Immersive Molecular Visualization with Omnidirectional Ray Tracing and Remote Rendering

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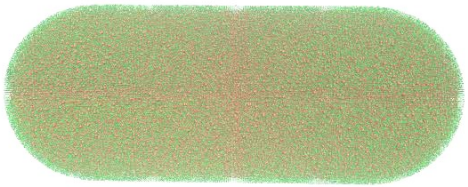
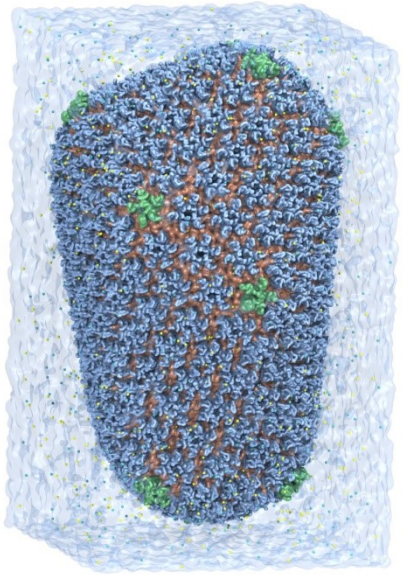
VMD – “Visual Molecular Dynamics”

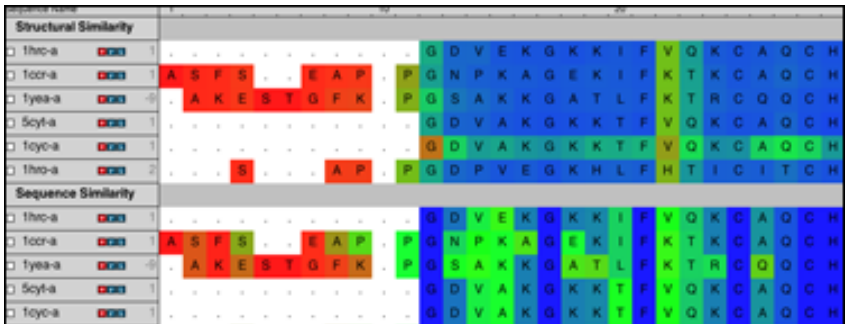
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting, plugins
- http://www.ks.uiuc.edu/Research/vmd/



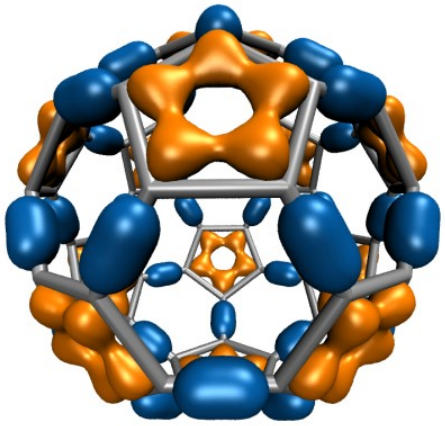
Whole Cell Simulation



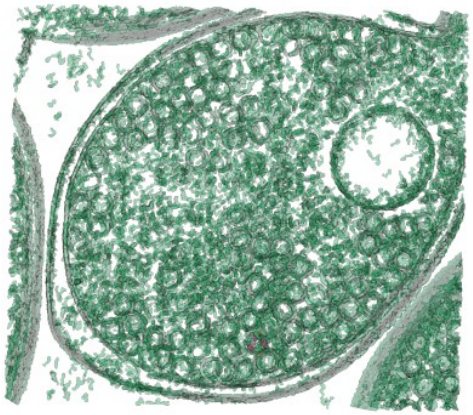
MD Simulations



Sequence Data



Quantum Chemistry

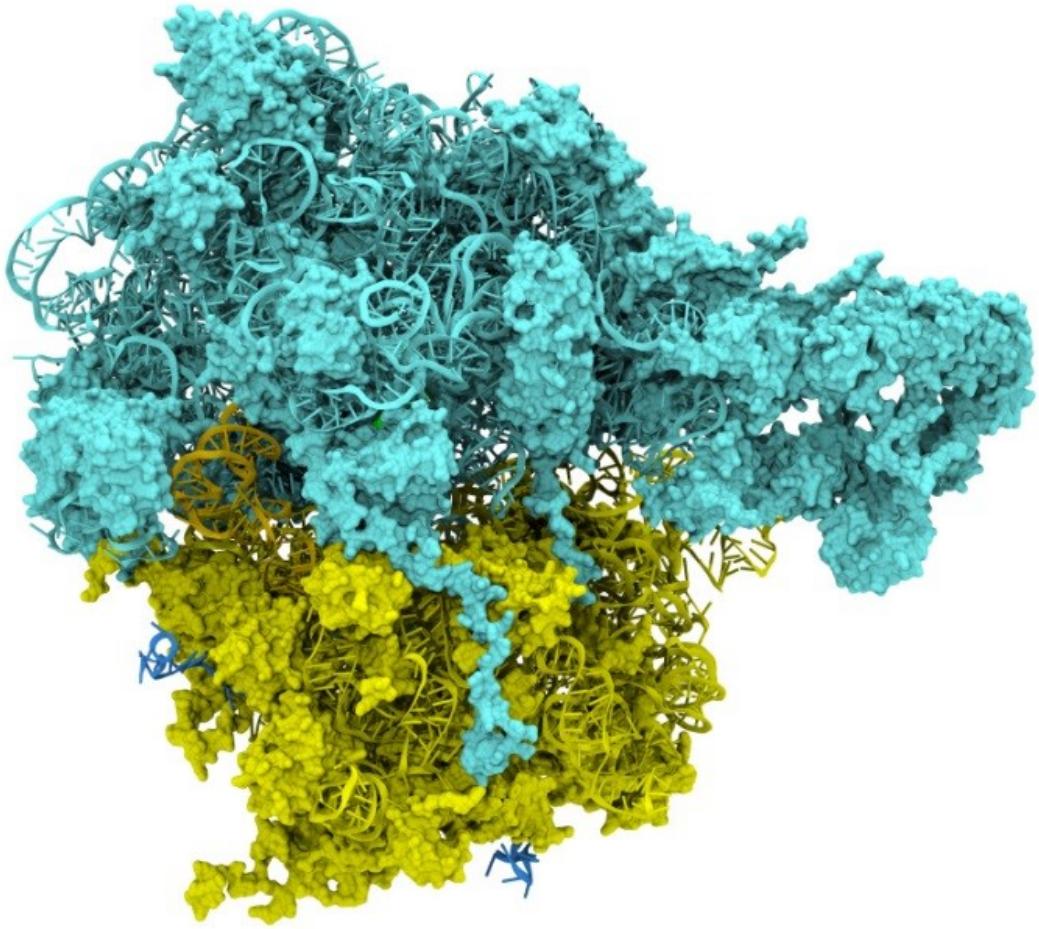


CryoEM, Cellular Tomography

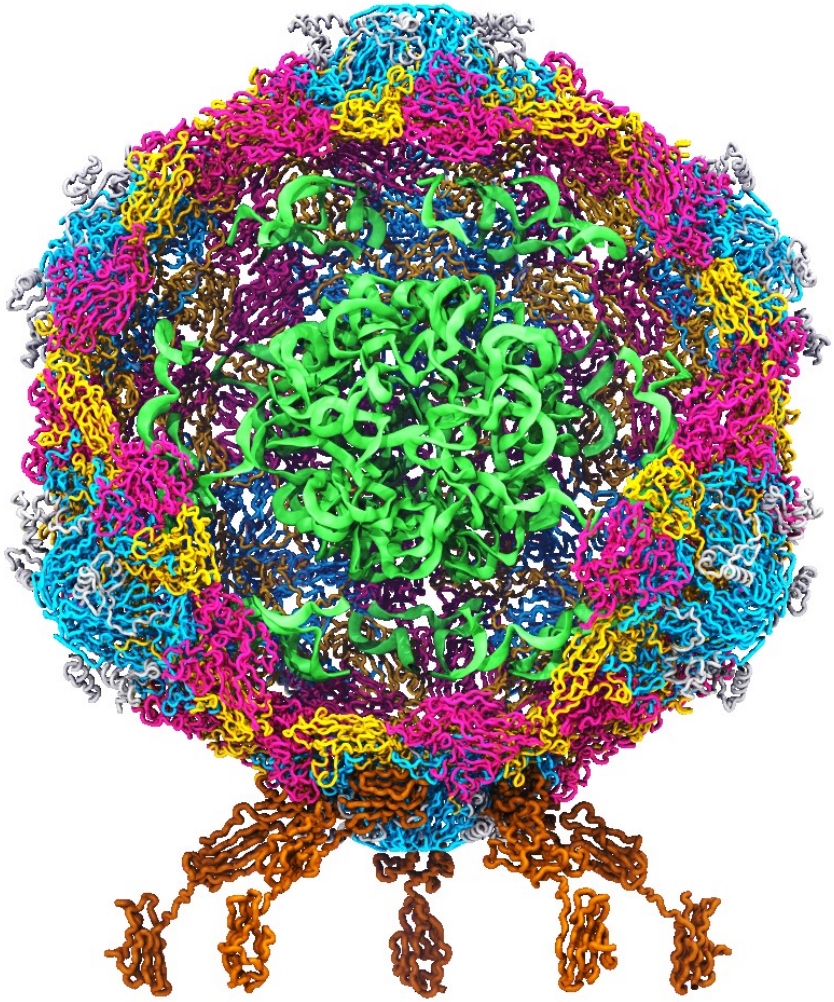
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

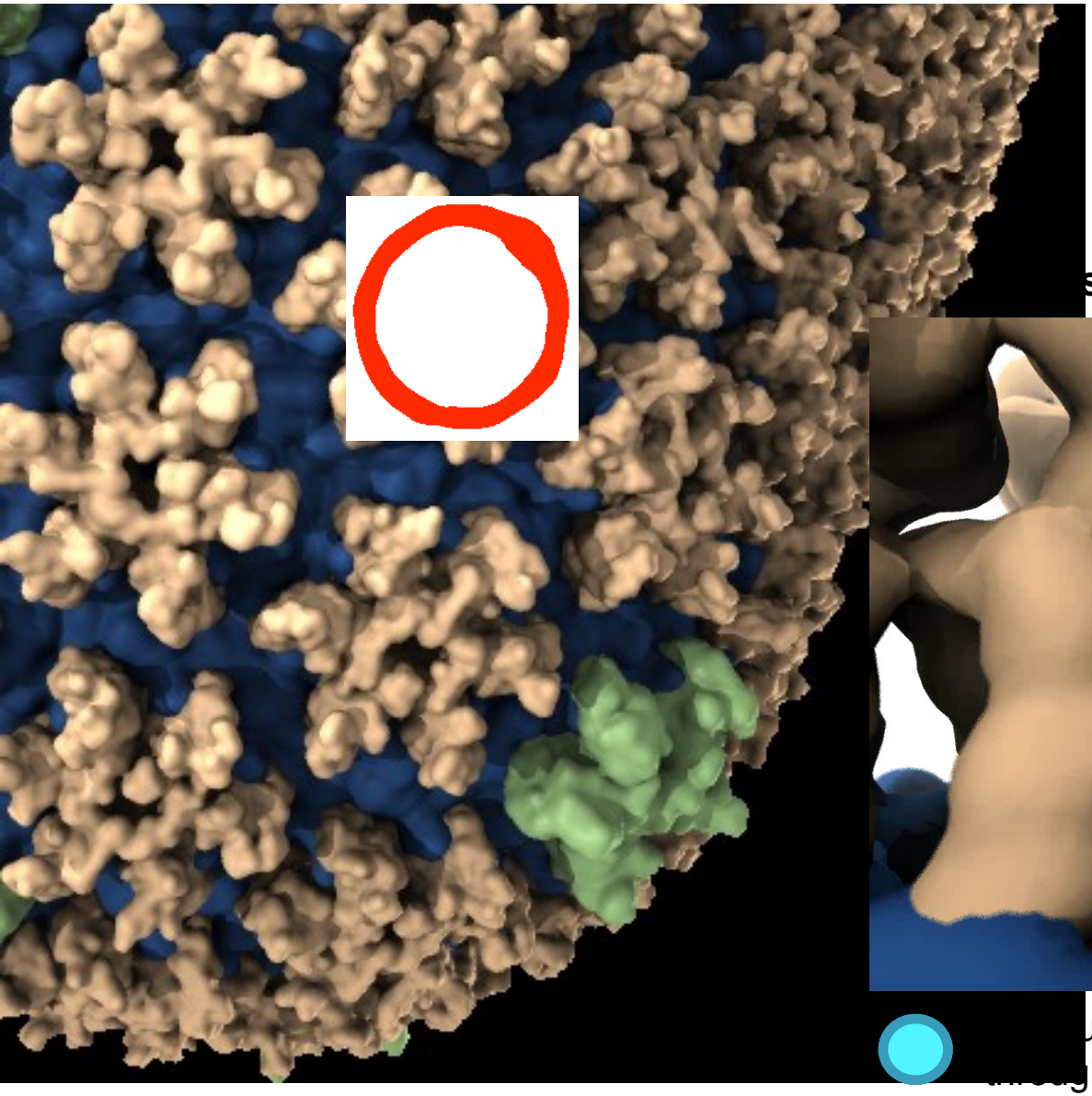


Immersive Viz. w/ VMD

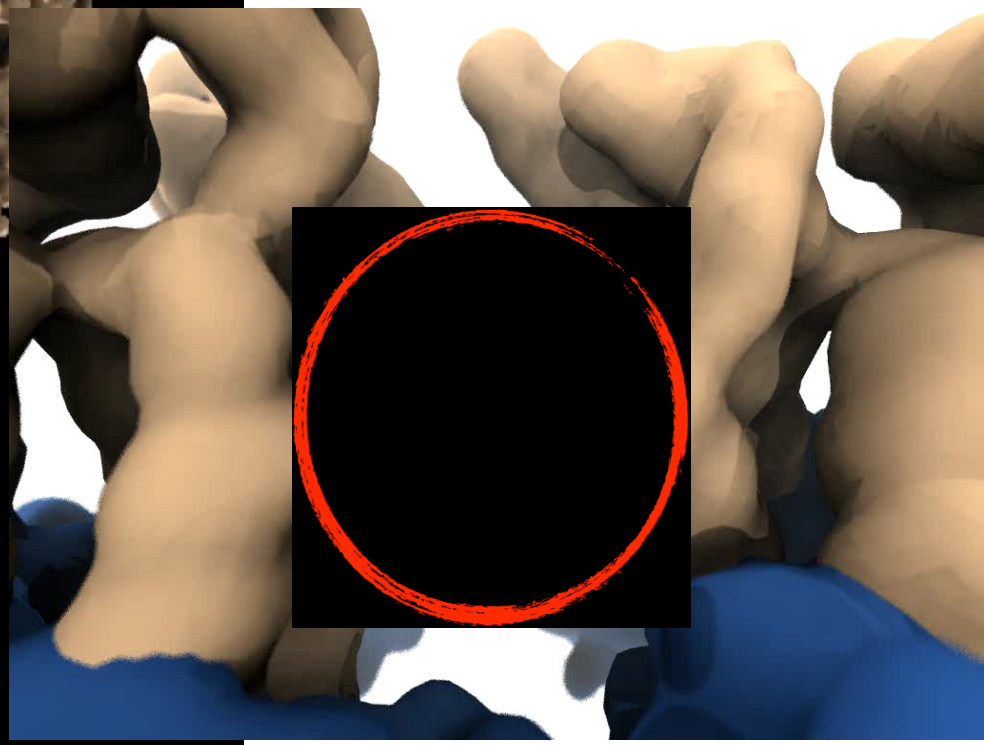
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability, convenience
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support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

VMD running in a CAVE

Goal: Intuitive interactive viz. in crowded molecular complexes



sults from 64 M atom, 1 μs sim!



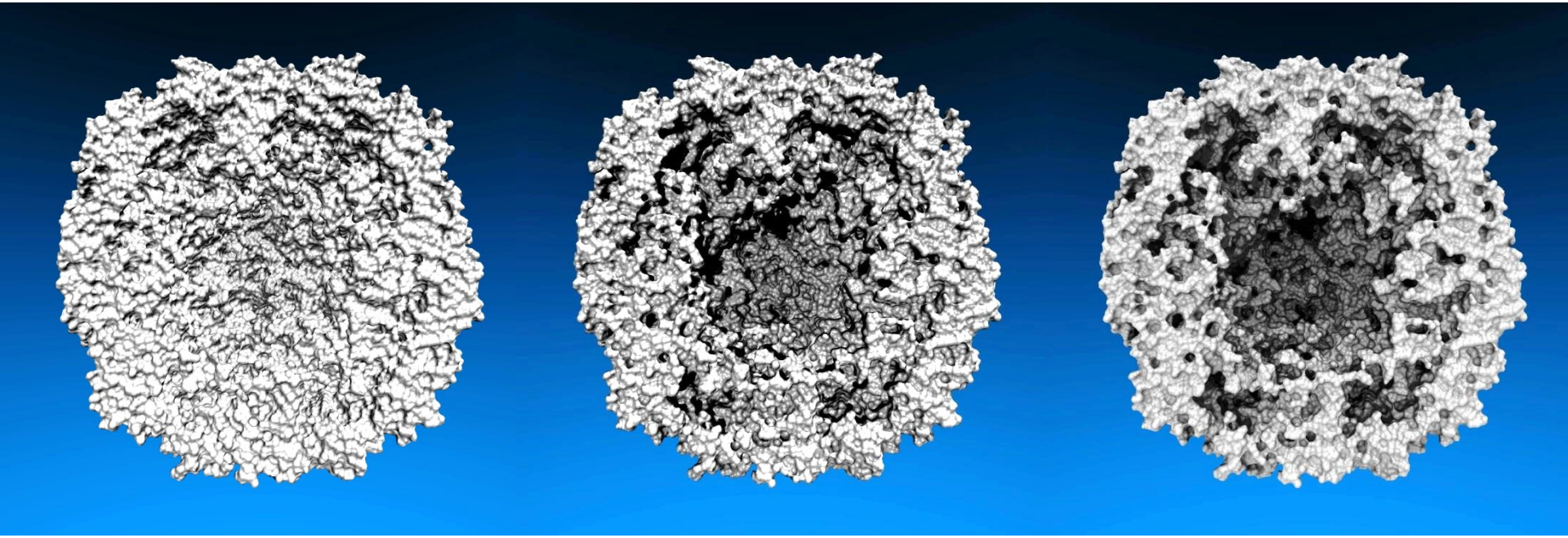
up view of chloride ions permeating
gh HIV-1 capsid hexameric centers

Lighting Comparison

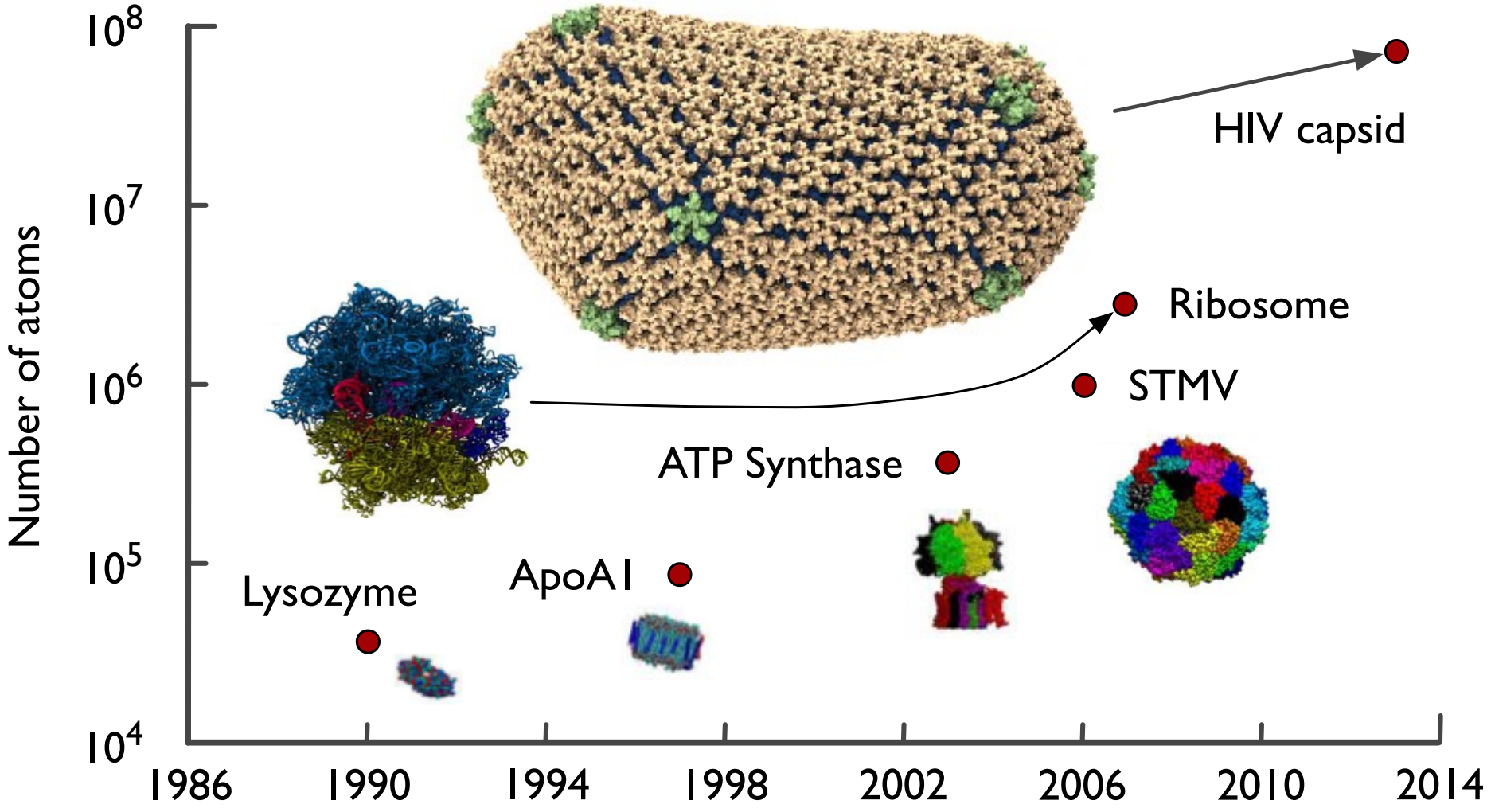
Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit

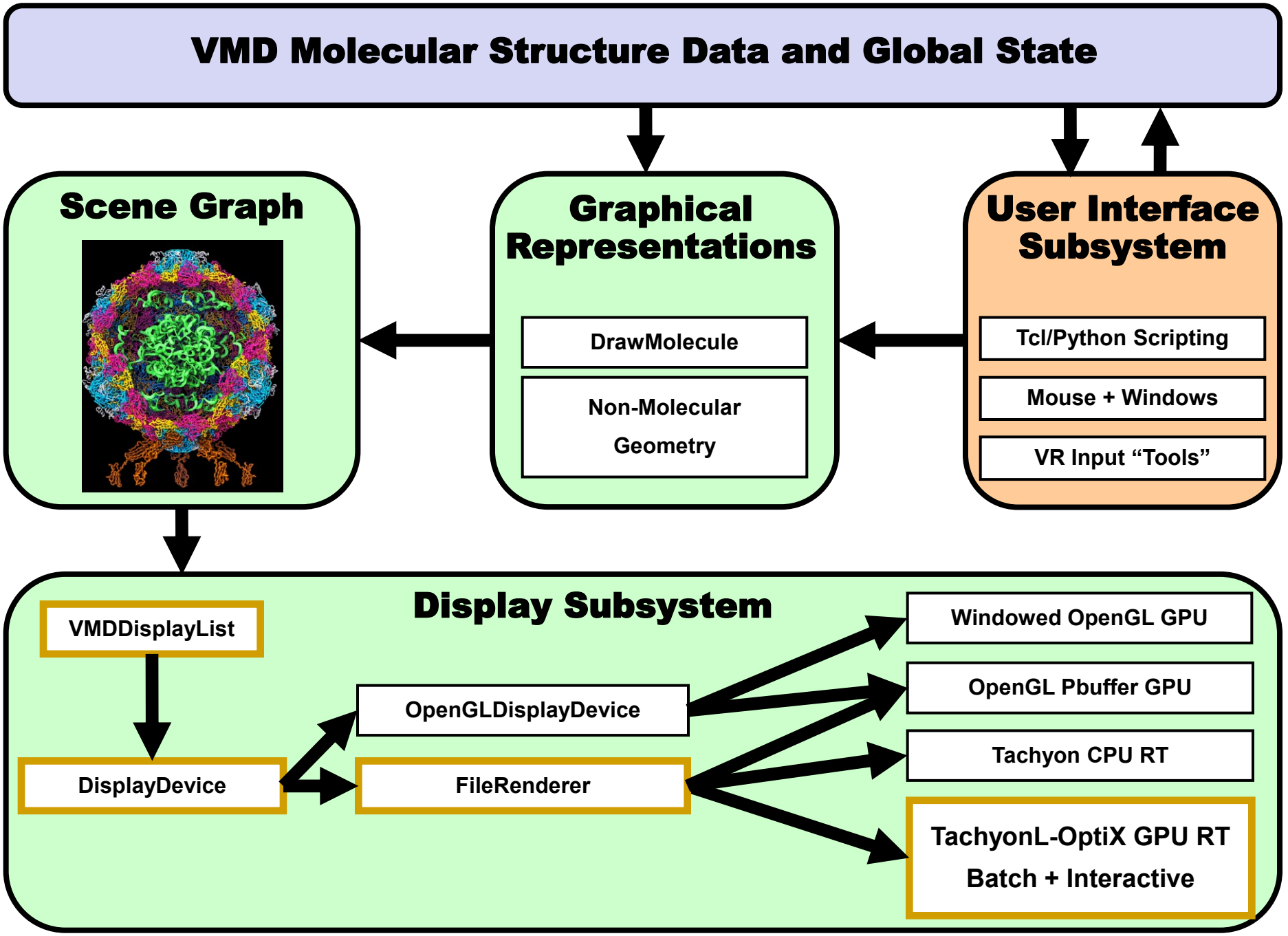


Computational Biology's Insatiable Demand for Processing Power

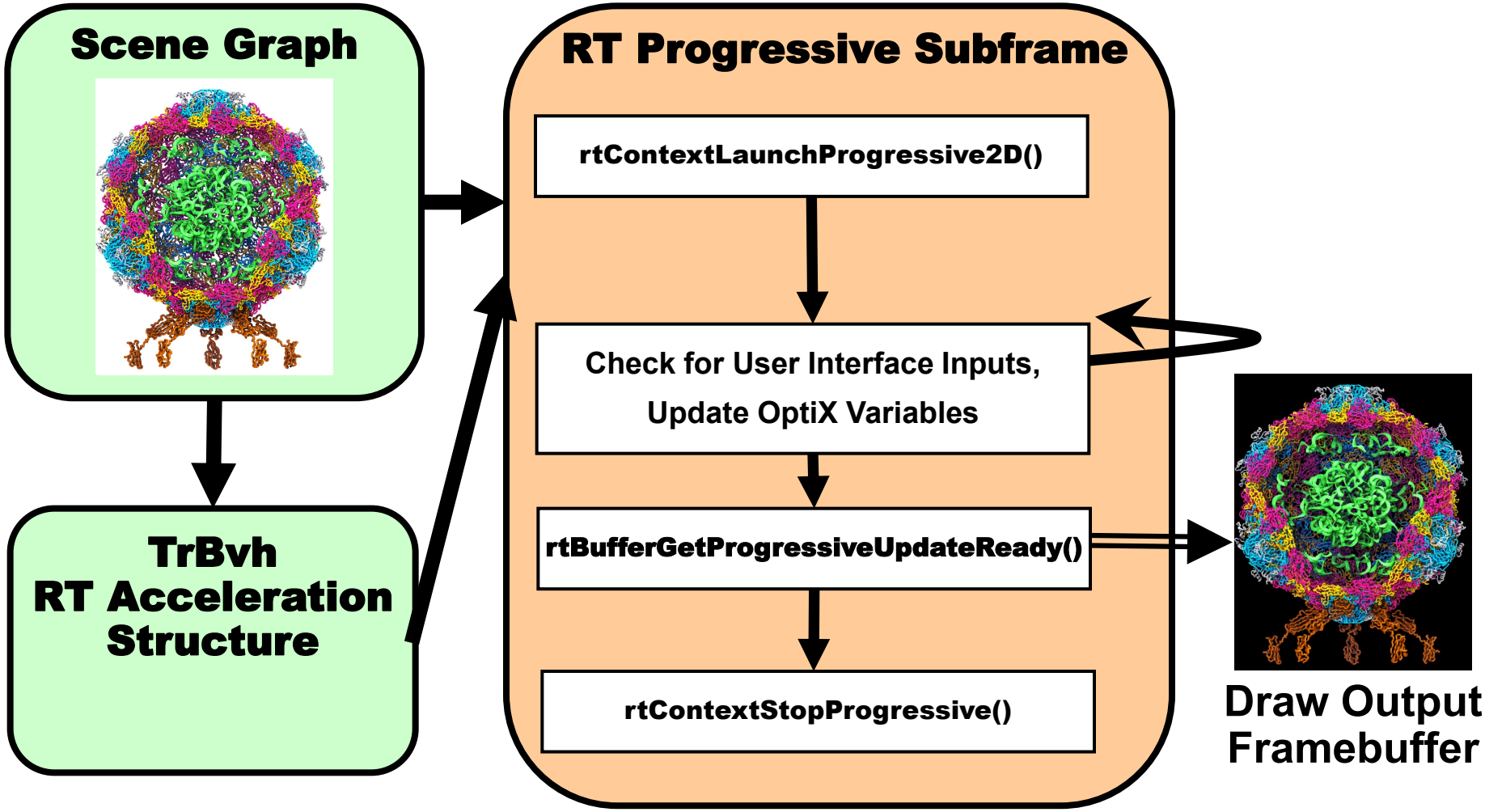


HMD Ray Tracing Challenges

- 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

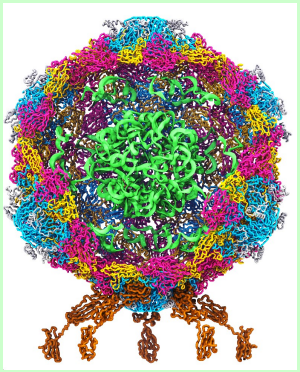

VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input "Tools"
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL 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

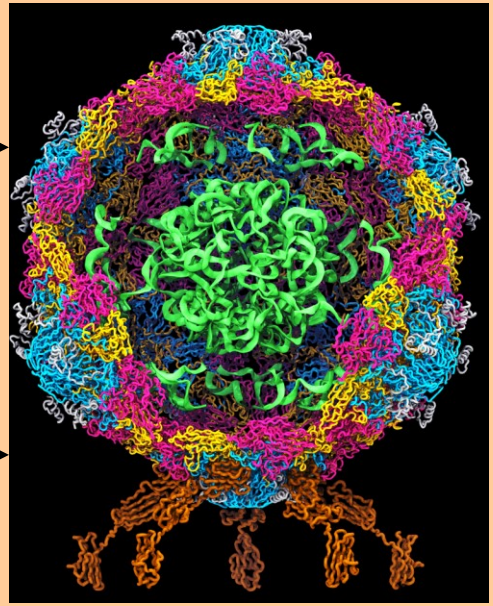
VMD Scene



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

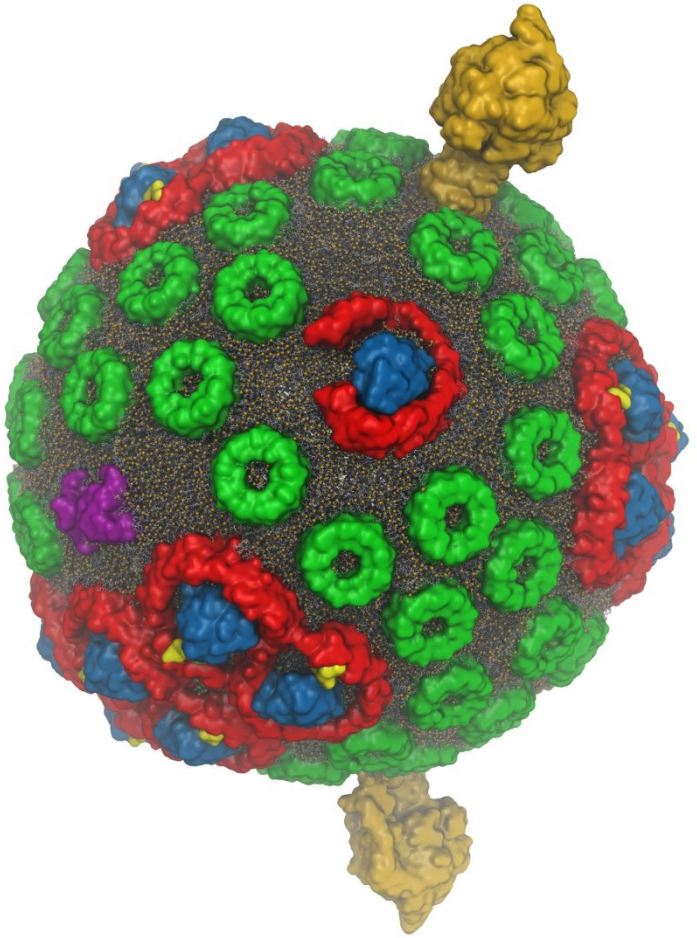
VCA 0:
8 M6000 GPUs

VCA N:
8 M6000 GPUs



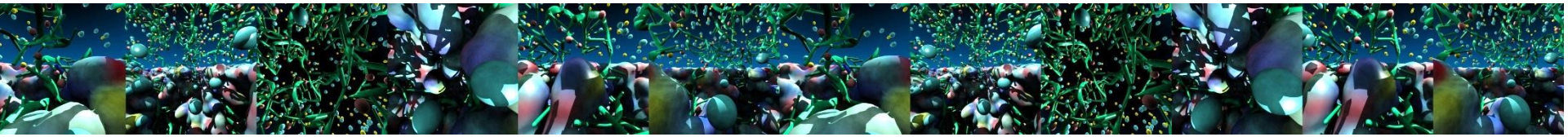
VMD 1.9.3 + OptiX 3.8/3.9 + CUDA 7.x ~1.5x Performance Increase

- 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**

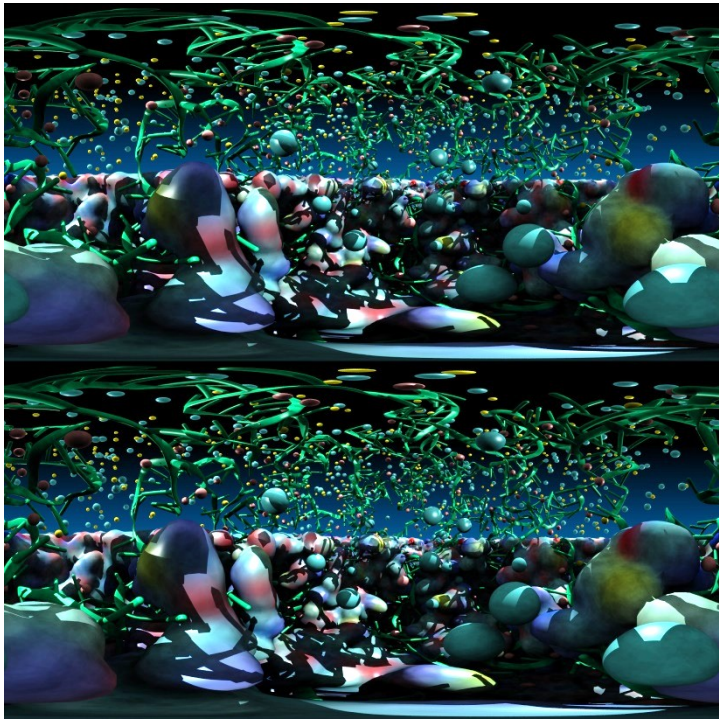


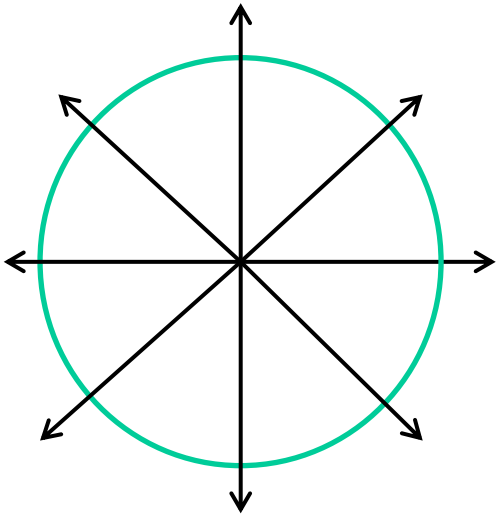
VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.

Stereoscopic Panorama Ray Tracing w/ OptiX

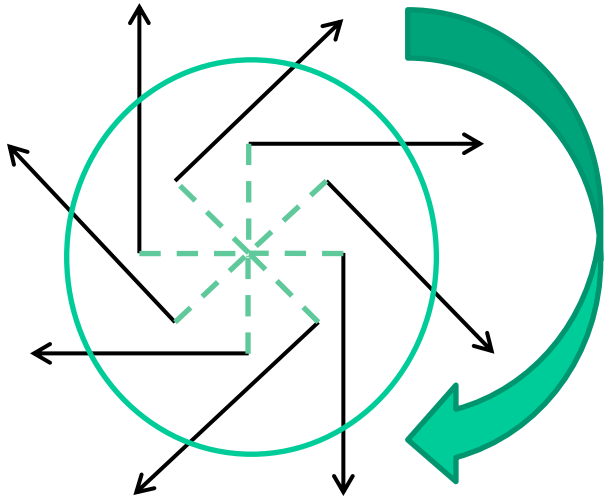


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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



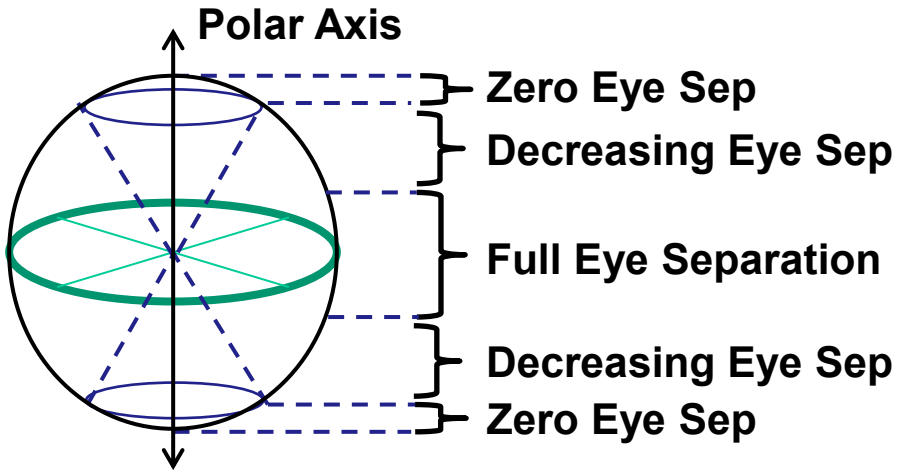


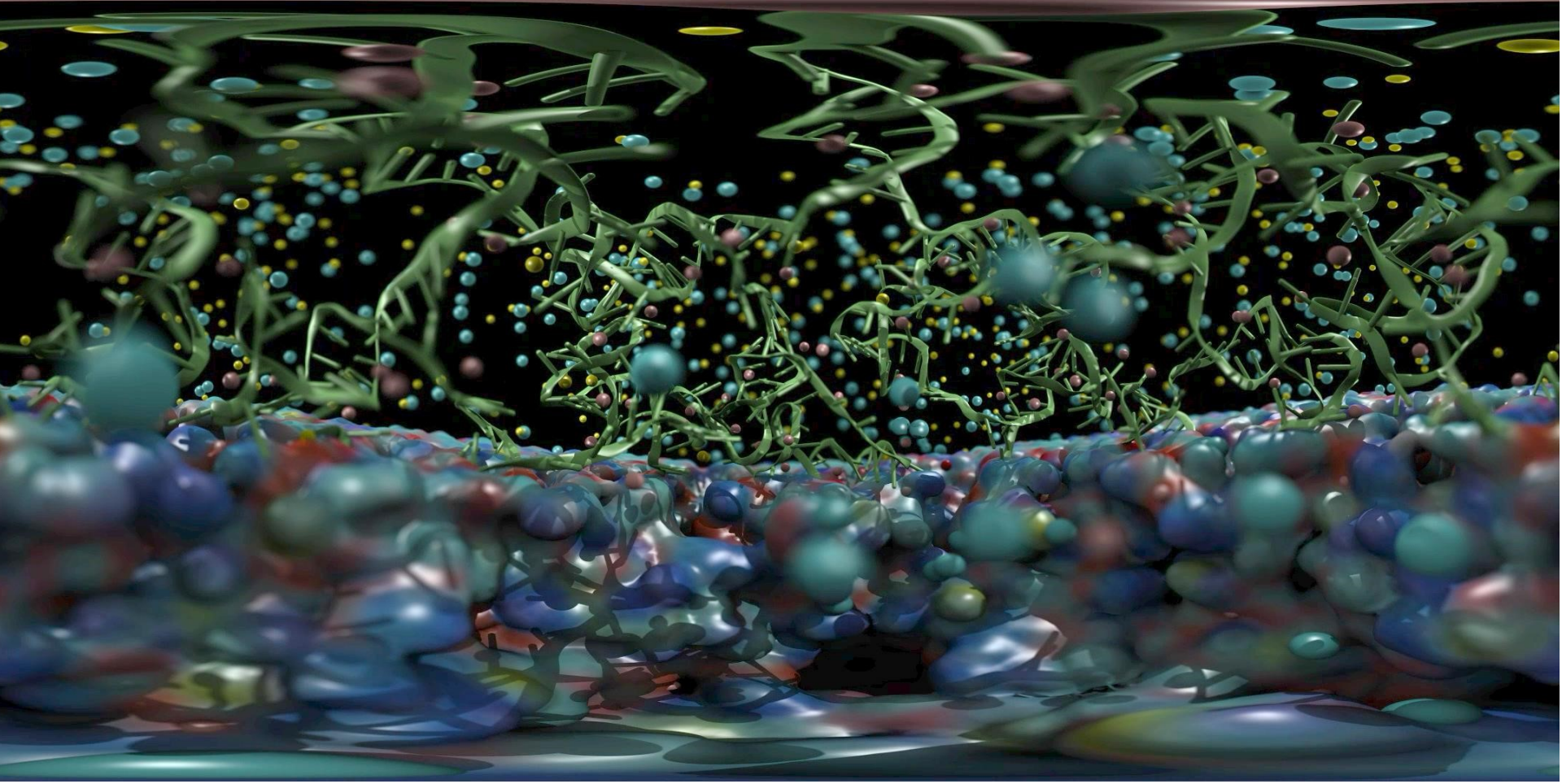
A) Monoscopic circular projection.
Eye at center of projection (COP).



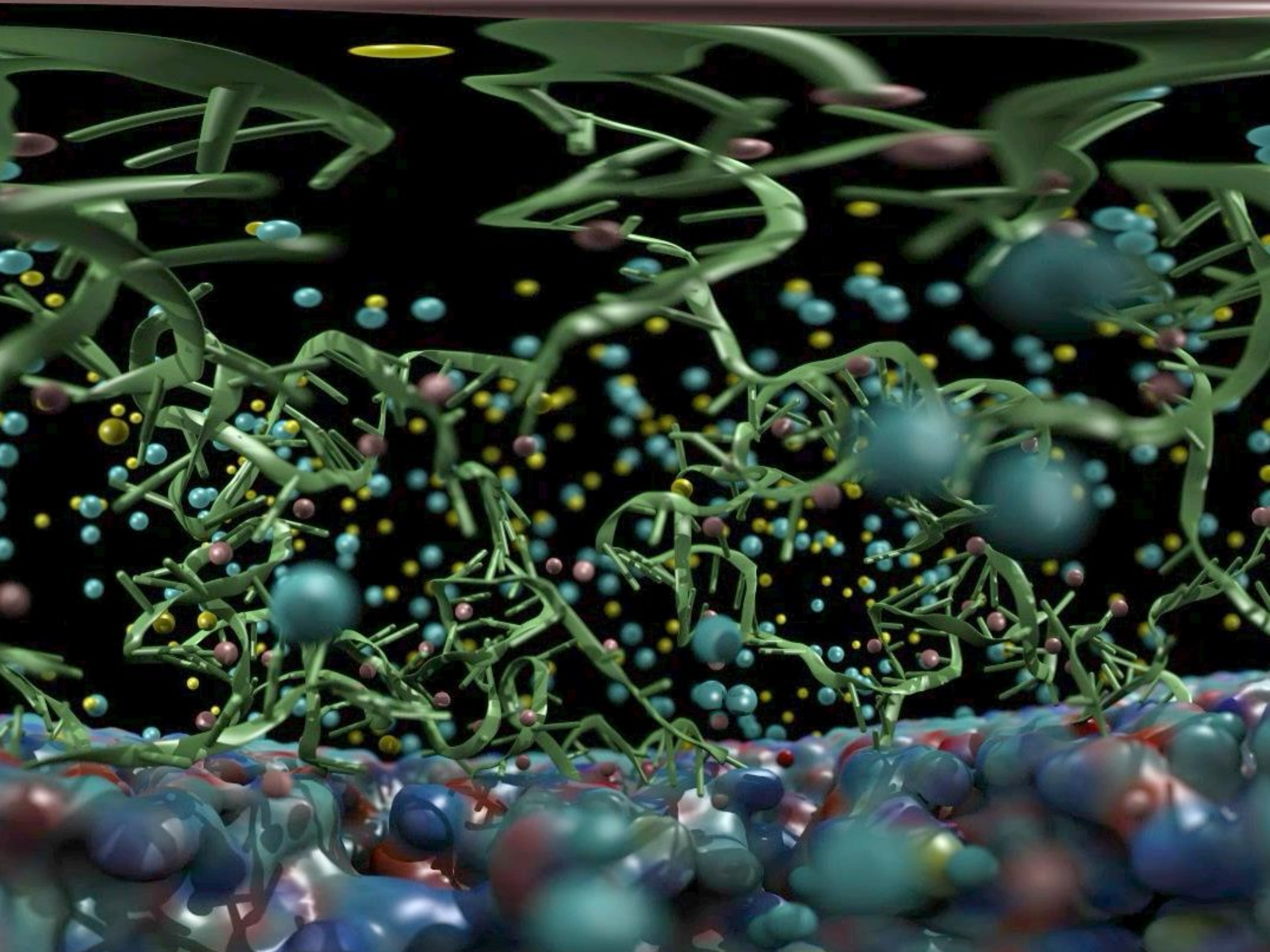
B) Left eye stereo circular projection.
Eye offset from COP by half of interocular distance.

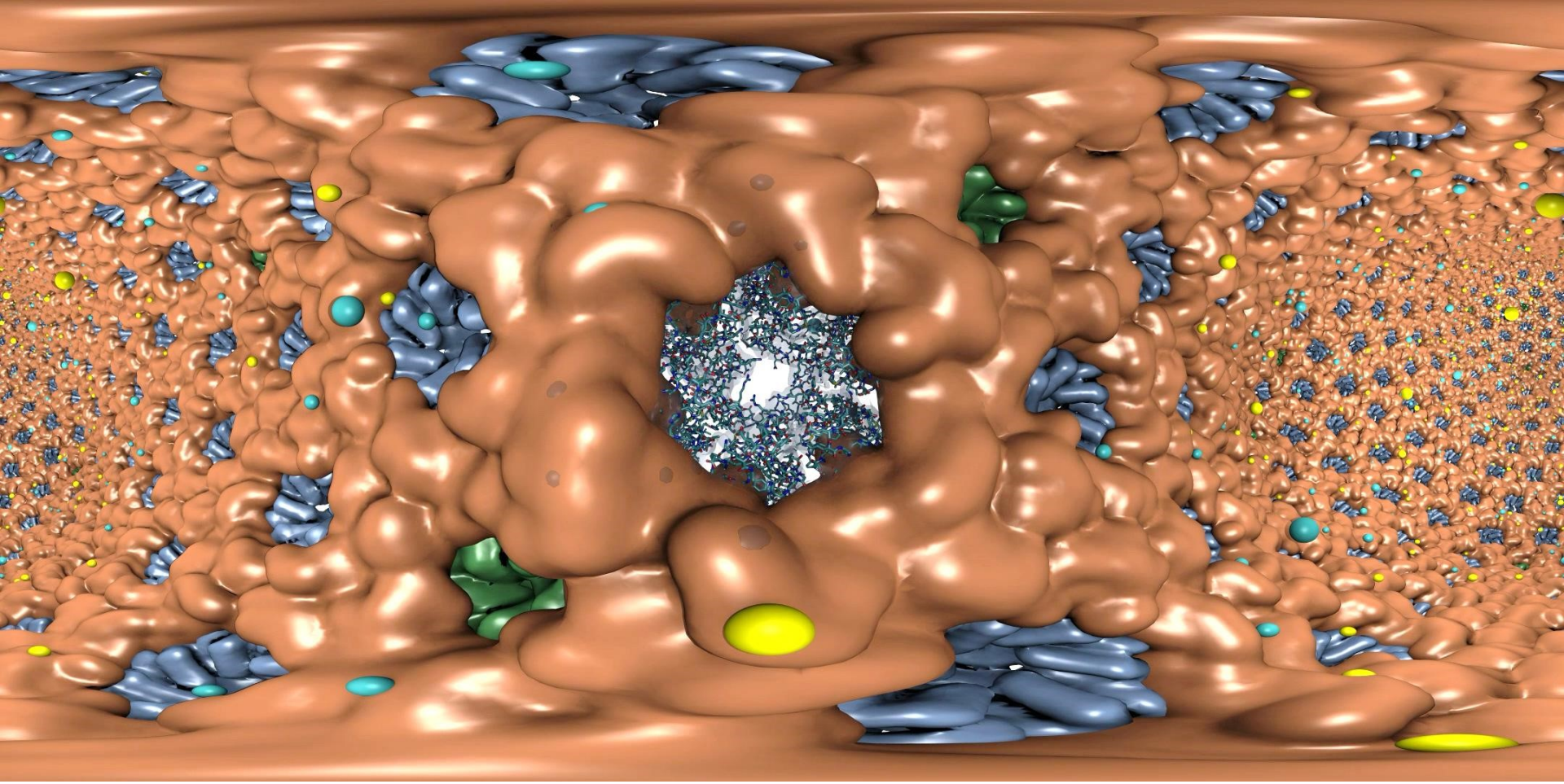
C) Stereo eye separation smoothly decreased to zero at zenith and nadir points on the polar axis to prevent incorrect stereo when HMD sees the poles.





Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …





HIV-1 Capsid, Capsid Hexamer Detail, and Ions
Range-Limited Ambient Occlusion Lighting, VR "Headlight", …

Progressive Ray Tracing Engine
Ray tracing loop runs continuously in new thread

Decodes H.264 video stream from remote VCA GPU cluster

Omnistereo Image Stream

Camera + Scene

HMD Display Loop
HMD loop runs in main VMD application thread at max OpenGL draw rate

View-dependent stereo reprojection for current HMD head pose

HMD distortion correction

RT Code + Camera + Scene

Omnistereo H.264 Video

VMD

HMD Video

HMD Pose

15Mbps Internet Link

Remote VCA GPU Cluster
Ray tracing runs continuously, streams H.264 video to VMD client

HMD

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 2:0 4:0	22.2 18.1 10.3
STMV Shadows+AO	1:1 1:2 1:4	18.2 16.1 12.4
STMV Shadows+AO+ DoF	1:1 2:1 2:2	16.1 11.1 8.5
HIV-1 Shadows	1:0 2:0 4:0	20.1 18.1 10.2
HIV-1 Shadows+AO	1:1 1:2 1:4	17.4 12.2 8.1

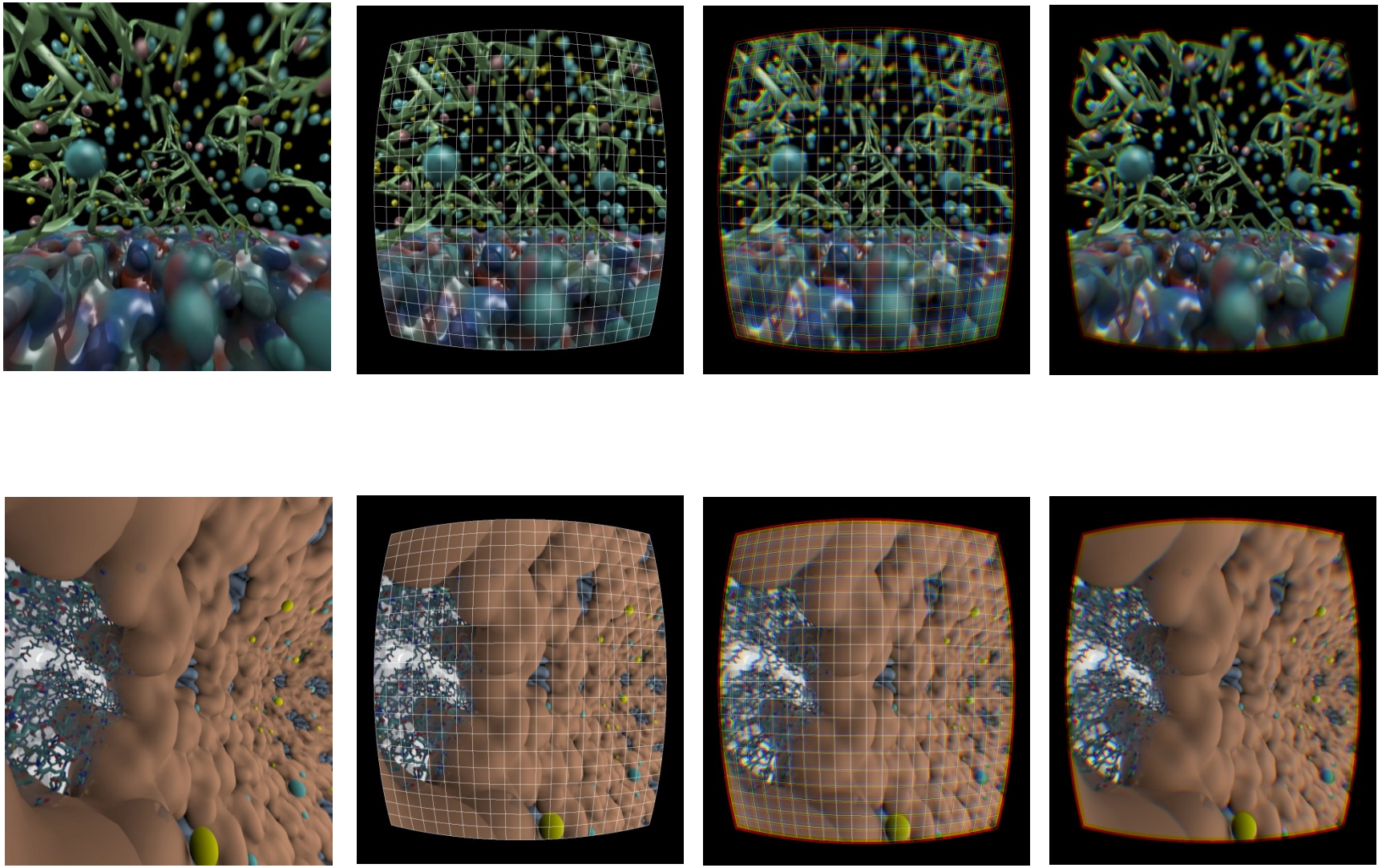
HMD View-Dependent Reprojection with OpenGL

- 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/

ZEISS
LENS CLEANER



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

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- NCSA Blue Waters team
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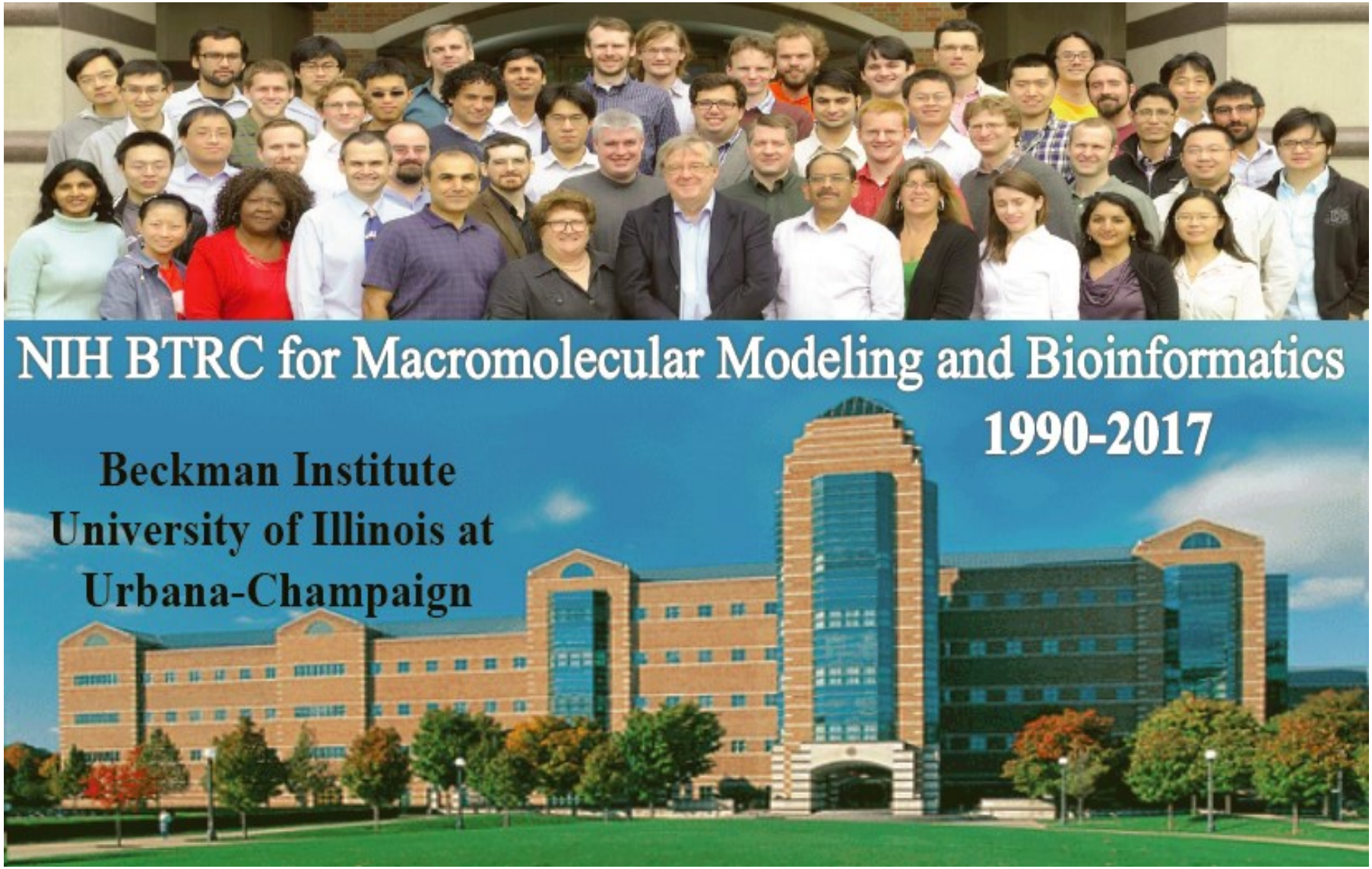
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- **Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering.** John E. Stone, William R. Sherman, and Klaus Schulten.High Performance Data Analysis and Visualization Workshop, IEEE International Parallel 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)**
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- **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.

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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**
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- **Unlocking the Full Potential of the Cray XK7 Accelerator.** M. D. Klein and J. E. Stone. Cray Users Group, Lugano Switzerland, May 2014.
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- **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.

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- **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.

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- **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

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- **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.
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- **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.