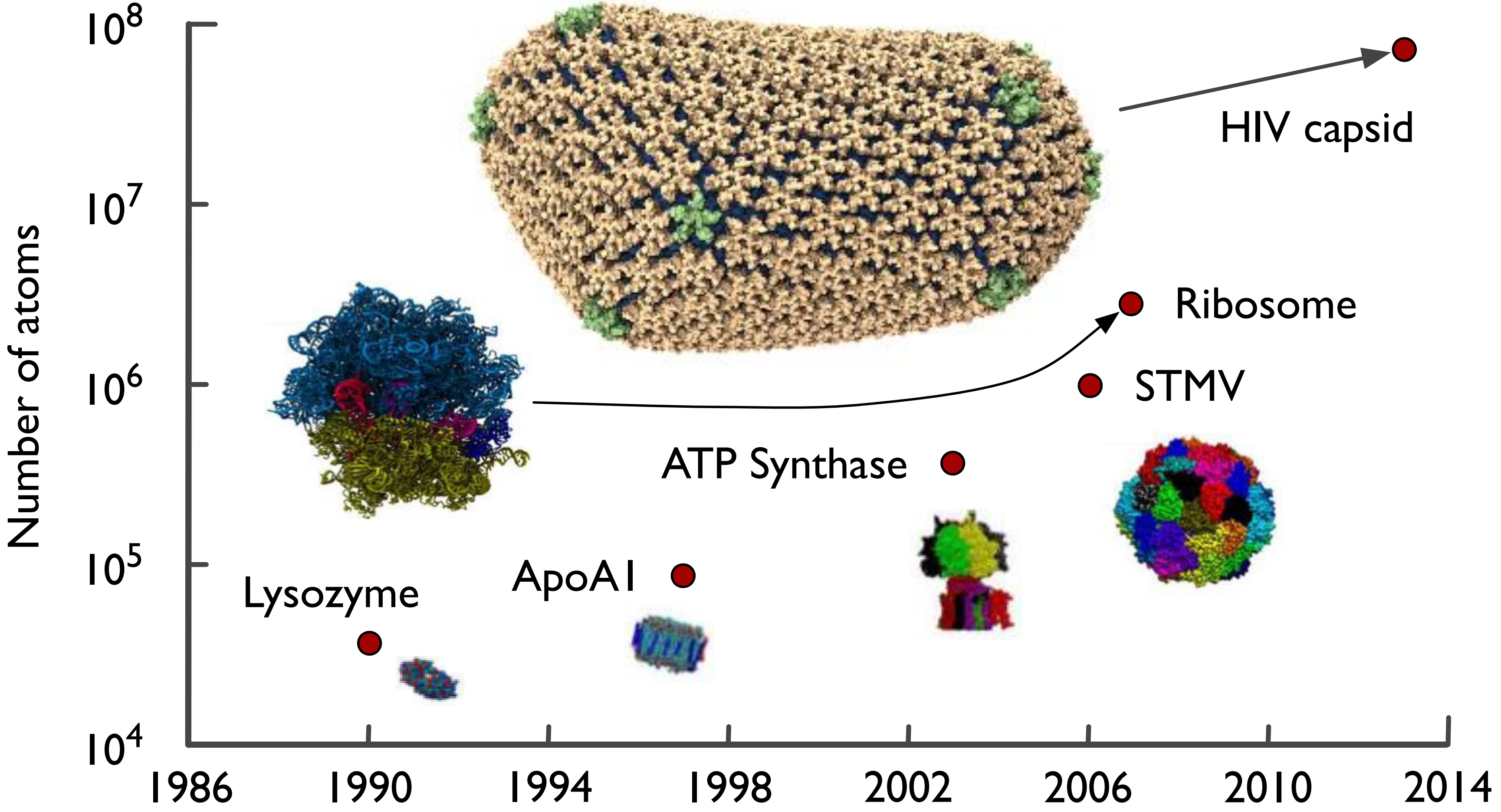
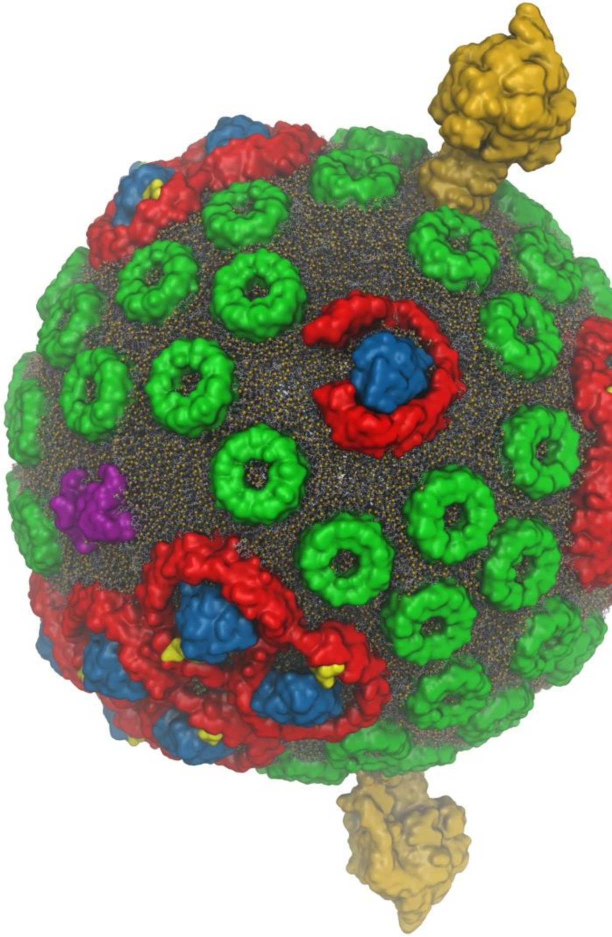
Computational Biology's Insatiable Demand for Processing Power

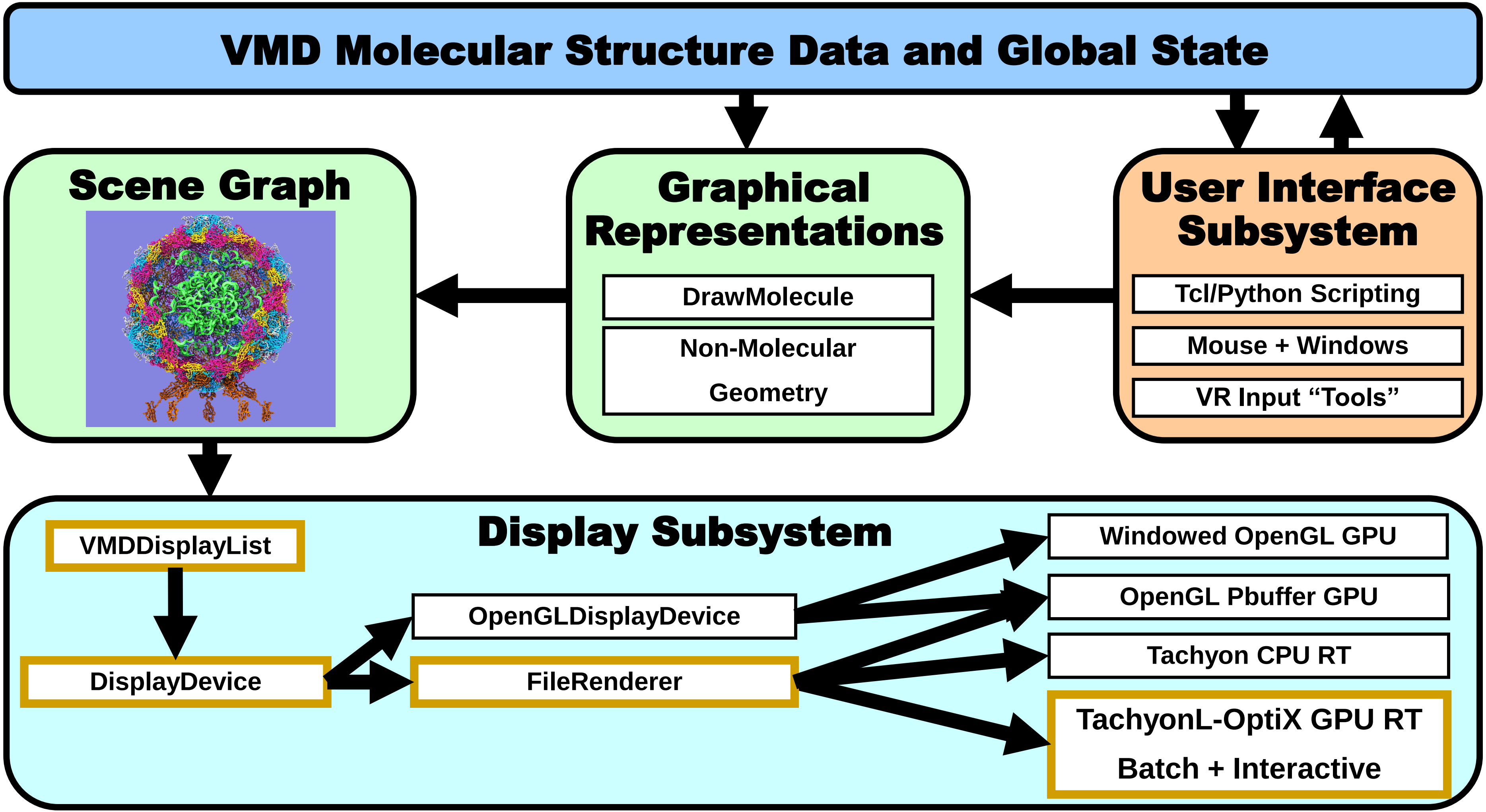


VMD 1.9.3 + OptiX 3.8 + CUDA 7.0
~1.5x Performance Increase

- 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**



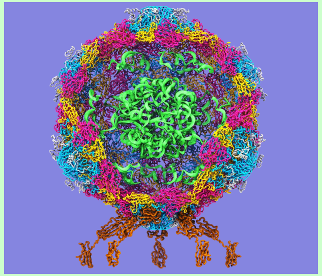
VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.



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

Scene Graph



TrBvh RT Acceleration Structure

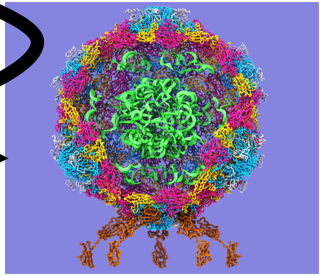
RT Progressive Subframe

rtContextLaunchProgressive2D()

Check for User Interface Inputs, Update OptiX Variables

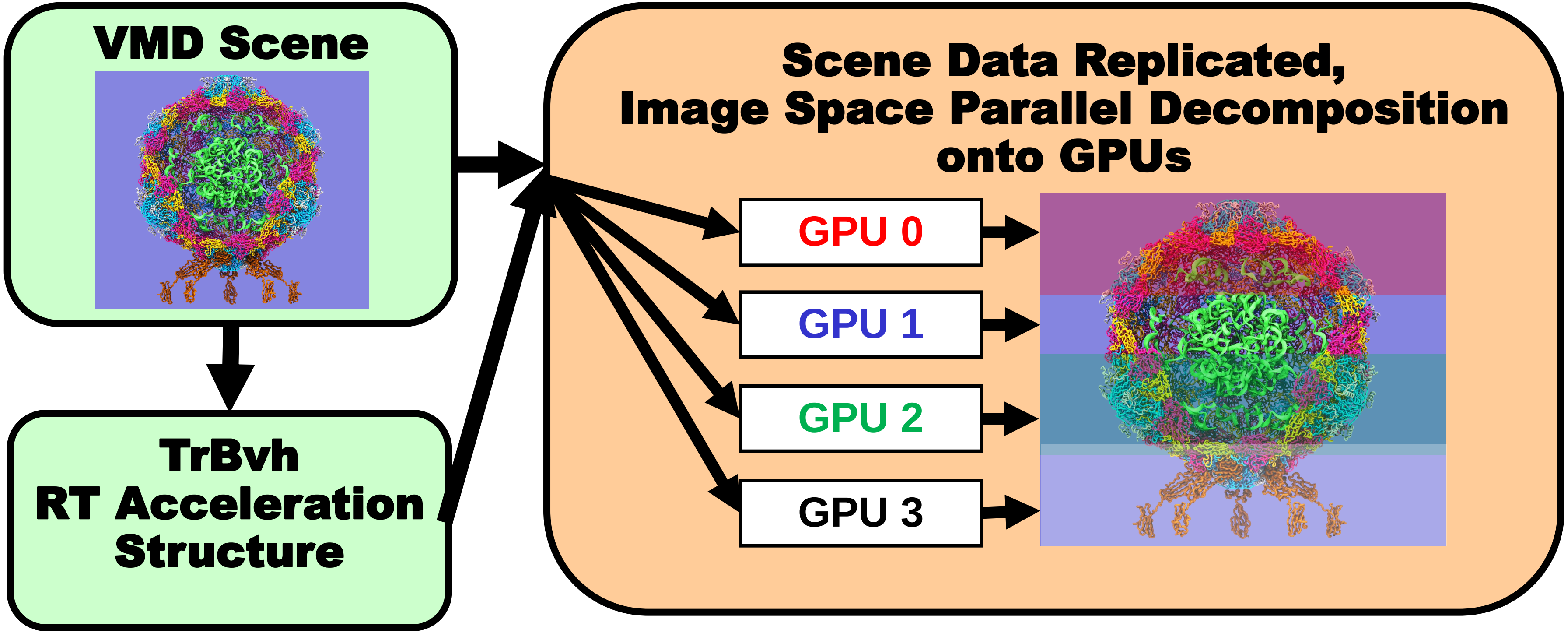
rtBufferGetProgressiveUpdateReady()

rtContextStopProgressive()



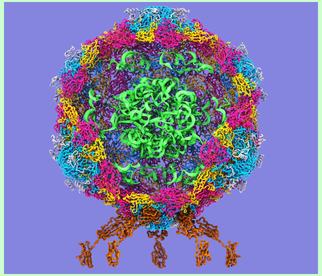
Draw Output Framebuffer

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



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

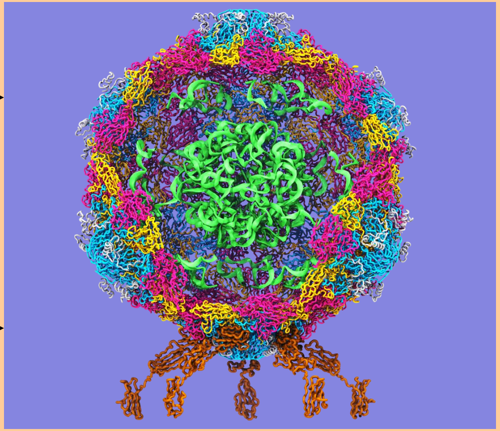
VMD Scene



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

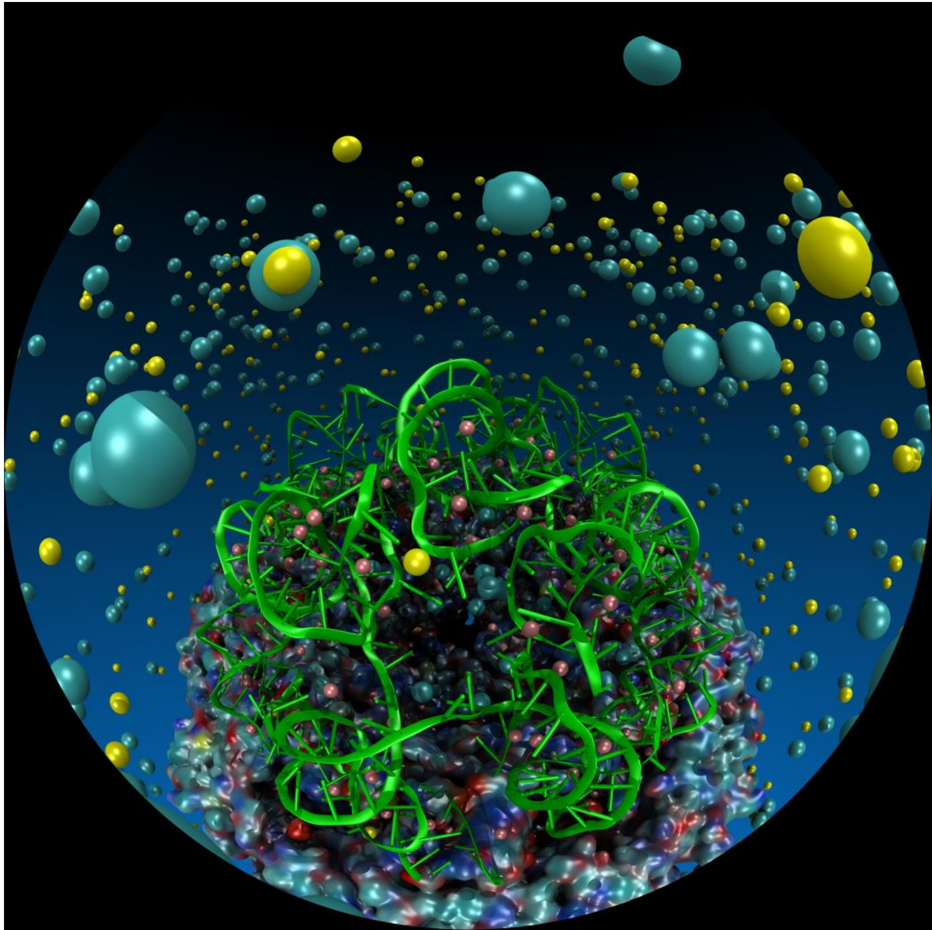
VCA 0:
8 K6000 GPUs

VCA N:
8 K6000 GPUs

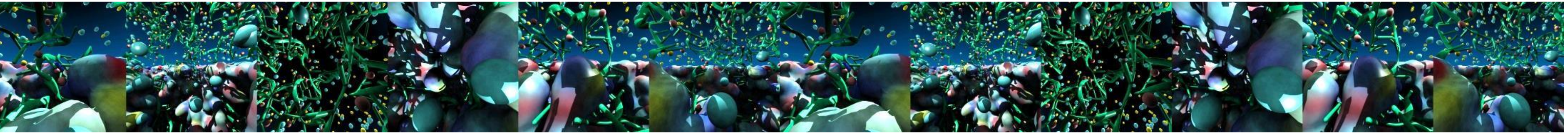


VMD Planetarium Dome Master Camera

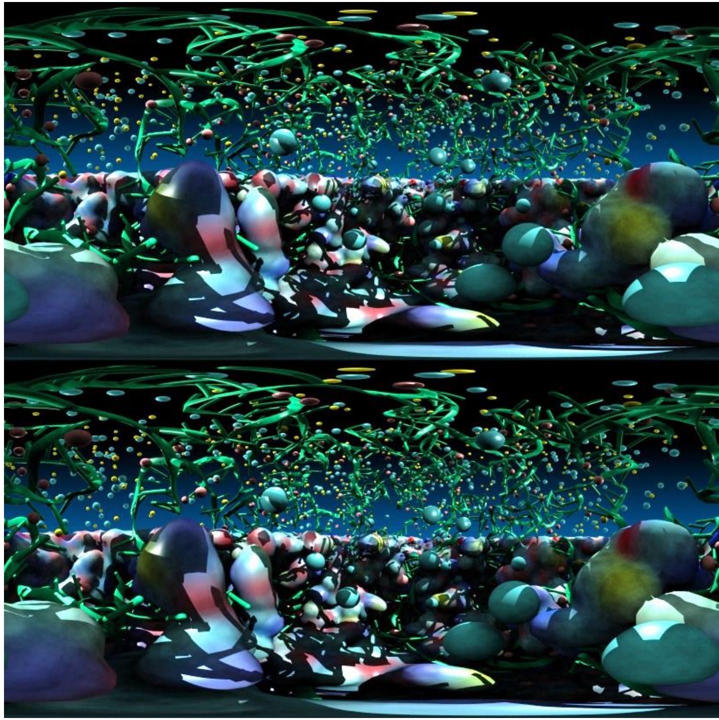
- RT-based dome projection -- rasterization poorly suited to non-planar projections
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required



Stereoscopic Panorama Ray Tracing w/ OptiX

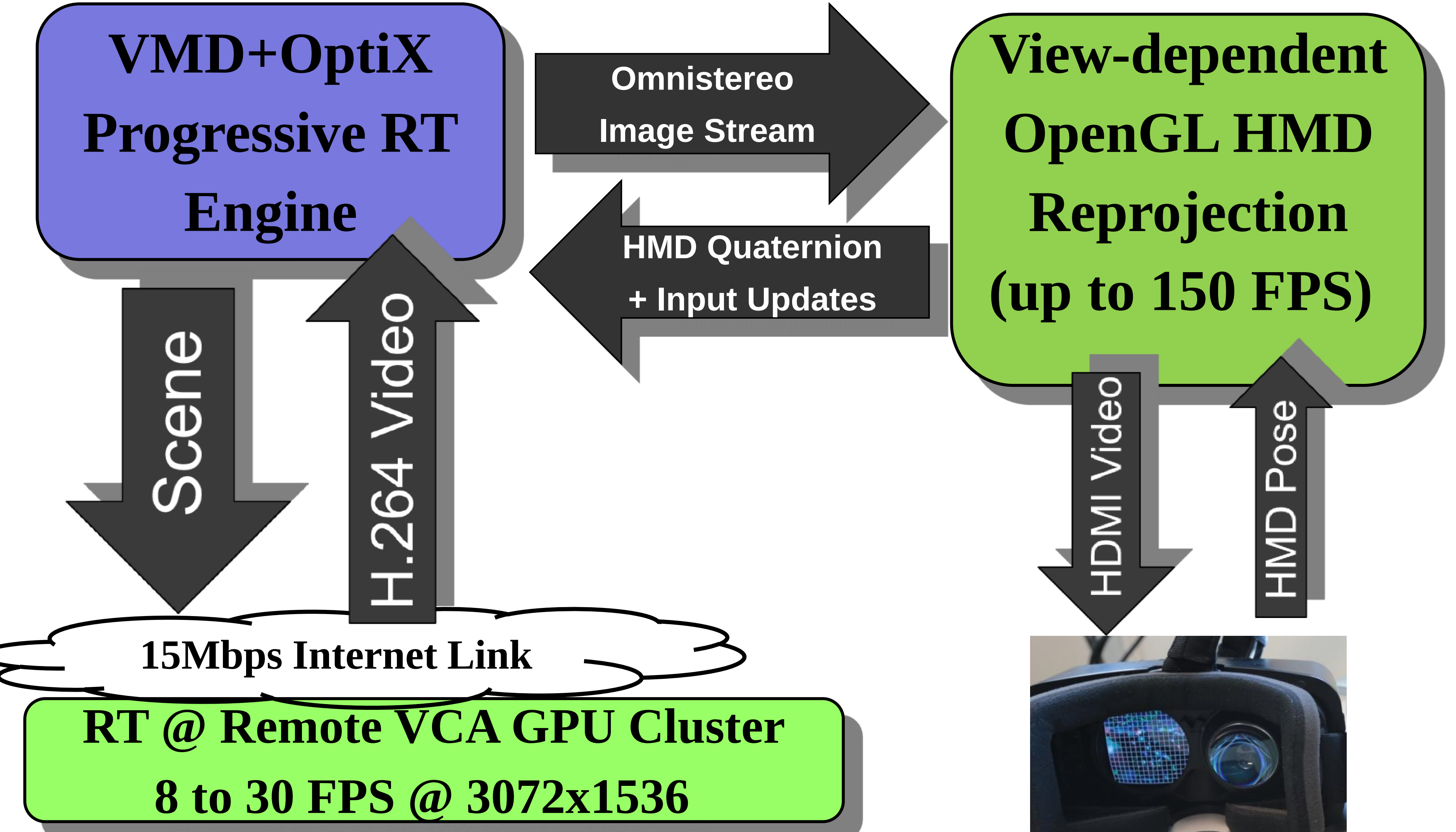


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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


VMD+OptiX Progressive RT Engine
Omnistereo Image Stream
HMD Quaternion + Input Updates
View-dependent OpenGL HMD Reprojection (up to 150 FPS)
Scene
H.264 Video
HDMI Video
HMD Pose
15Mbps Internet Link
RT @ Remote VCA GPU Cluster
8 to 30 FPS @ 3072x1536

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

VMD can support a variety of HMD lens designs, e.g.

http://research.microsoft.com/en-us/um/redmond/projects/lensfactory/oculus/

Come See A Live Demo!

- Demo shown by collaborators in Indiana U. booth on and off throughout exhibition
- RT @ NVIDIA VCA cluster in Santa Clara, thousands of miles away
- Work-in-progress:
  - 6DOF controller UI
  - Alternative HMD lens designs

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

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 SchultenSC'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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