VMD+OptiX: Bringing Interactive Molecular 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/

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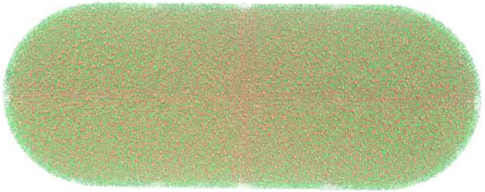
NVIDIA GTC Theater, NVIDIA Booth #1021,

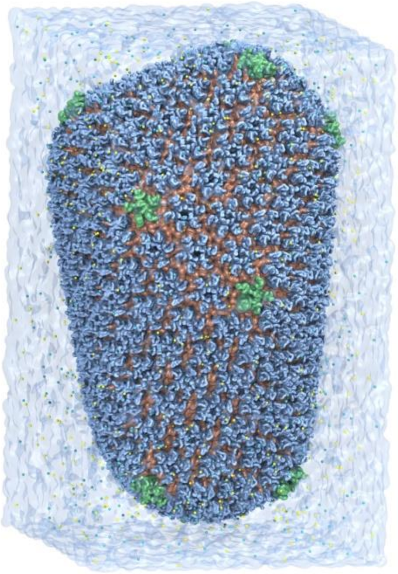
Supercomputing 2015, Austin, TX

VMD – “Visual Molecular Dynamics”

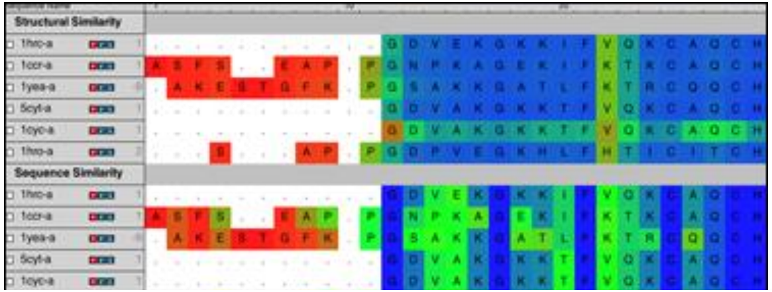
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



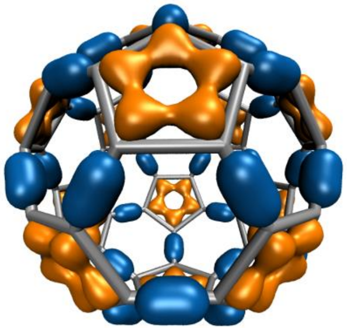
Whole Cell Simulation



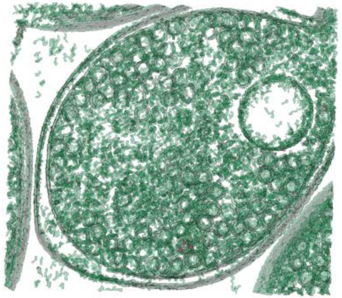
MD Simulations



Sequence Data



Quantum Chemistry

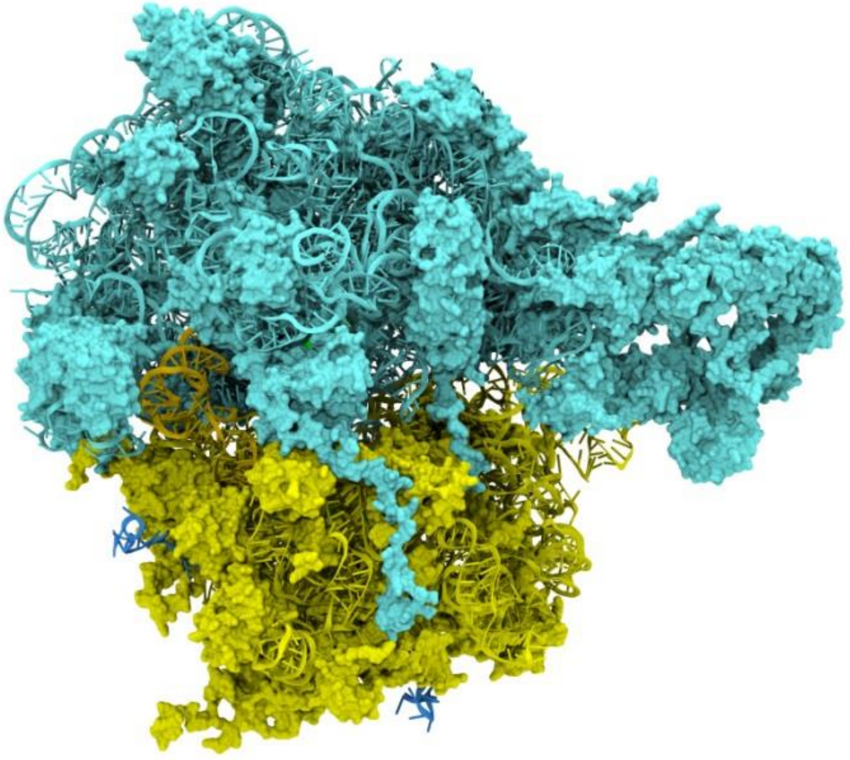


CryoEM, Cellular Tomography

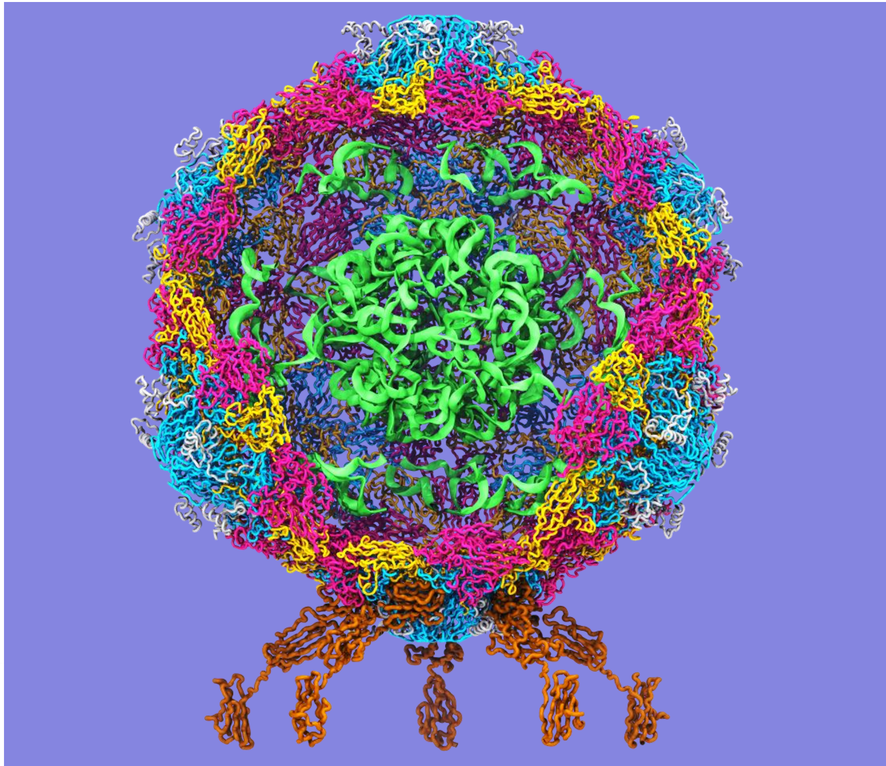
Goal: A Computational Microscope

Study the molecular machines in living cells

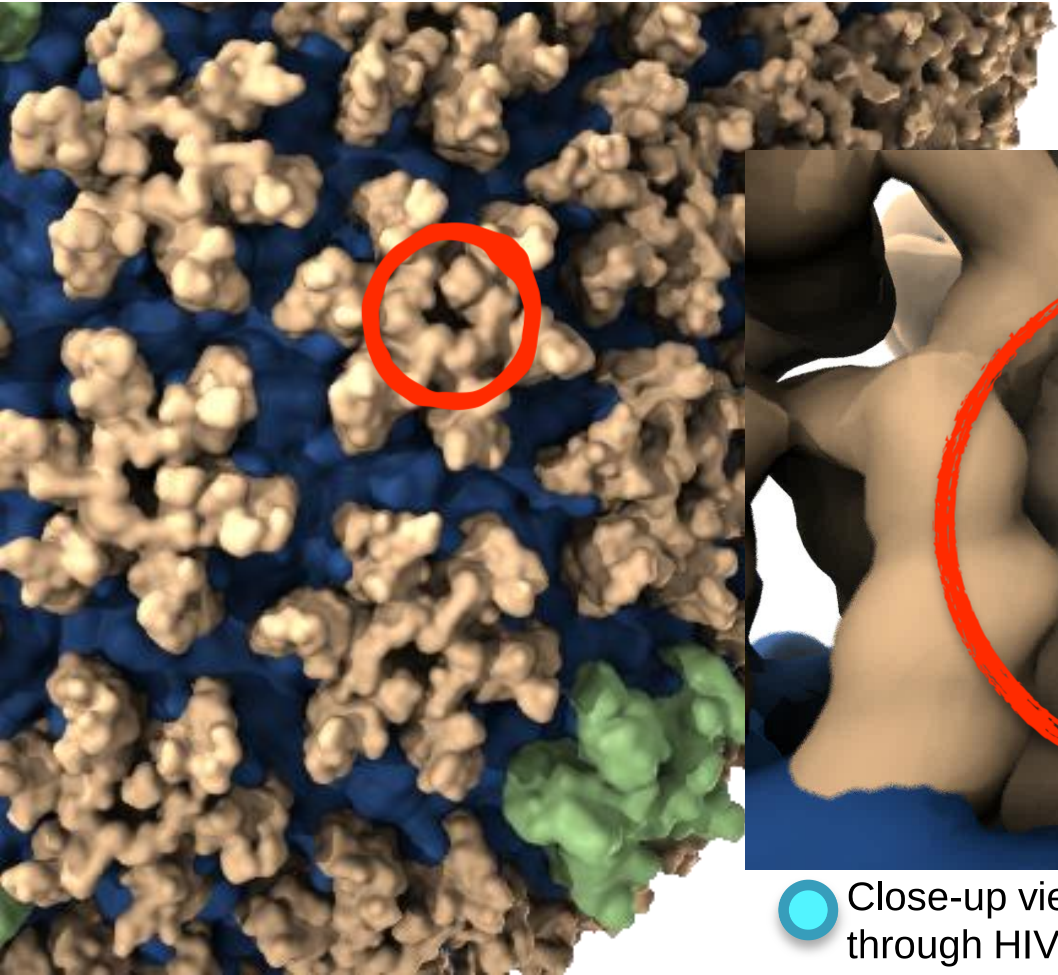
Ribosome: target for antibiotics



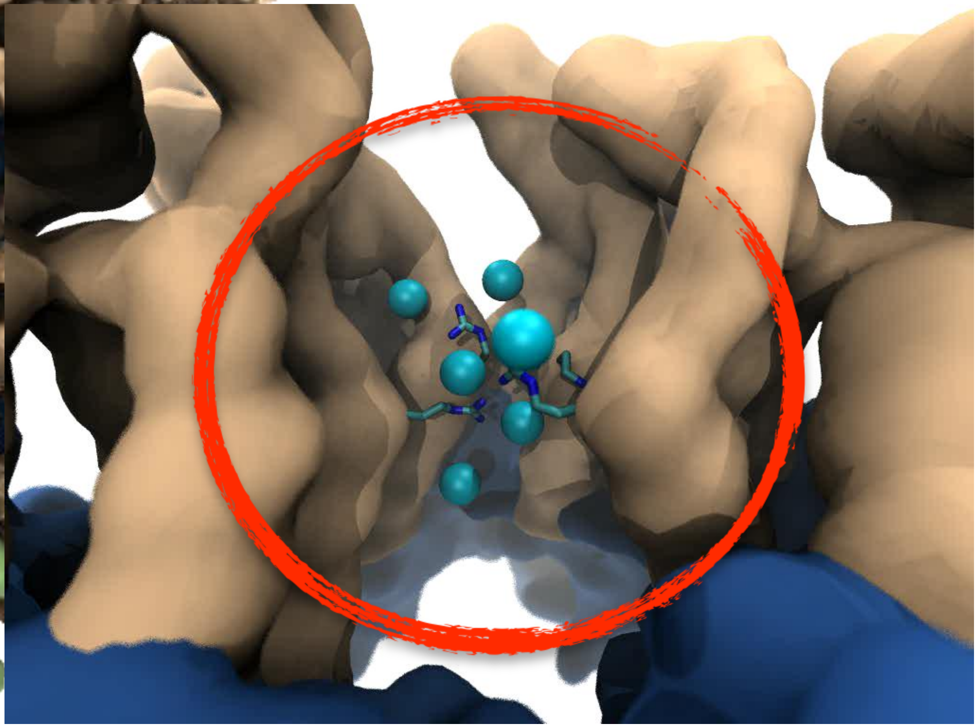
Poliovirus



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

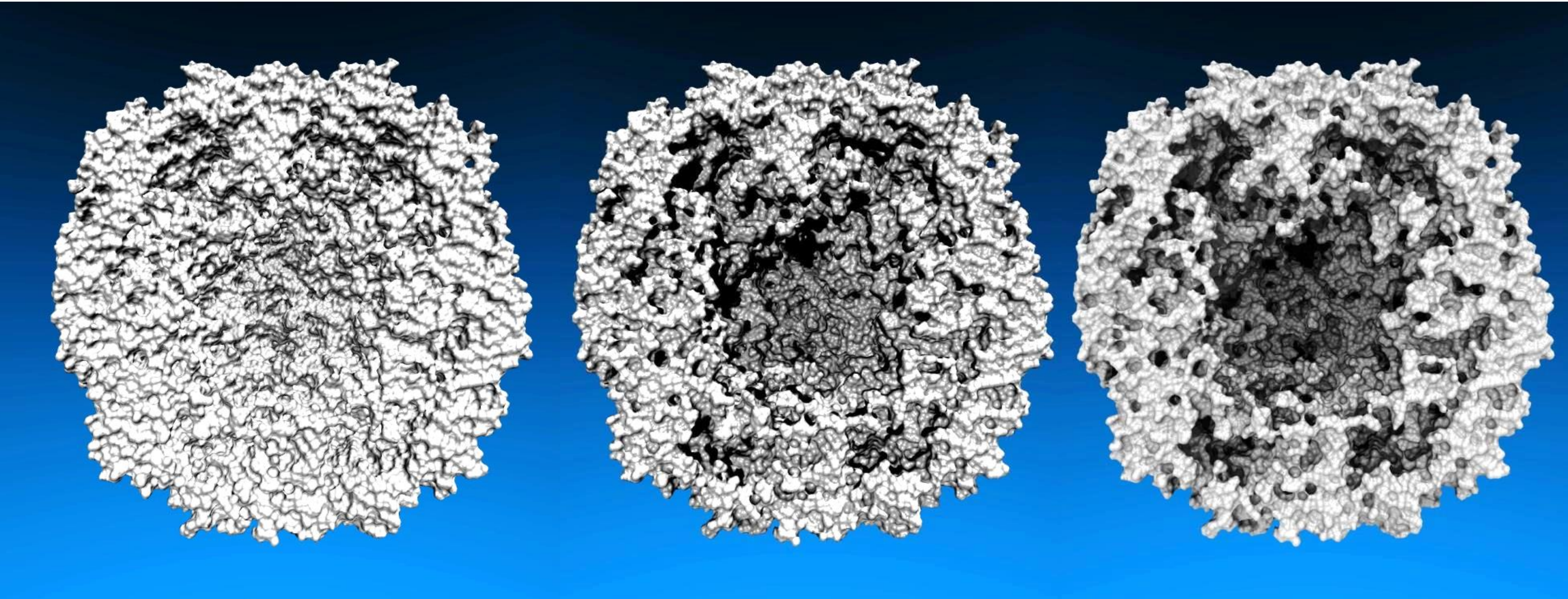
VMD running in a CAVE w/ VR Juggler

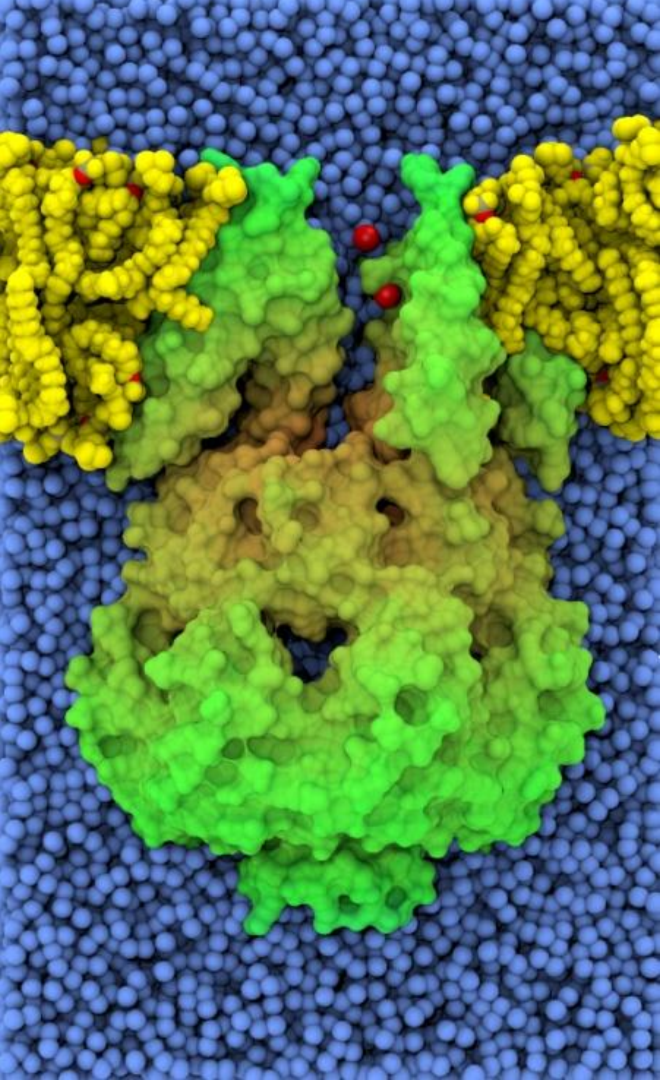
Lighting Comparison

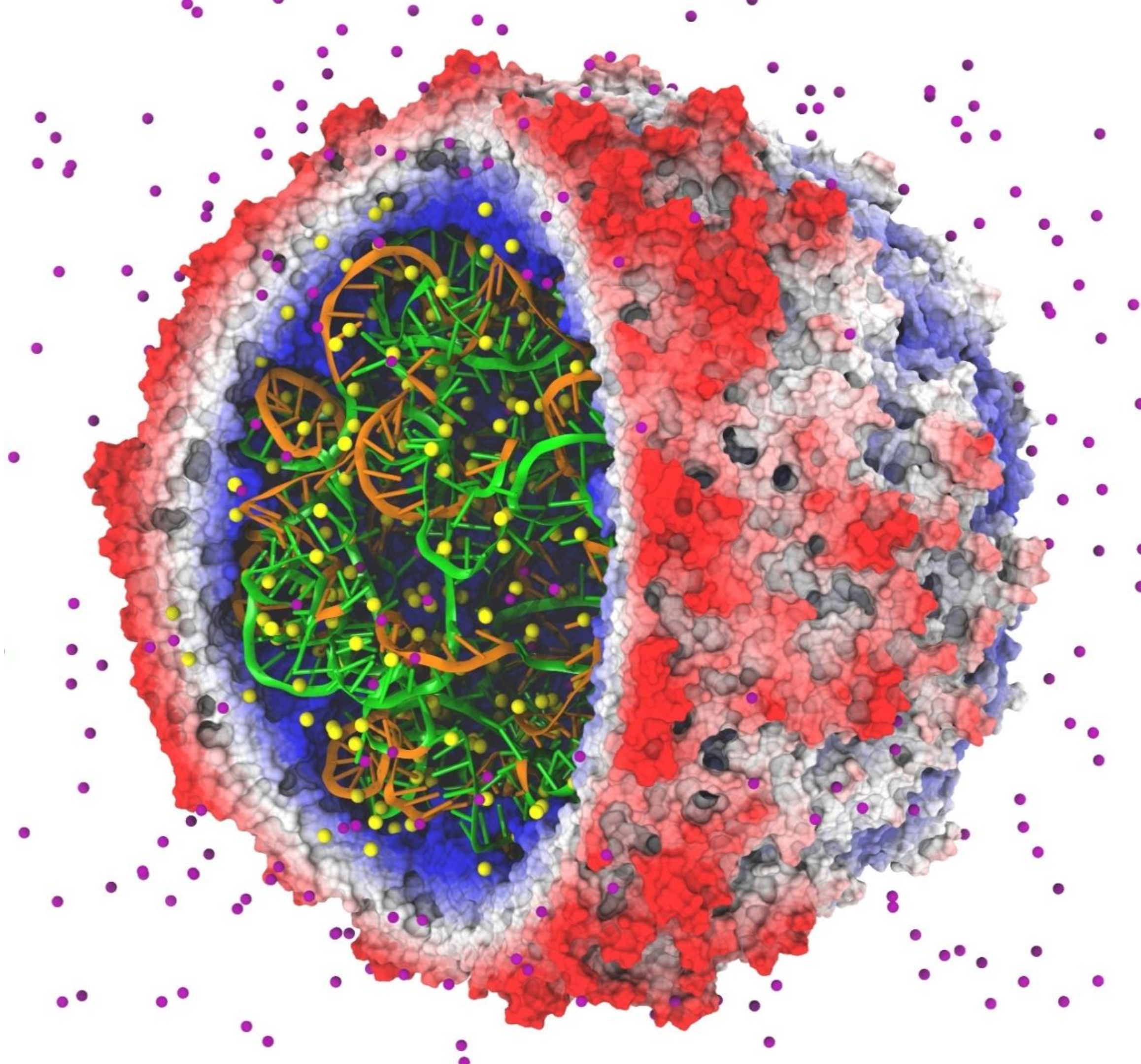
Two lights, no shadows

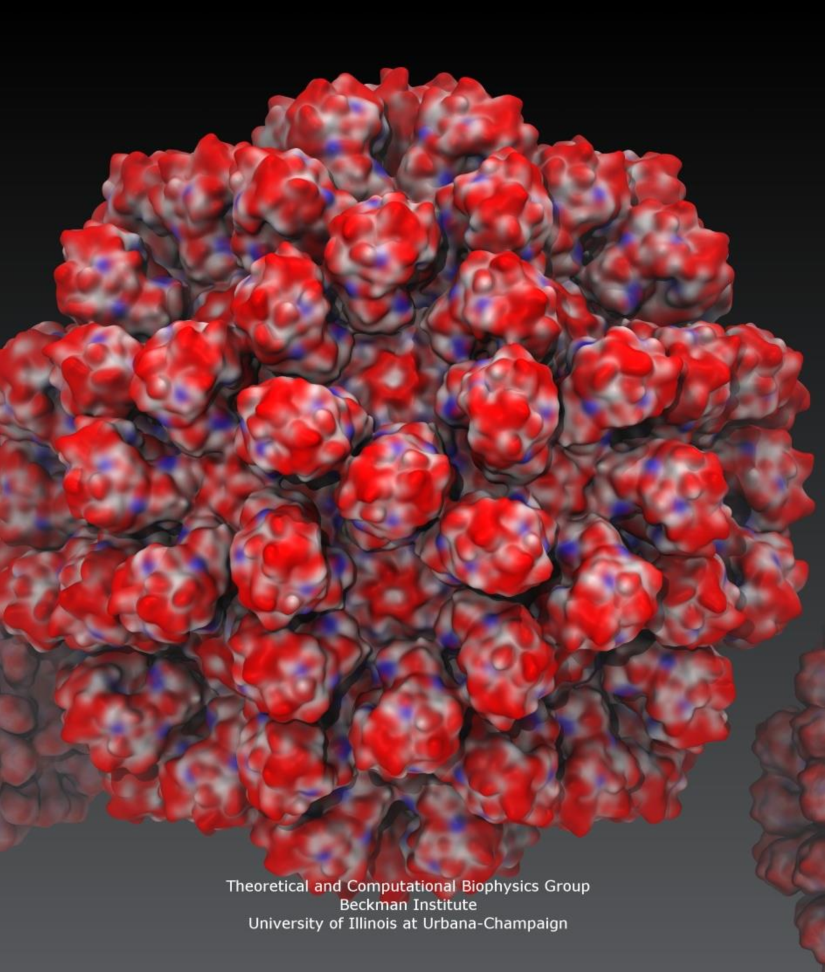
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit





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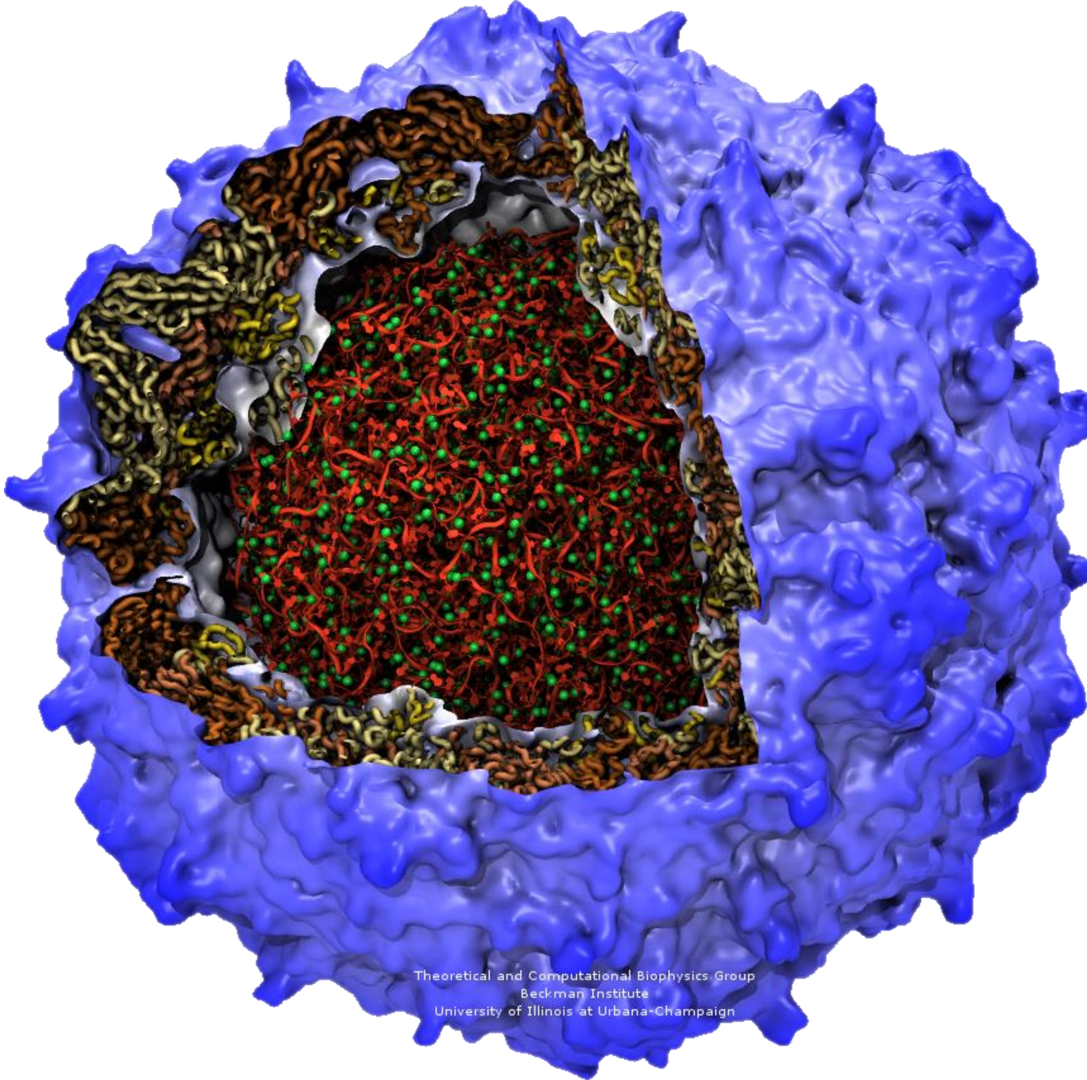
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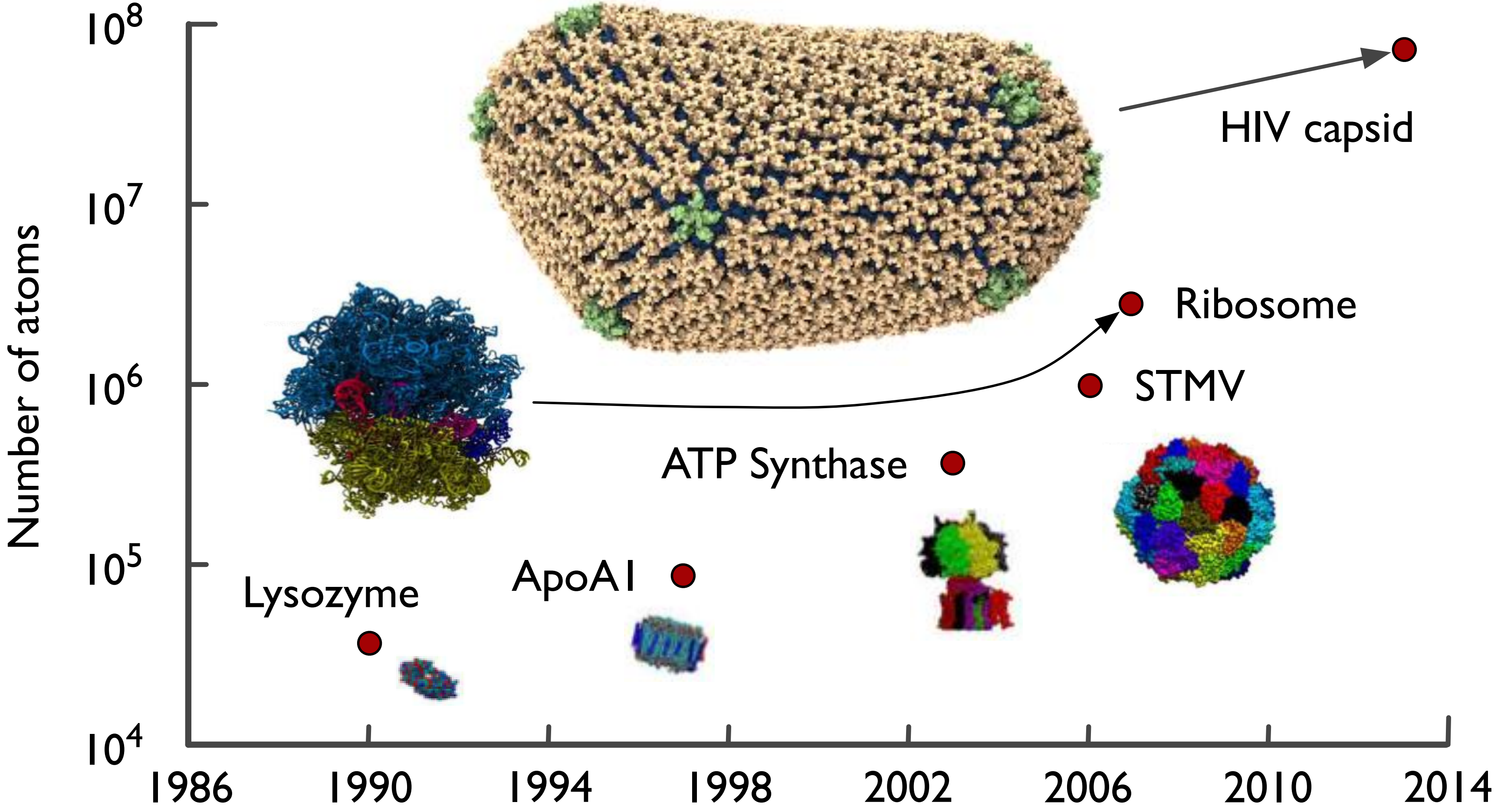
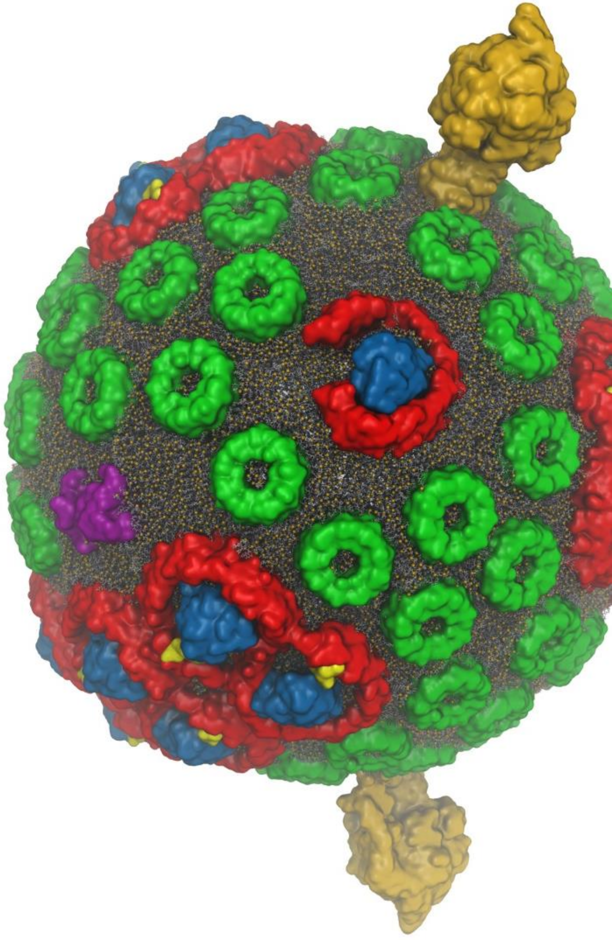
Computational Biology's Insatiable Demand for Processing Power

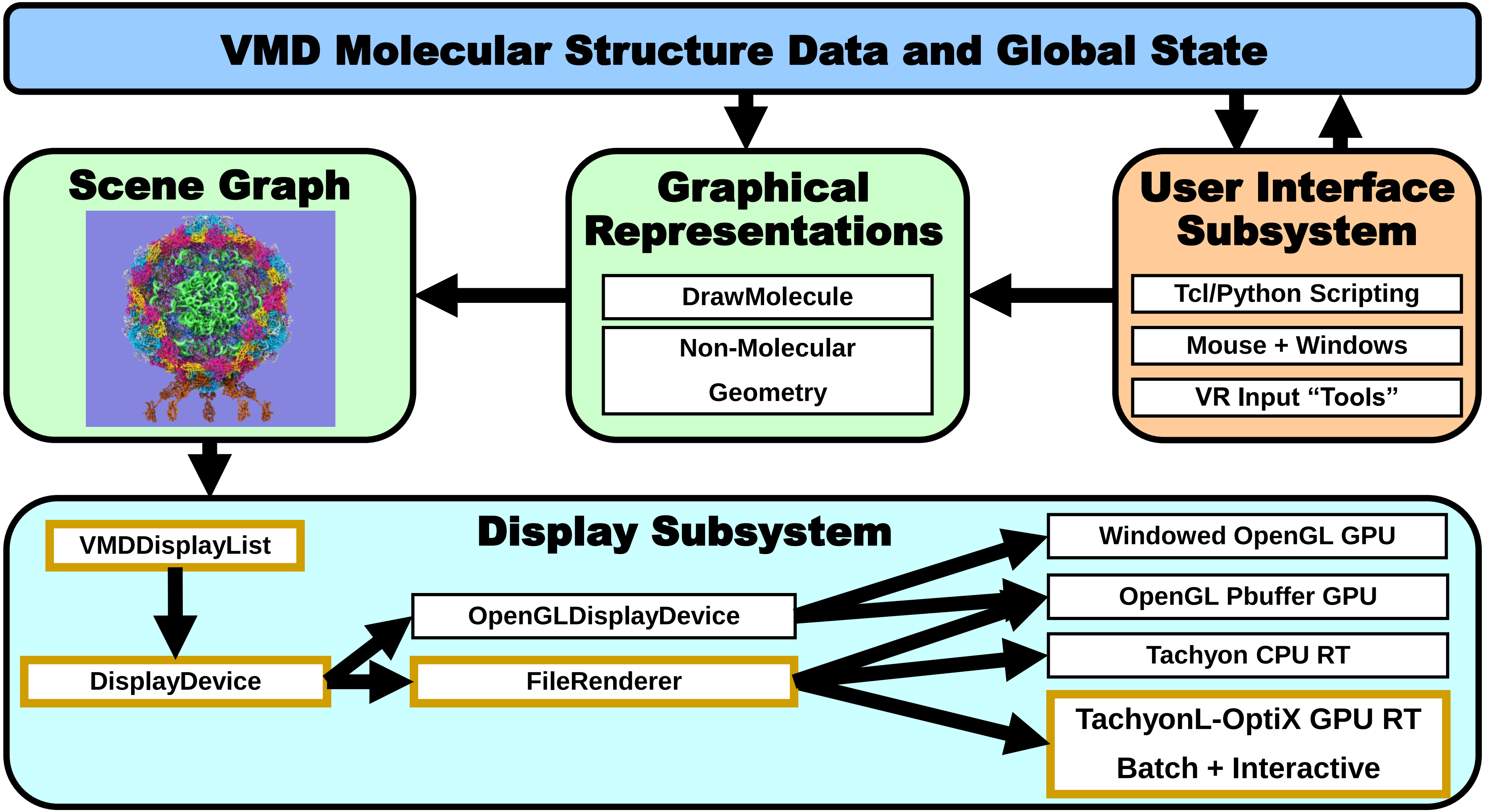


VMD 1.9.3 + OptiX 3.8 + CUDA 7.0
~1.5x Performance Increase

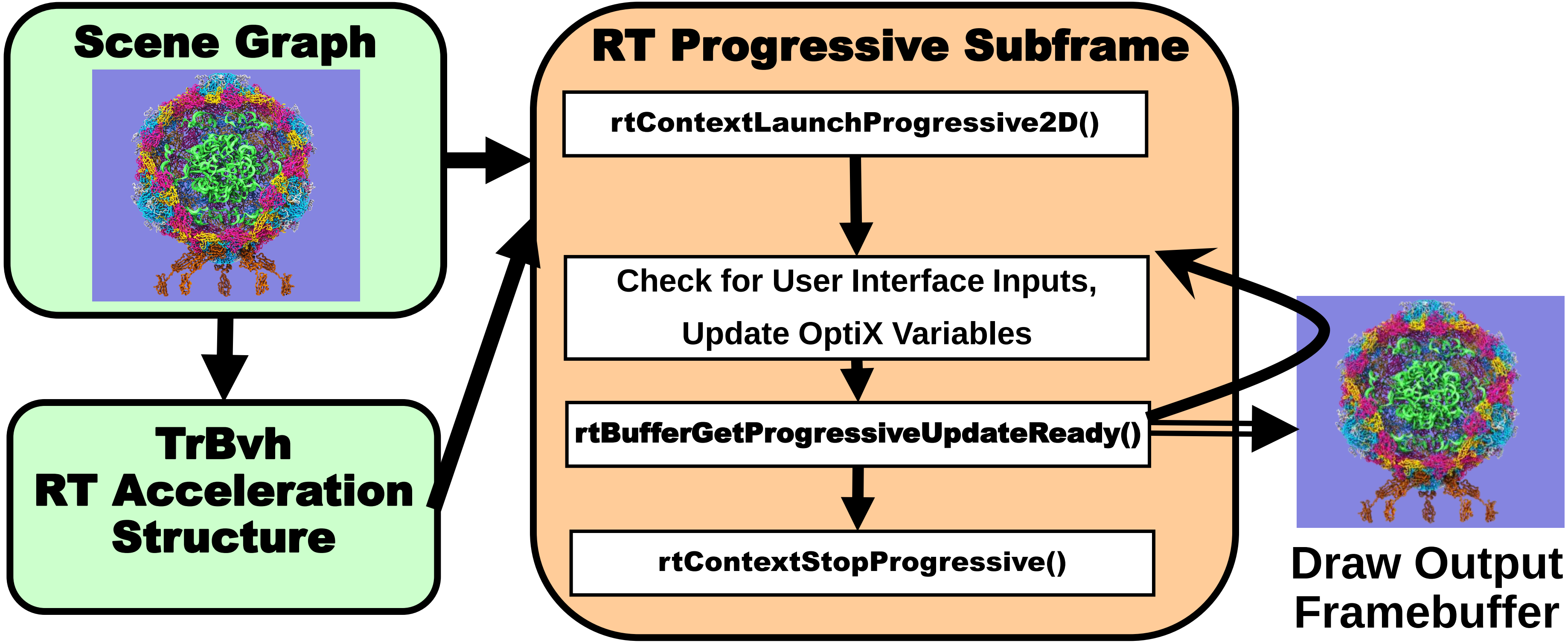
- OptiX GPU-native **“Trbvh” acceleration structure builder** yields substantial perf increase vs. CPU builders running on Opteron 6276 CPUs
- New optimizations in VMD TachyonL-OptiX RT engine:
  - **CUDA C++ Template specialization of RT kernels**
    - **Combinatorial expansion of ray-gen and shading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



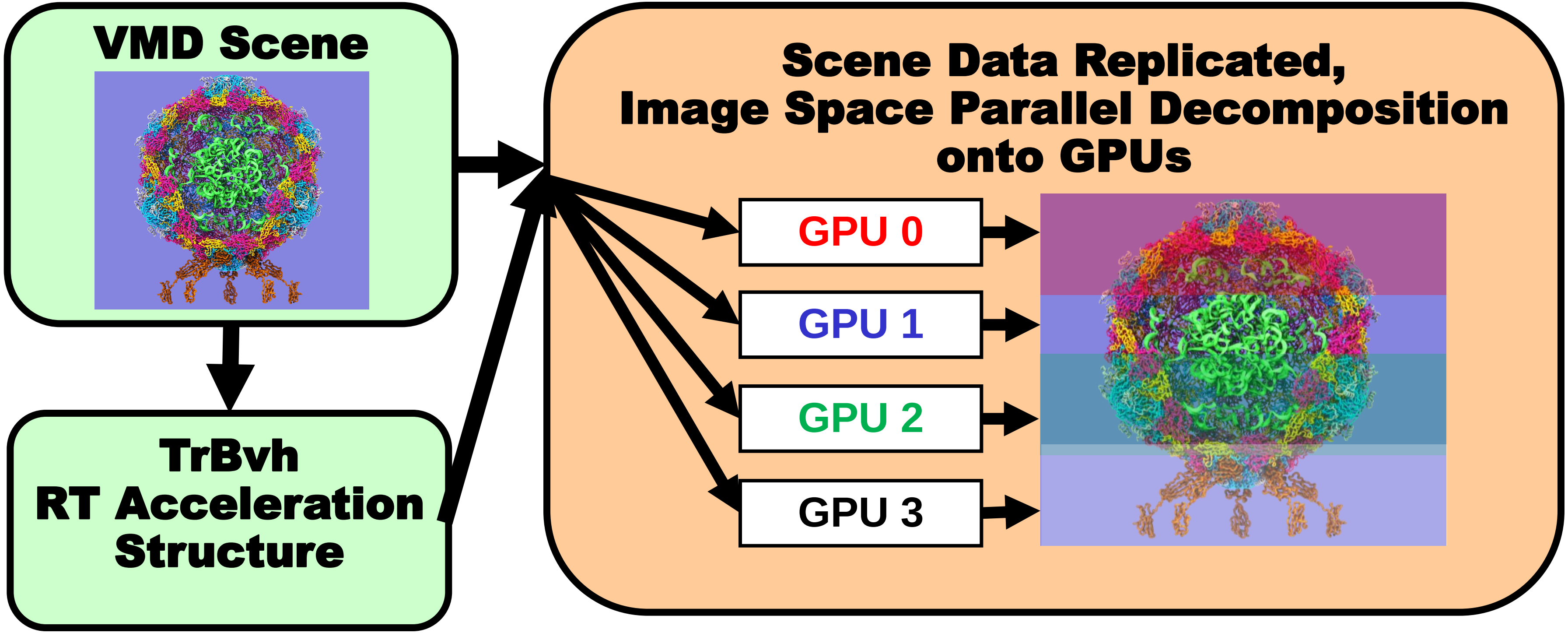
VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.


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

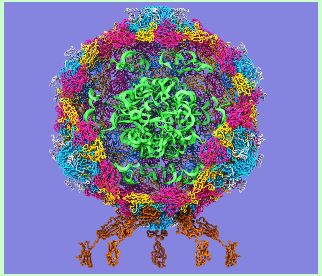


VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node



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

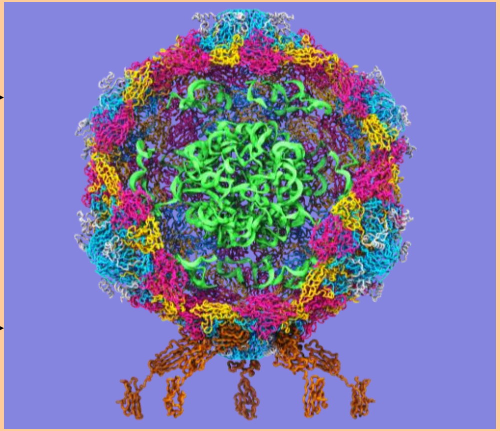
VMD Scene



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

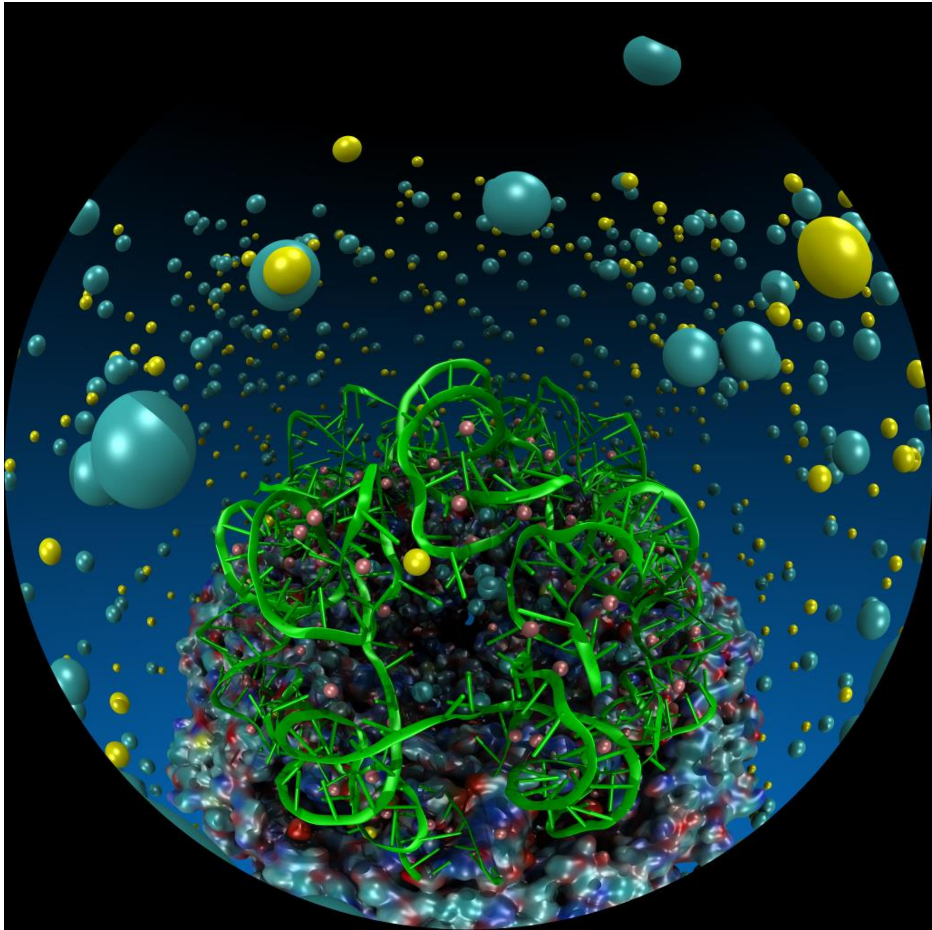
VCA 0:
8 K6000 GPUs

VCA N:
8 K6000 GPUs

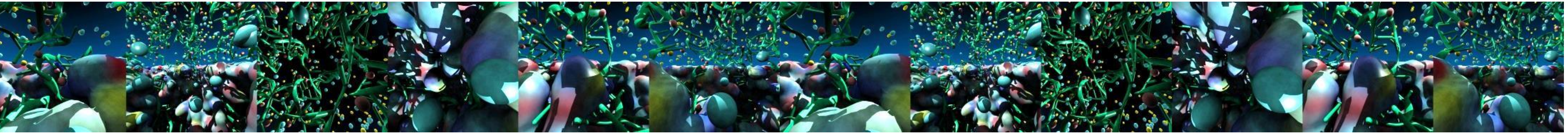


VMD Planetarium Dome Master Camera

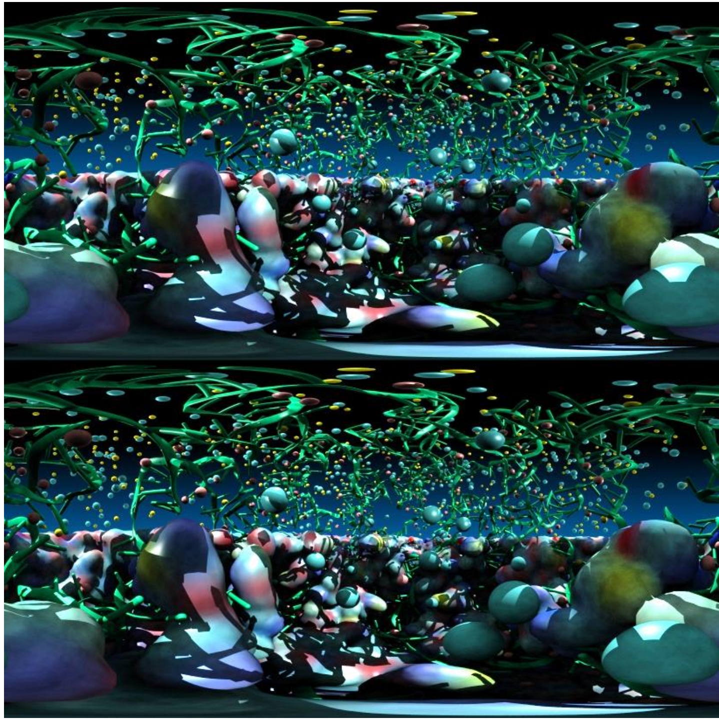
- RT-based dome projection -- rasterization poorly suited to non-planar projections
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required



Stereoscopic Panorama Ray Tracing w/ OptiX

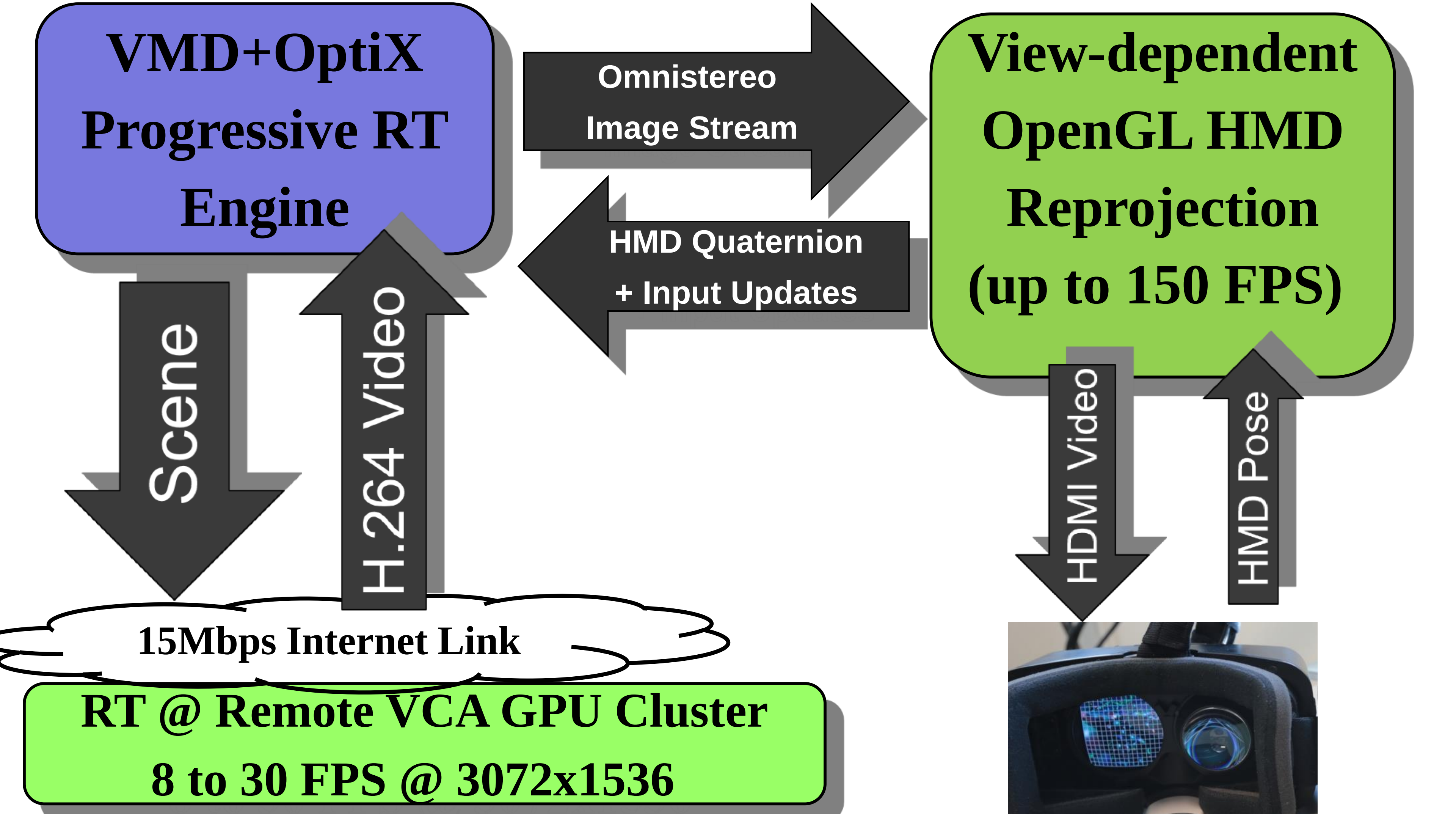


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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