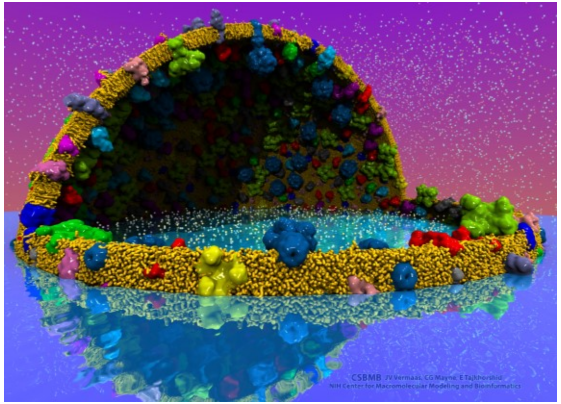
GPU-Accelerated OptiX Ray Tracing for Scientific Visualization

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/Research/gpu/

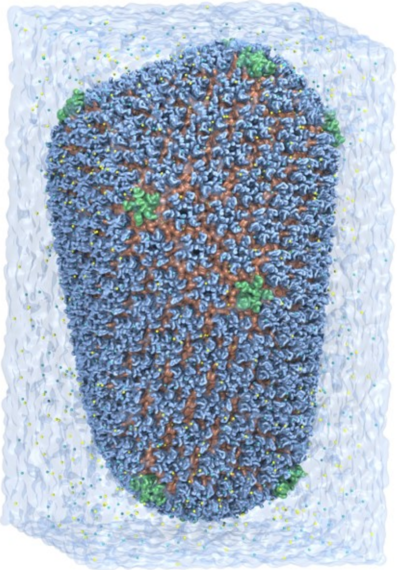
10:00-10:25, NVIDIA Theater, Siggraph 2018
Vancouver BC, Canada, Thursday August 16th, 2018

VMD – "Visual Molecular Dynamics"

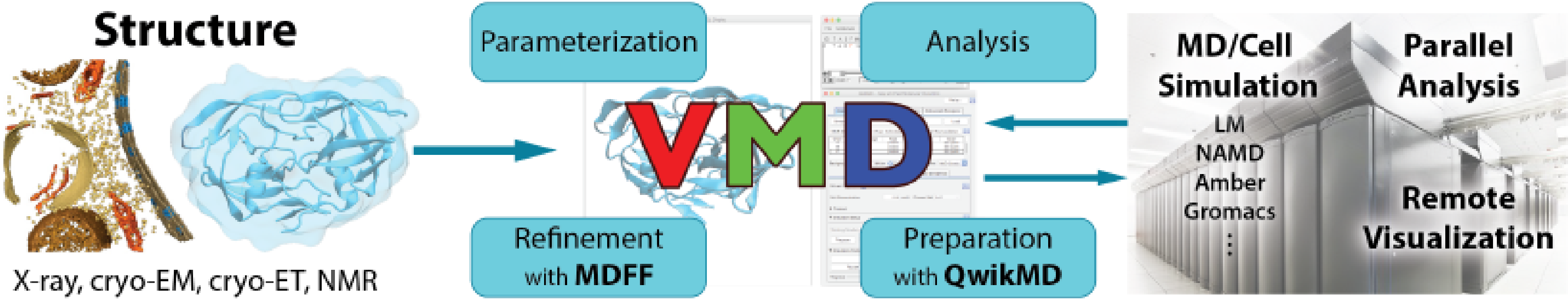
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
  - Sequence information
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



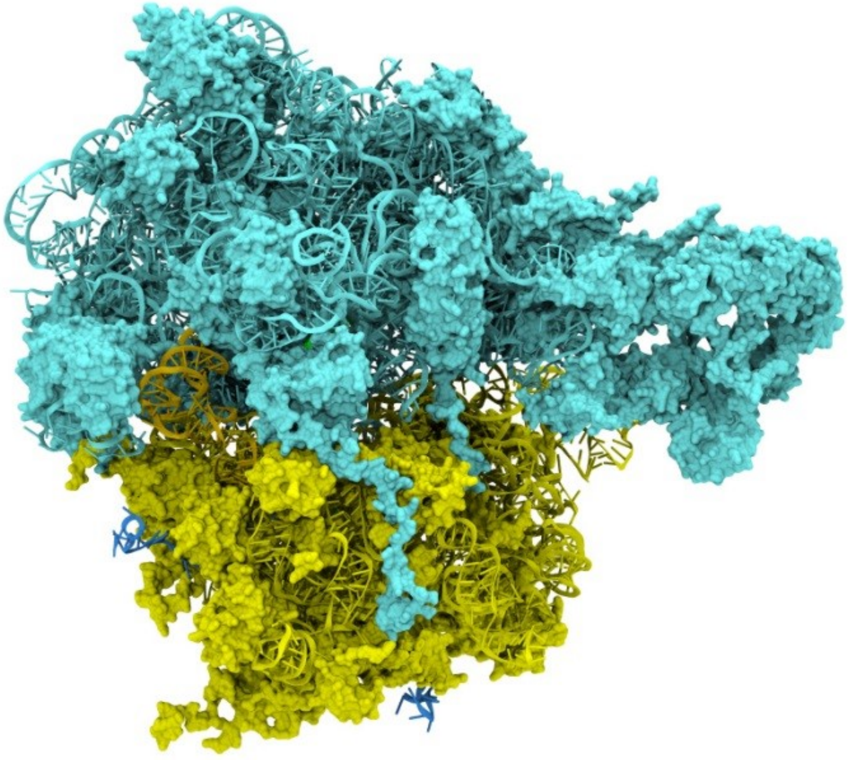
MD Simulation



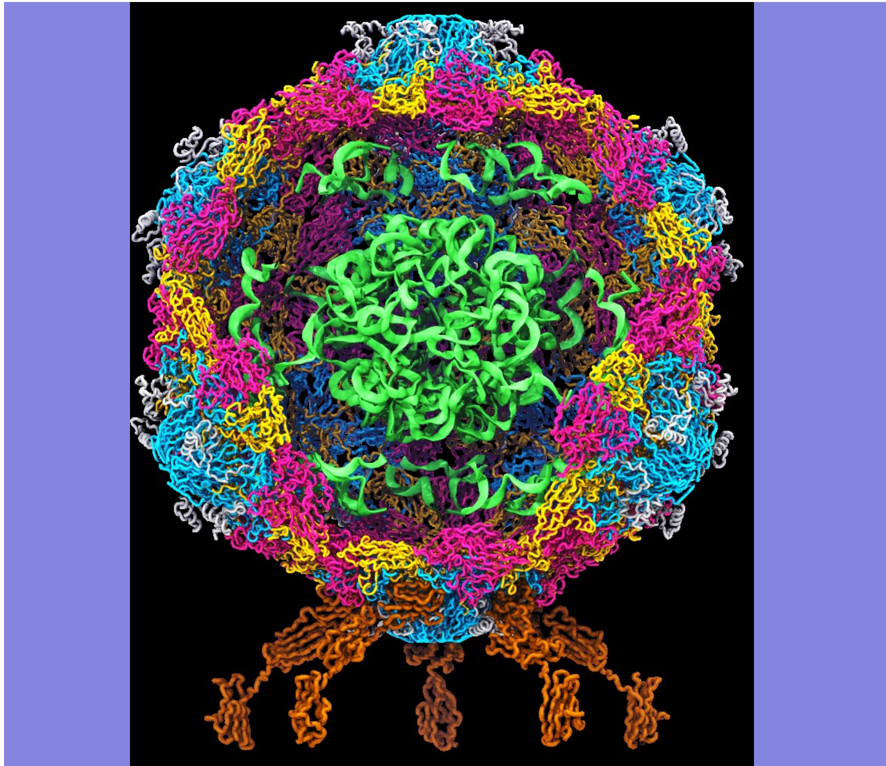
Goal: A Computational Microscope

Study the molecular machines in living cells

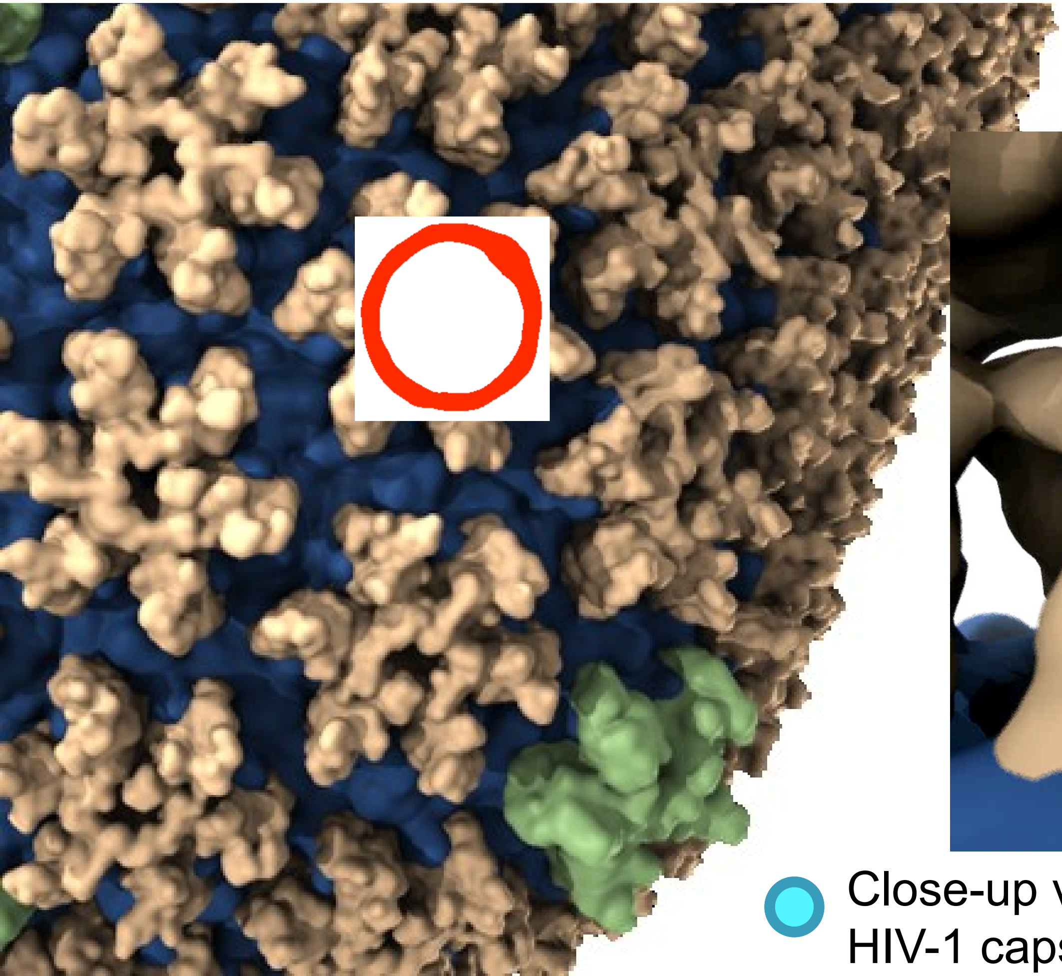
Ribosome: target for antibiotics



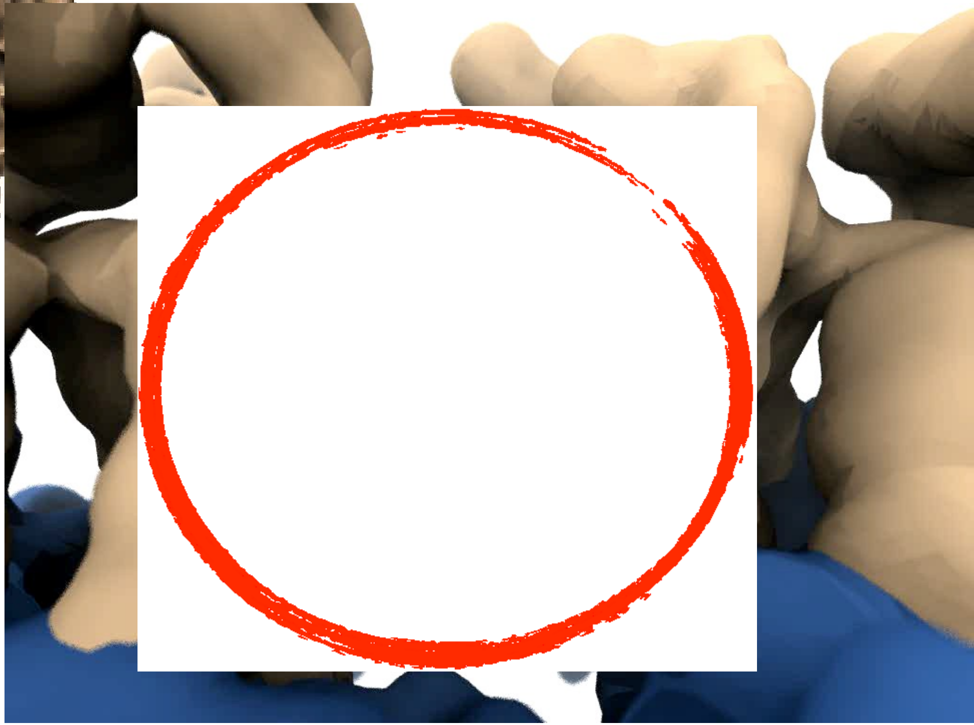
Poliovirus



Goal: Intuitive interactive viz. in crowded molecular complexes



Results from 64M atom, 1 μs sim!



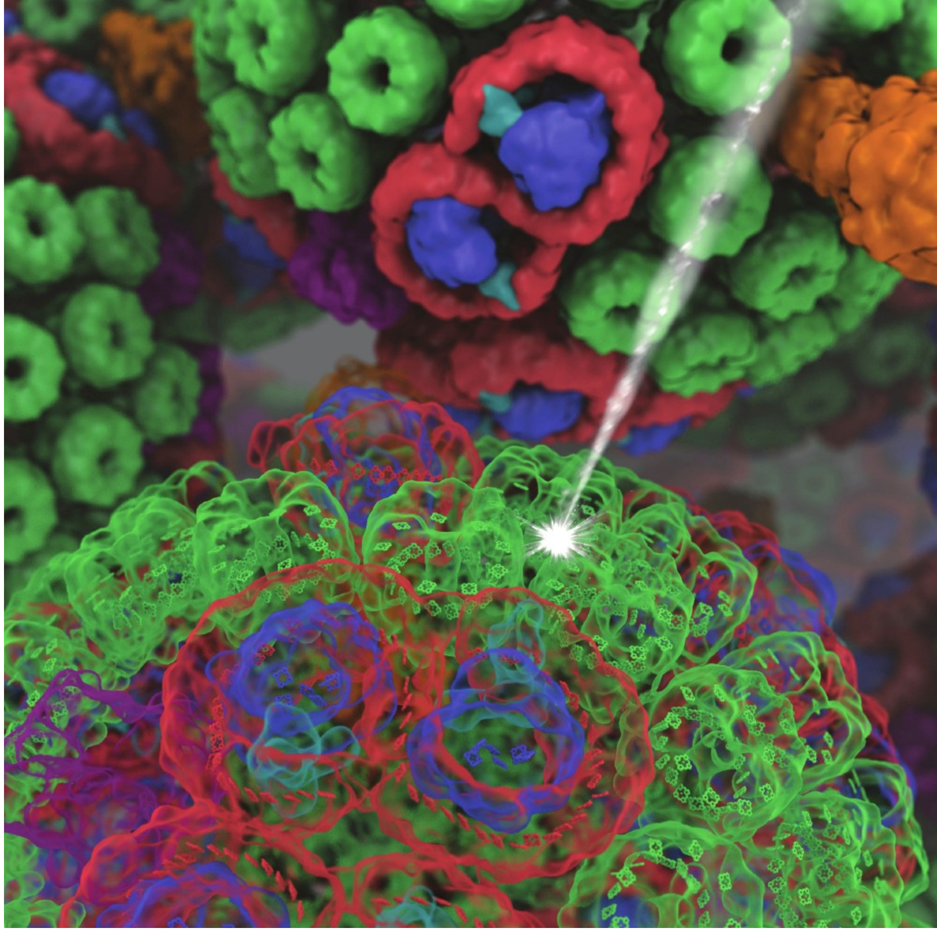
- Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers

High Fidelity Ray Tracing with OptiX

- Advanced rendering techniques save scientists time, produce images that are easier to interpret
- Ambient Occlusion, Depth of Field, high quality transparency, instancing, ….

- **Interactive RT** on laptop, desk, cloud
- Interactivity is critically important for scientists that need to obtain results without becoming a graphics expert

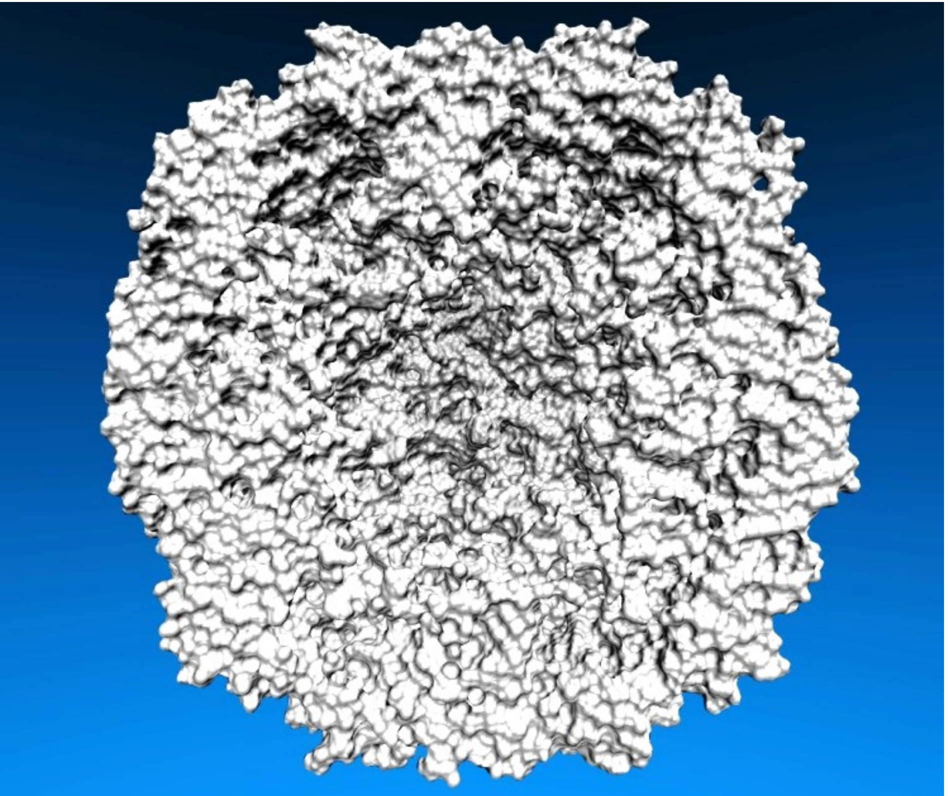
- Large-scale parallel rendering: in situ or post hoc visualization tasks
- **Stereoscopic panorama and full-dome projections**
- **Omnidirectional VR: YouTube, HMDs**



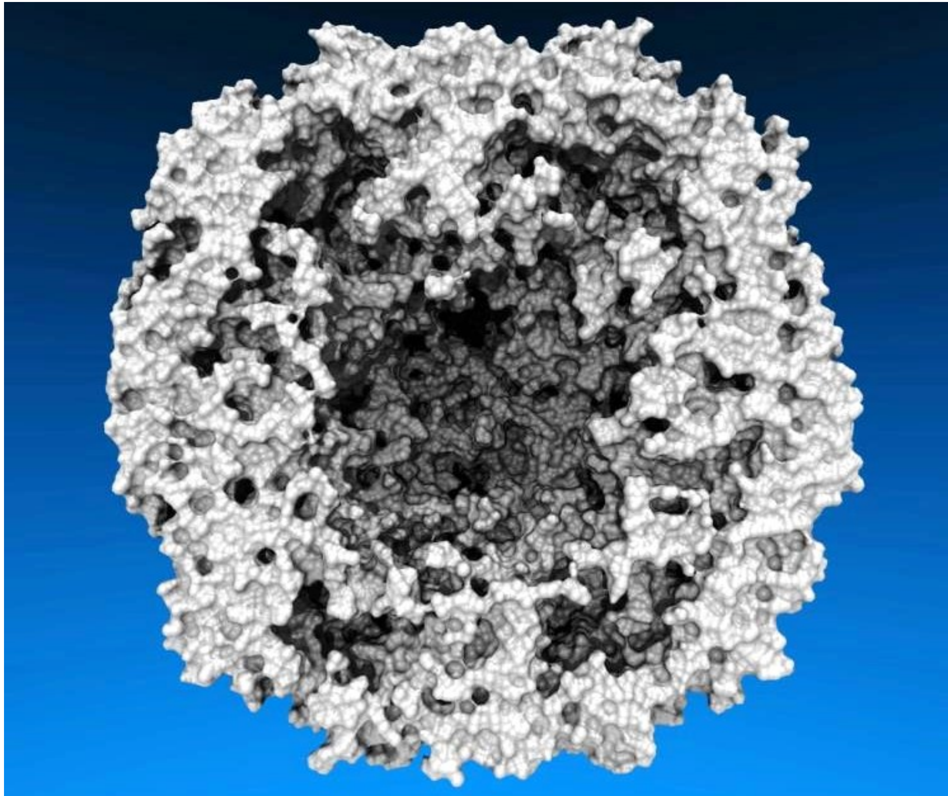
VMD/OptiX all-atom Chromatophore

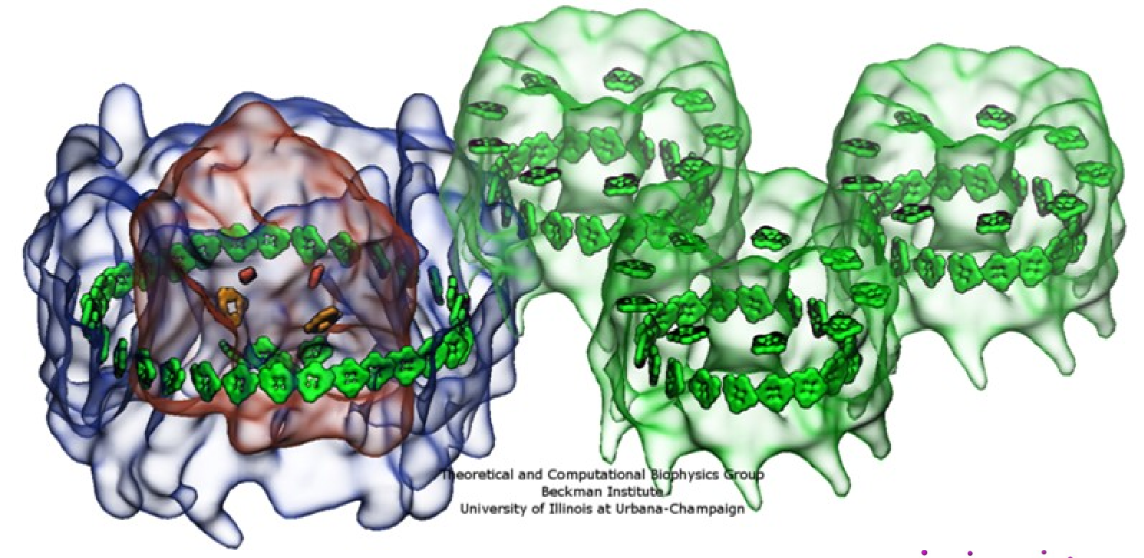
Lighting Comparison, STMV Capsid

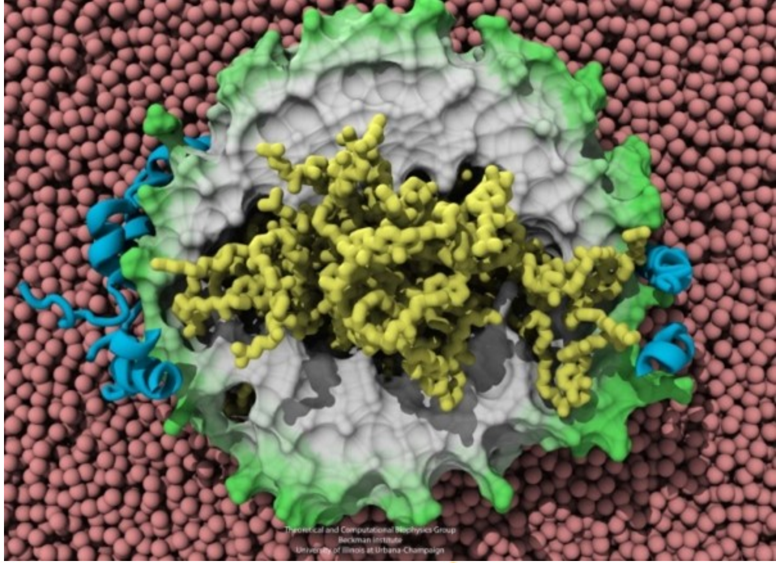
Two lights, no shadows

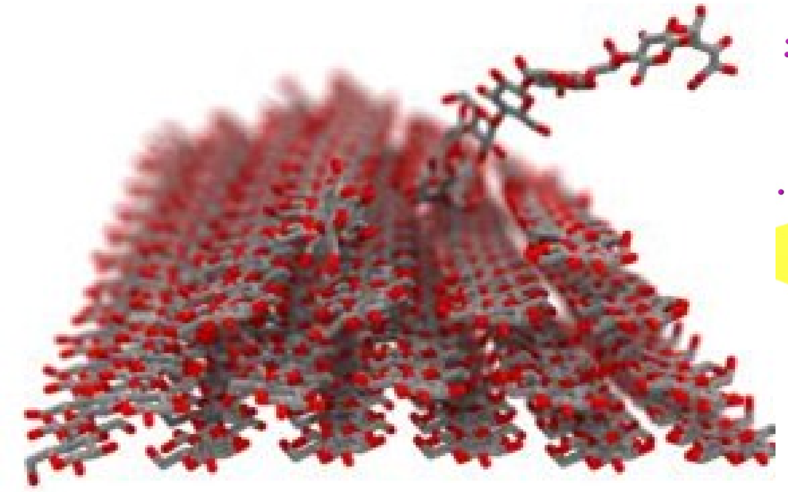


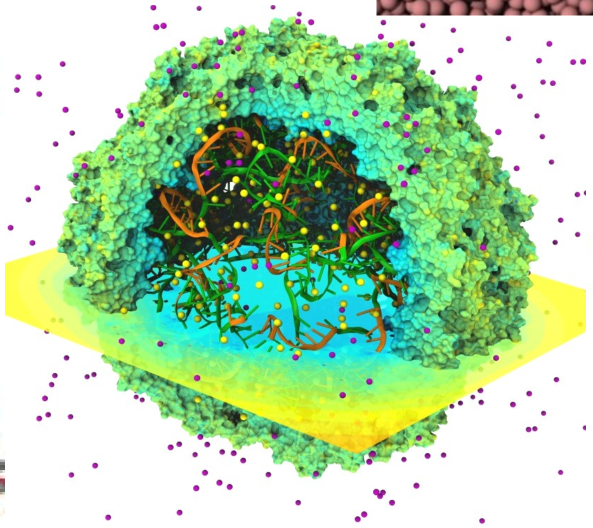
Ambient occlusion + two lights, 144 AO rays/hit

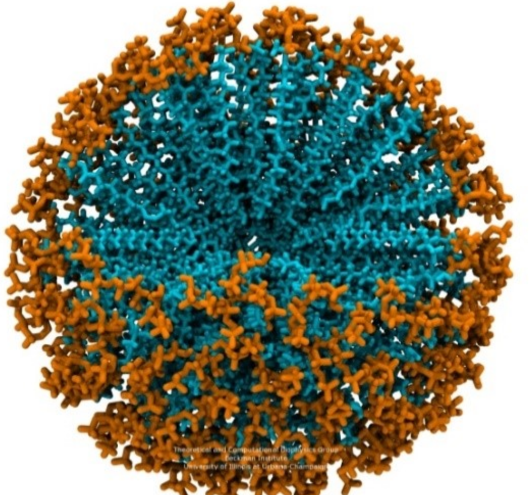



Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign



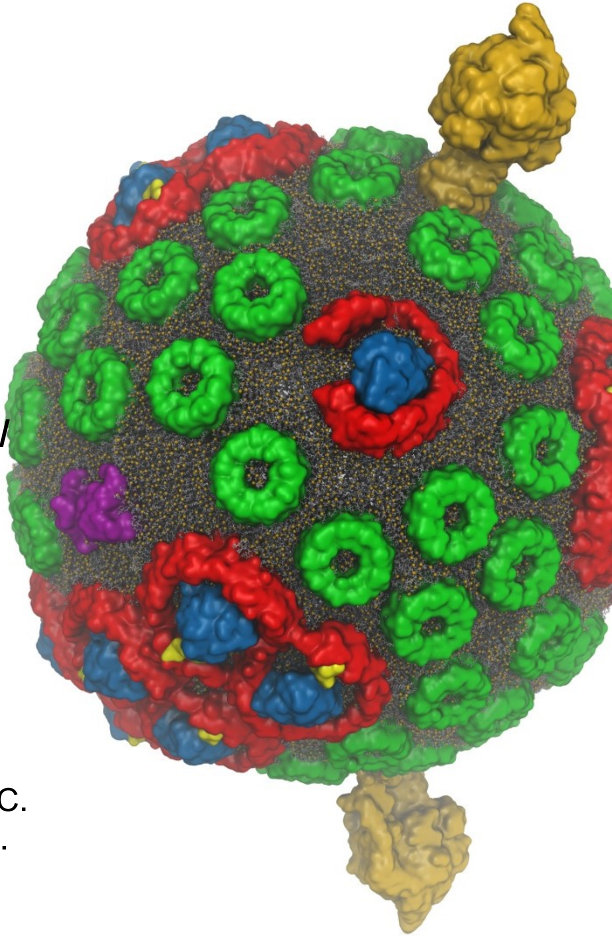






VMD w/ OptiX

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization
- Remote RT on NVIDIA GPU clusters
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- **GPU memory sharing via NVLink on Quadro, Tesla GPUs**
- **VMD+OptiX 5, NVIDIA NGC container: https://ngc.nvidia.com/registry/**
- **In-progress:**
  - **OptiX denoising support: fast turnaround w/ AO, DoF, etc**

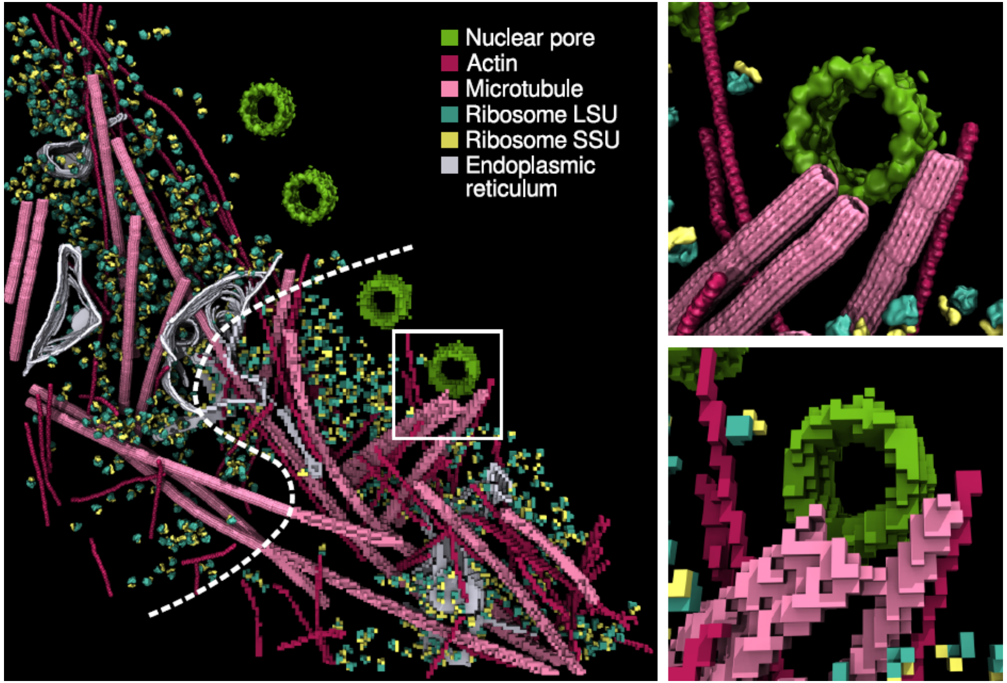


VMD/OptiX GPU Ray Tracing of all-atom Chromatophore w/ lipids.

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.

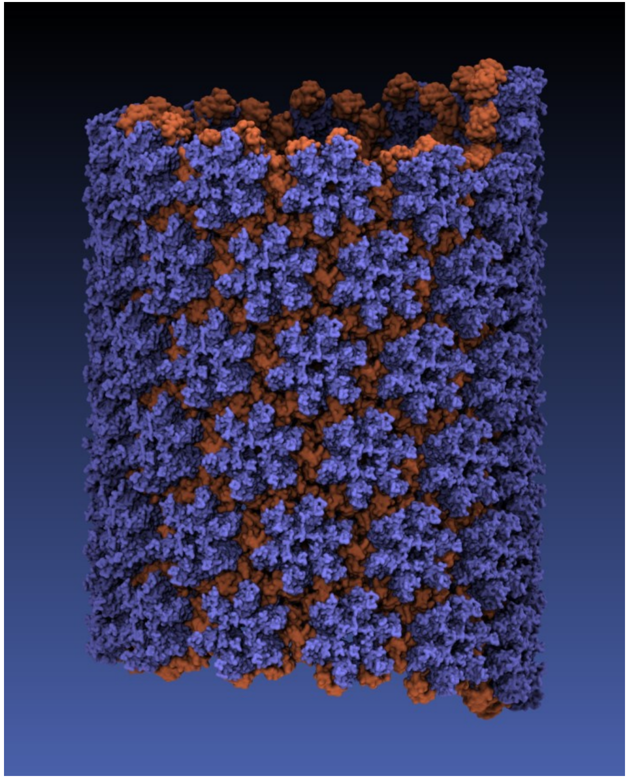
Interactive Ray Tracing of Cells

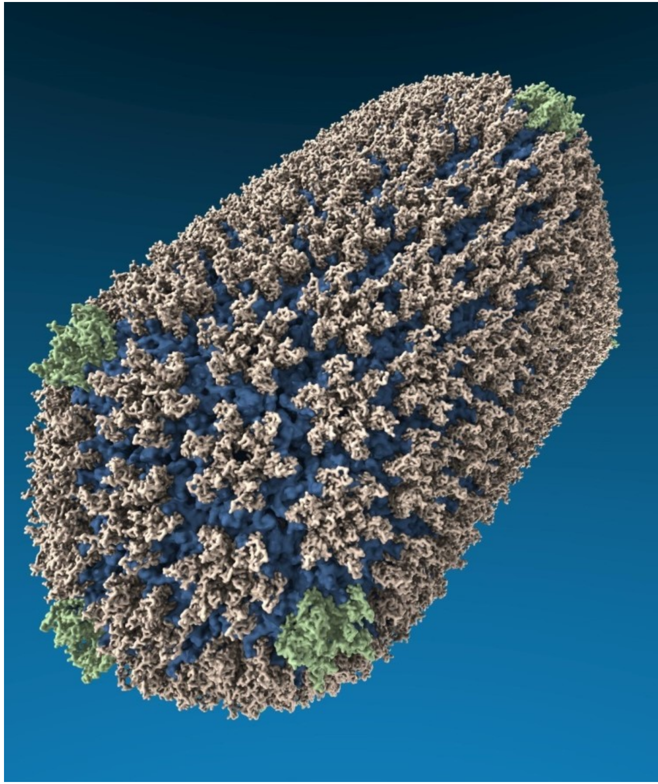
- High resolution cellular tomograms, **billions of voxels**
- Even isosurface or lattice site graphical representations involve ~100M geometric primitives
- 24GB GPUs allow interactive RT of large cellular tomograms
- **VMD exploits GPUs with NVLink and OptiX distribution of scene data across multiple GPUs for greater capacity and higher performance**



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

VMD "QuickSurf" Representation, Ray Tracing

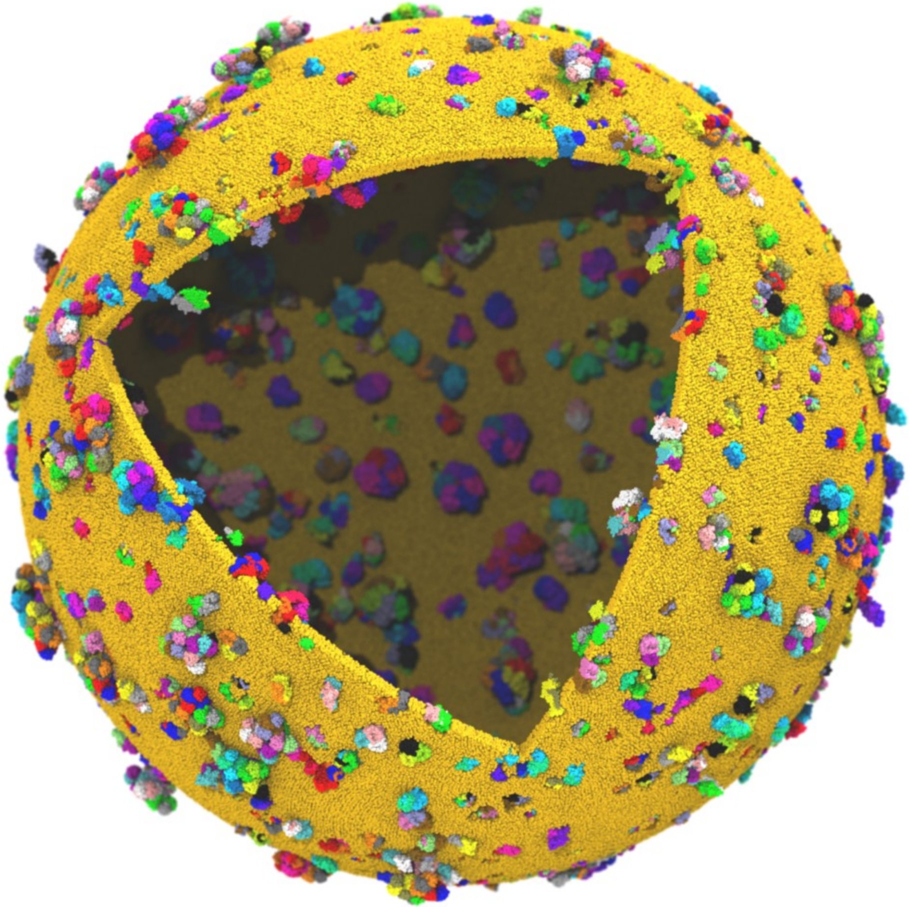




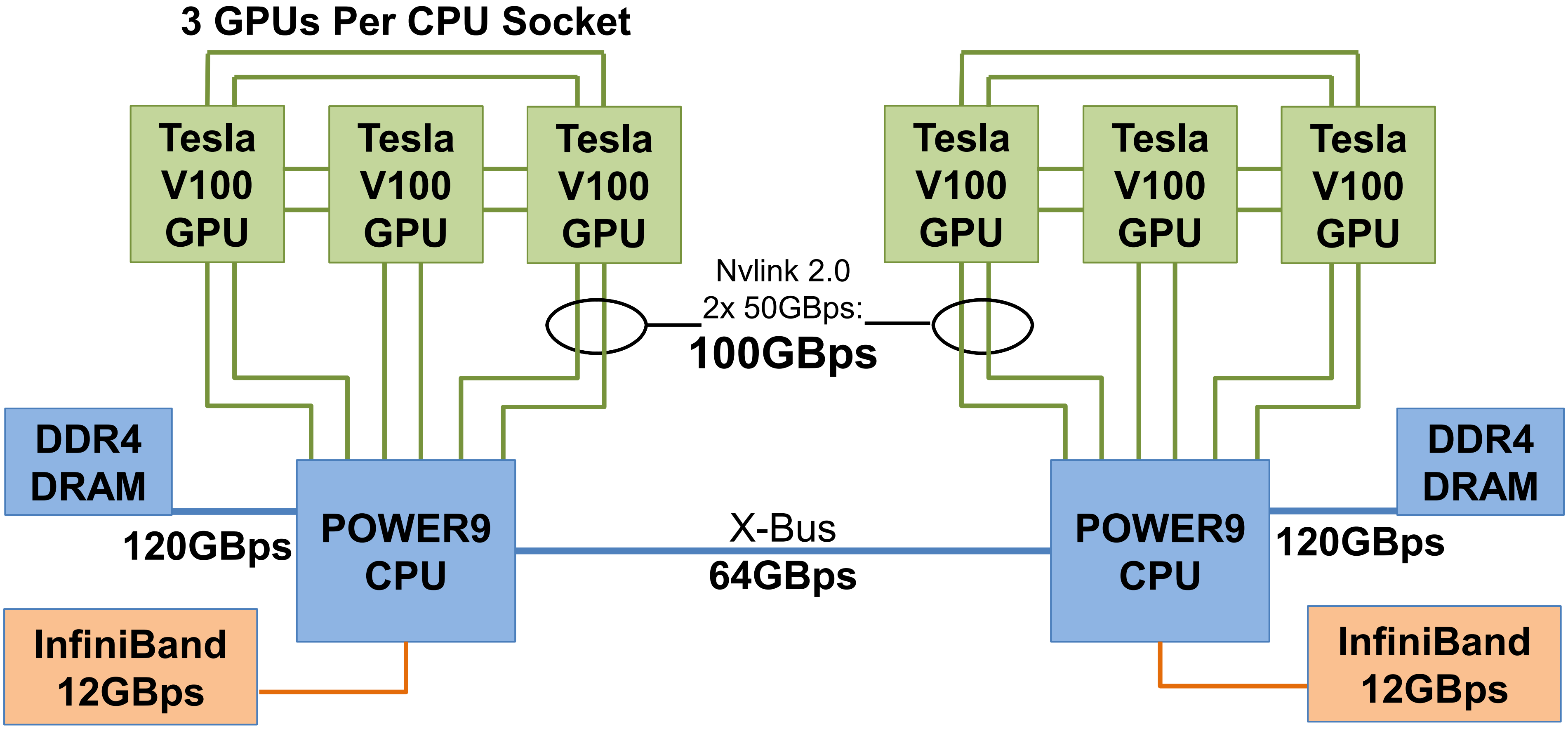
All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

Next Generation: Simulating a Proto-Cell

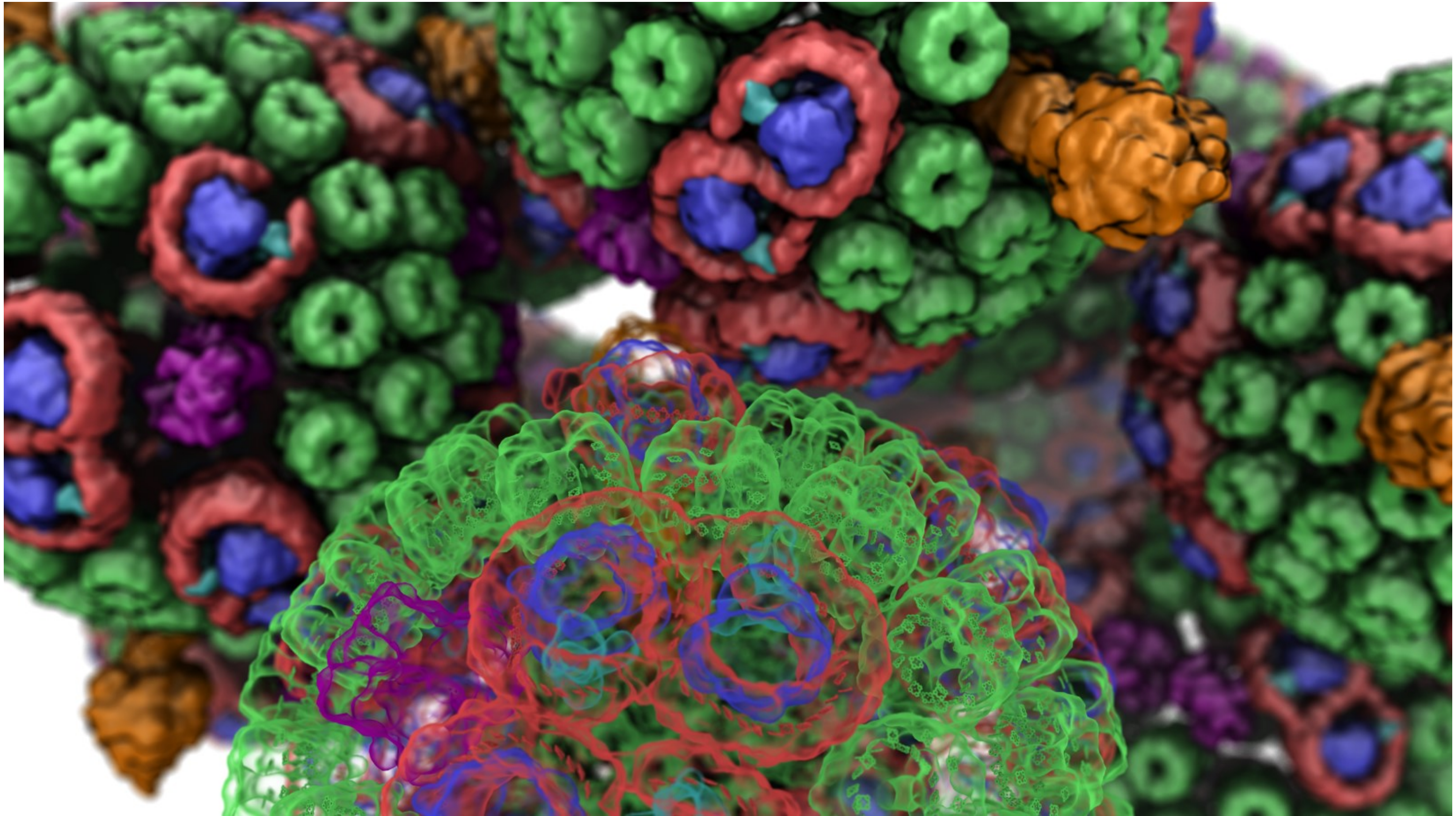
- **ORNL Summit: NVLink-connected Tesla V100 GPUs enable next-gen visualizations**
- 200nm diameter
- ~1 billion atoms w/ solvent
- ~1400 proteins in membrane



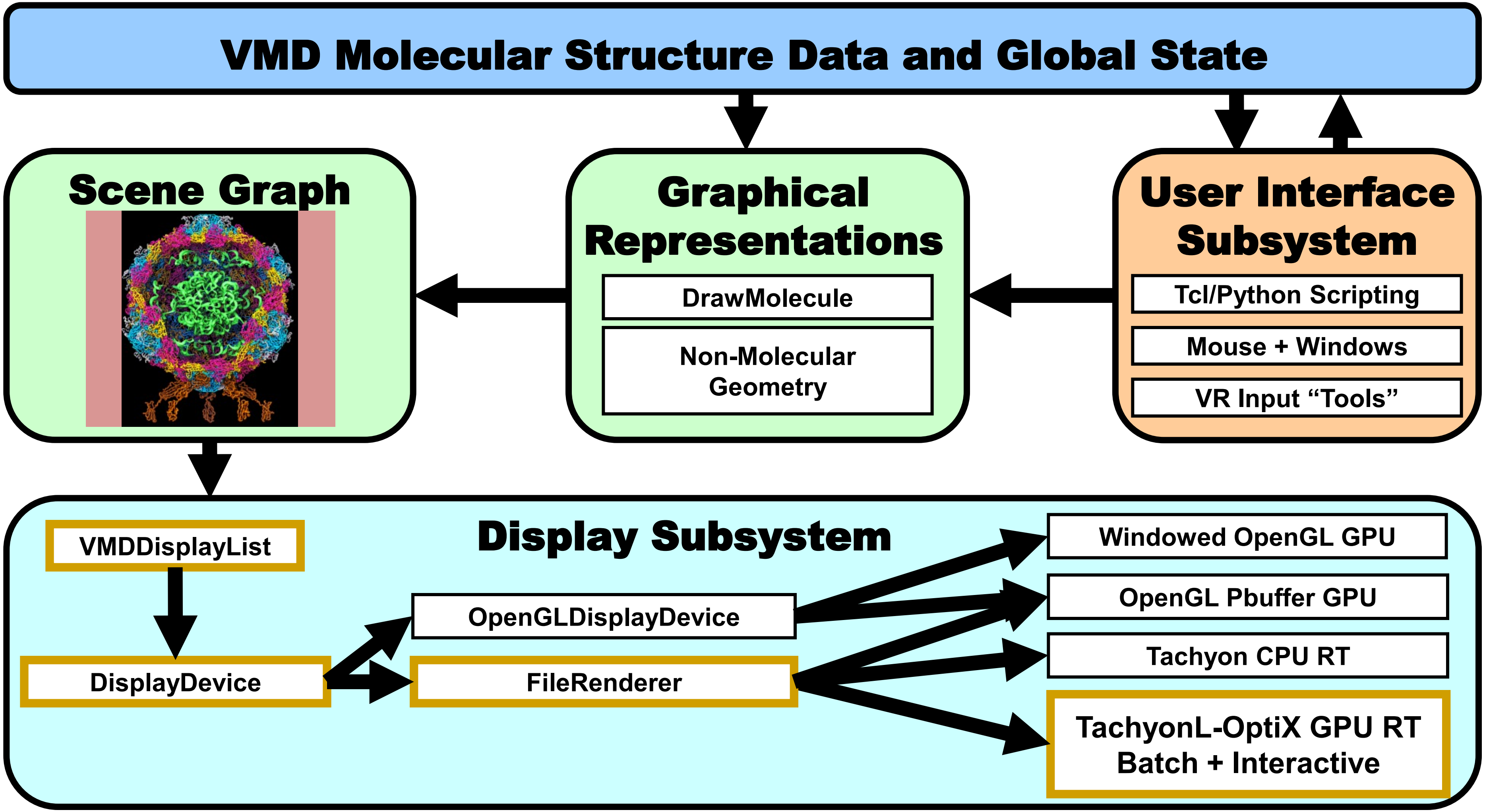
IBM AC922, ORNL Summit Node



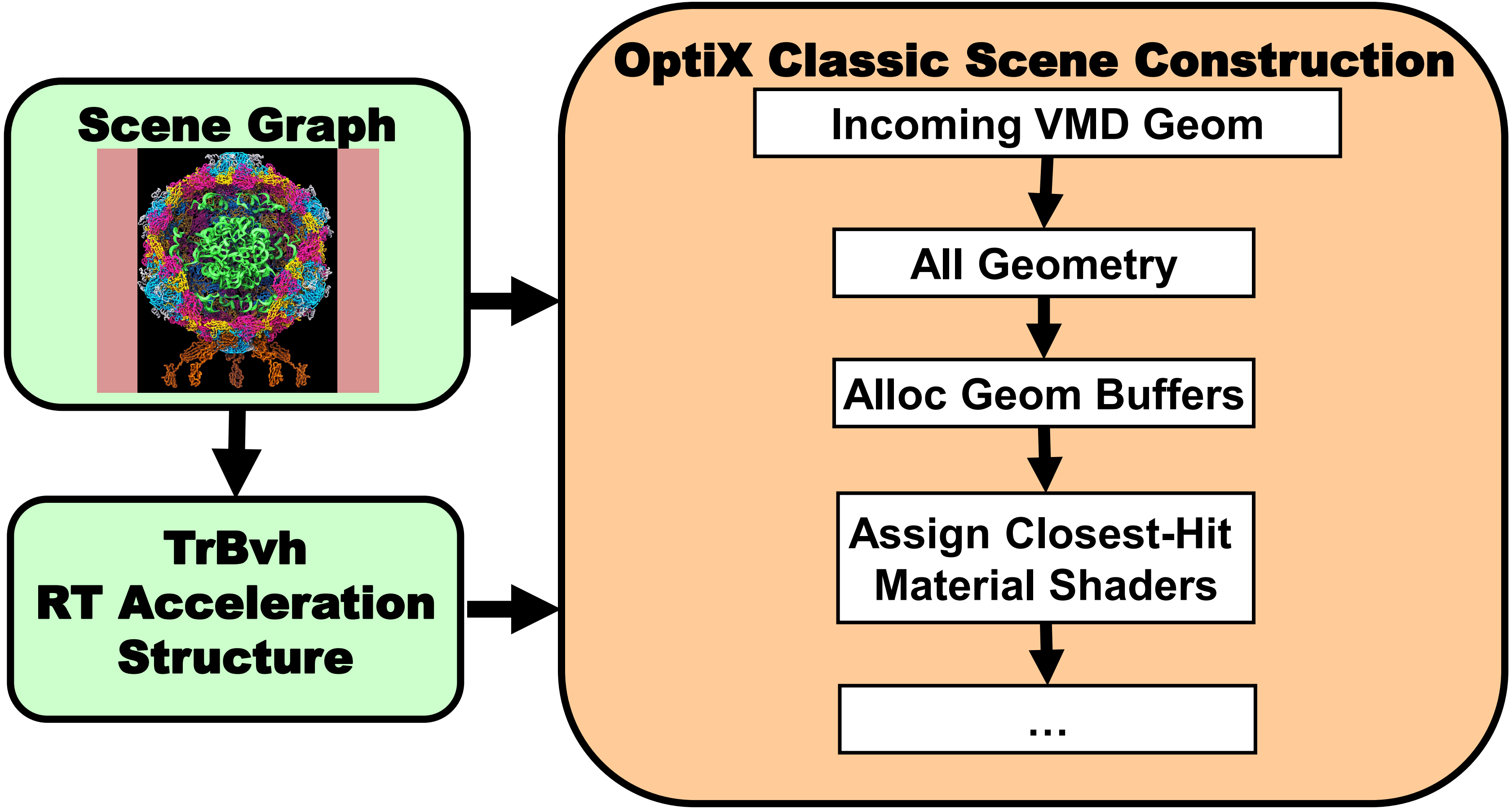
VMD/OpiX RTX Acceleration



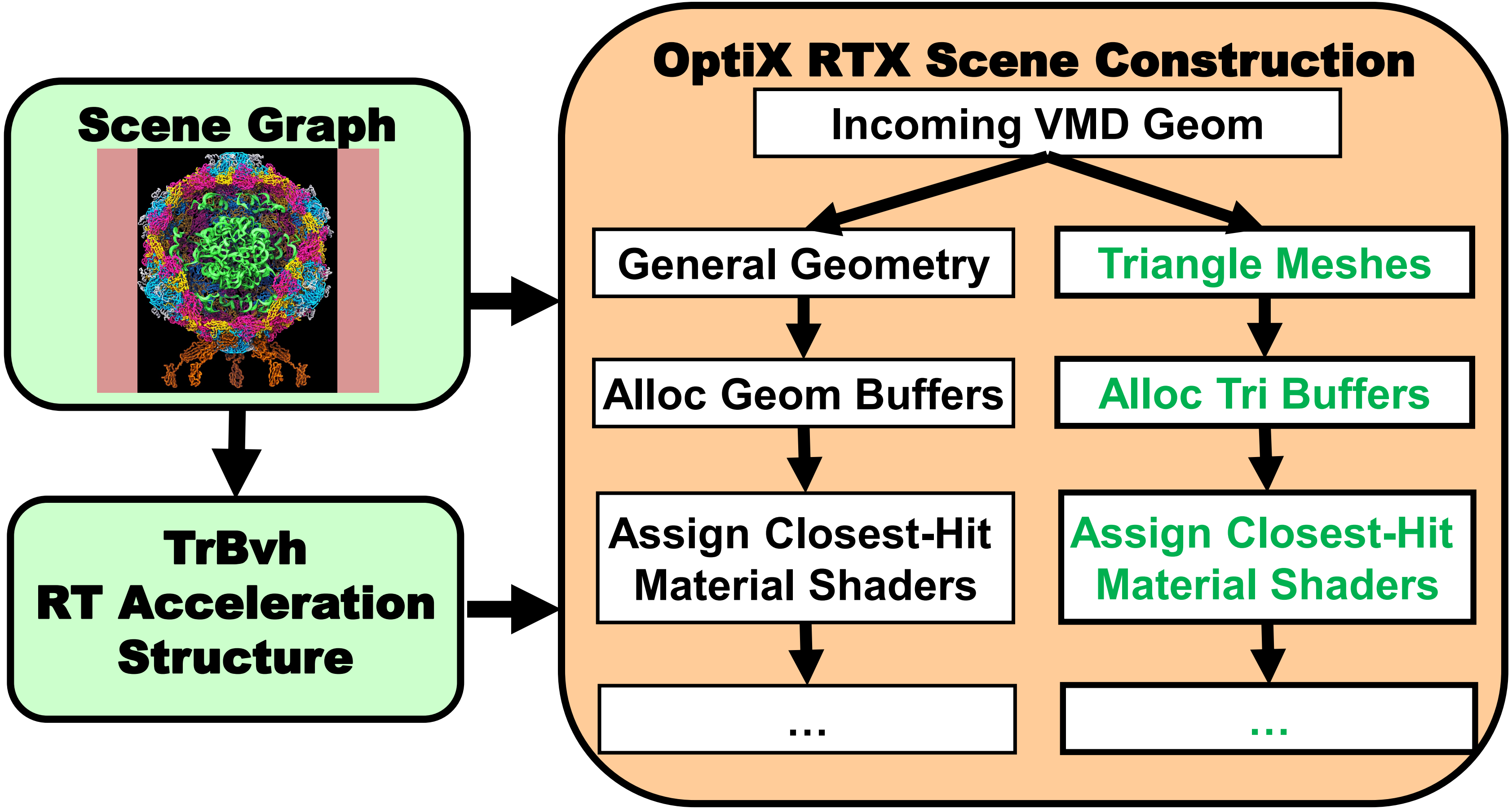
NIH


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

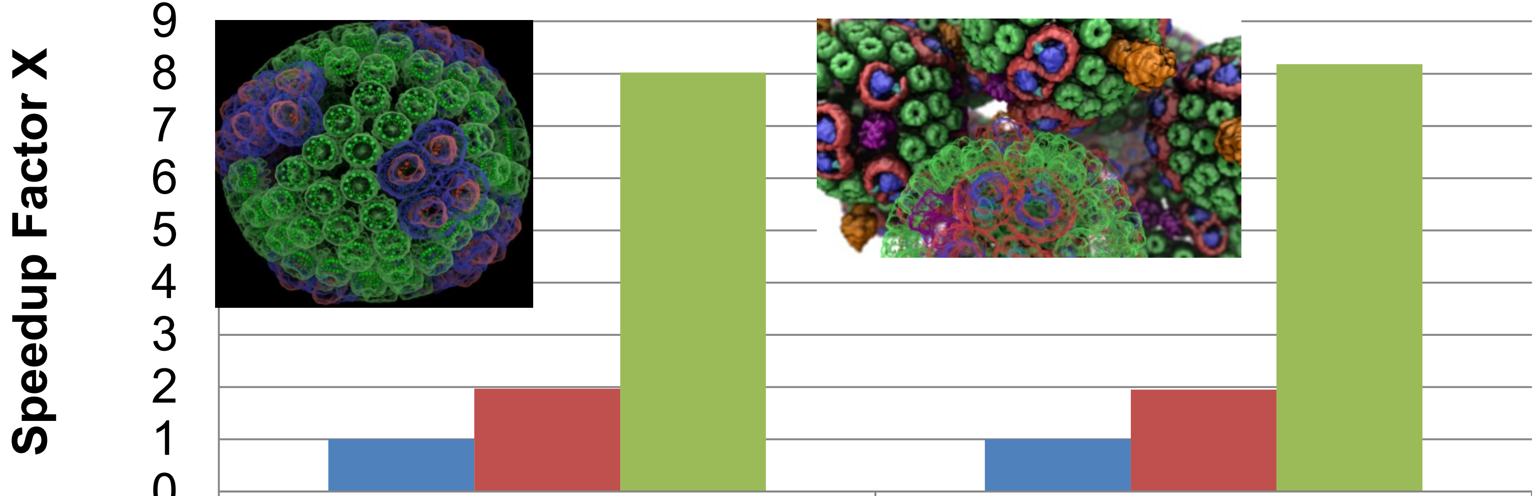
VMD Scene w/ OptiX Classic APIs



VMD Scene w/ OptiX RTX APIs



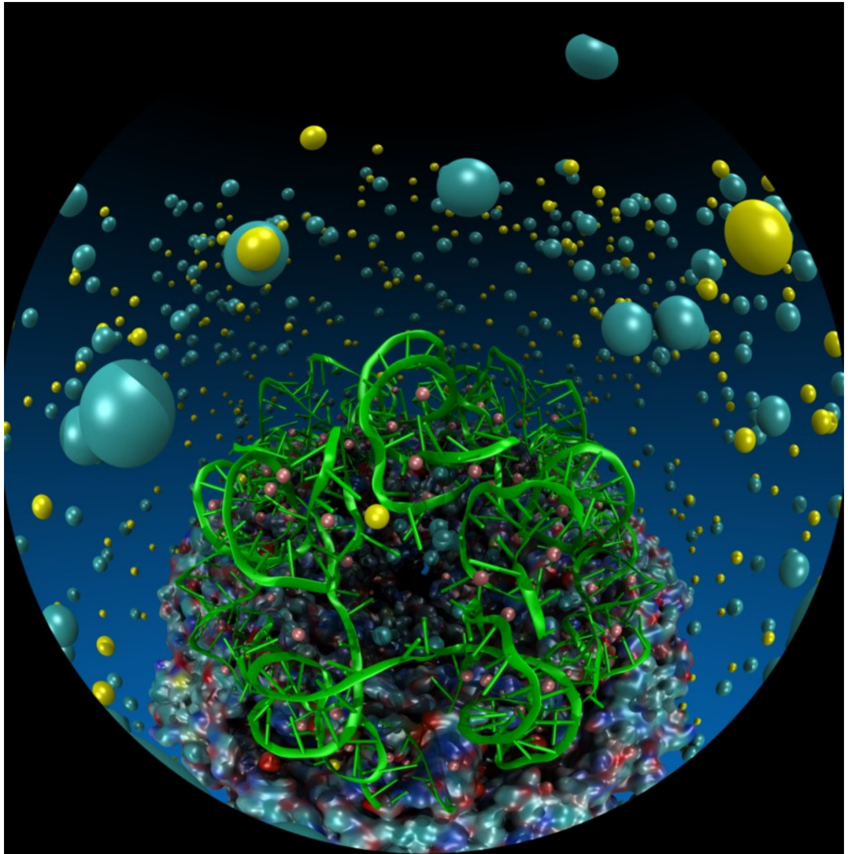
VMD OptiX RT performance on Quadro RTX 6000

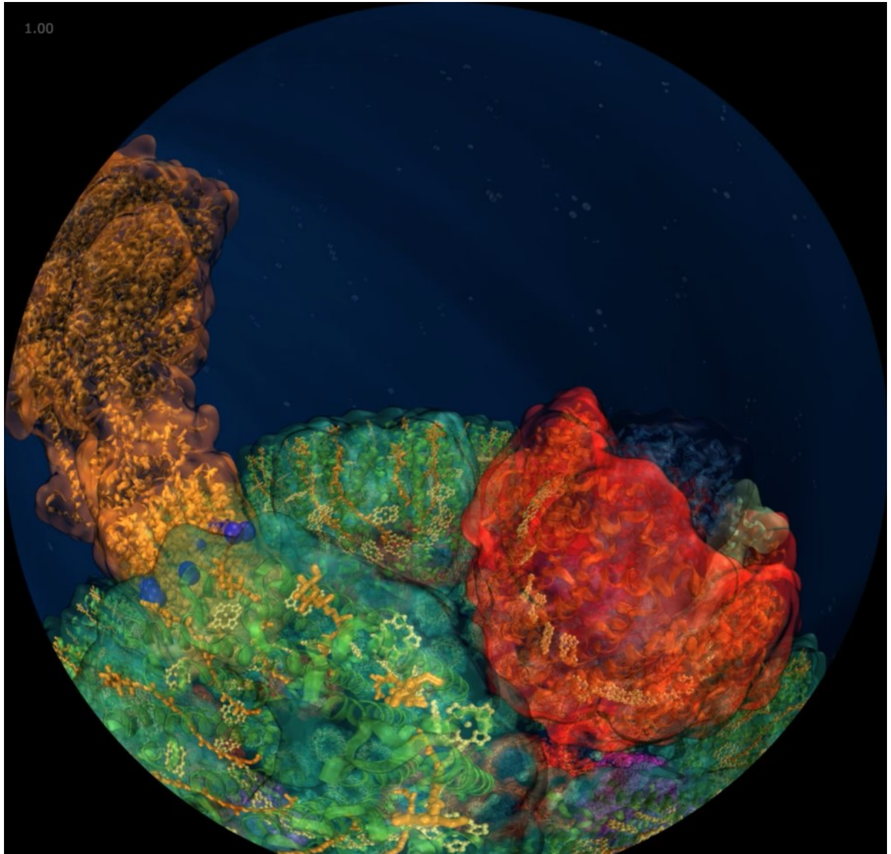


	Chromatophore @ 4Kx4K	Chrom Cell, 512x DoF @ 1080p
Quadro GV100	1	1
2x Quadro GV100	1.97	1.95
Quadro RTX 6000	8.02	8.18

Planetarium Dome Master Projections

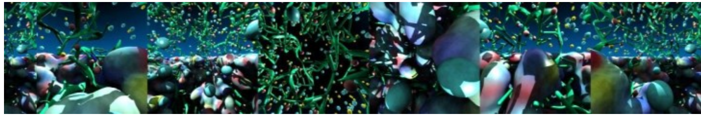
NSF CADENS Dome Show w/ NCSA AVL

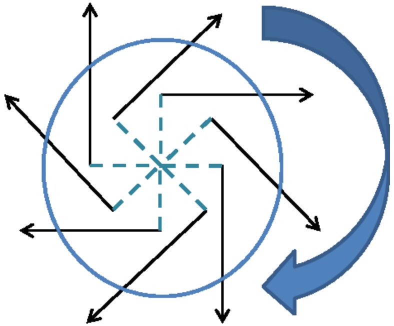


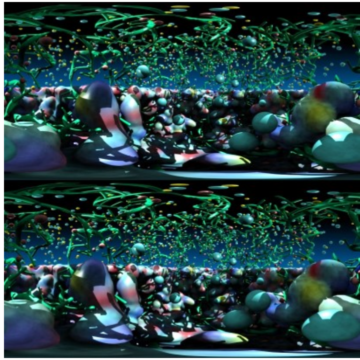


Omnidirectional Stereoscopic Ray Tracing

- **Ray trace 360° images and movies for Desk and VR HMDs: Oculus, Vive, Cardboard**
- Stereo spheremaps or cubemaps allow very high-frame-rate interactive OpenGL display
- **AO lighting, depth of field**, shadows, transparency, curved geometry, …

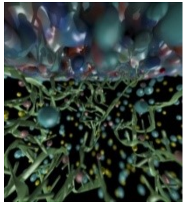


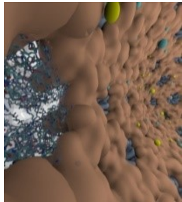


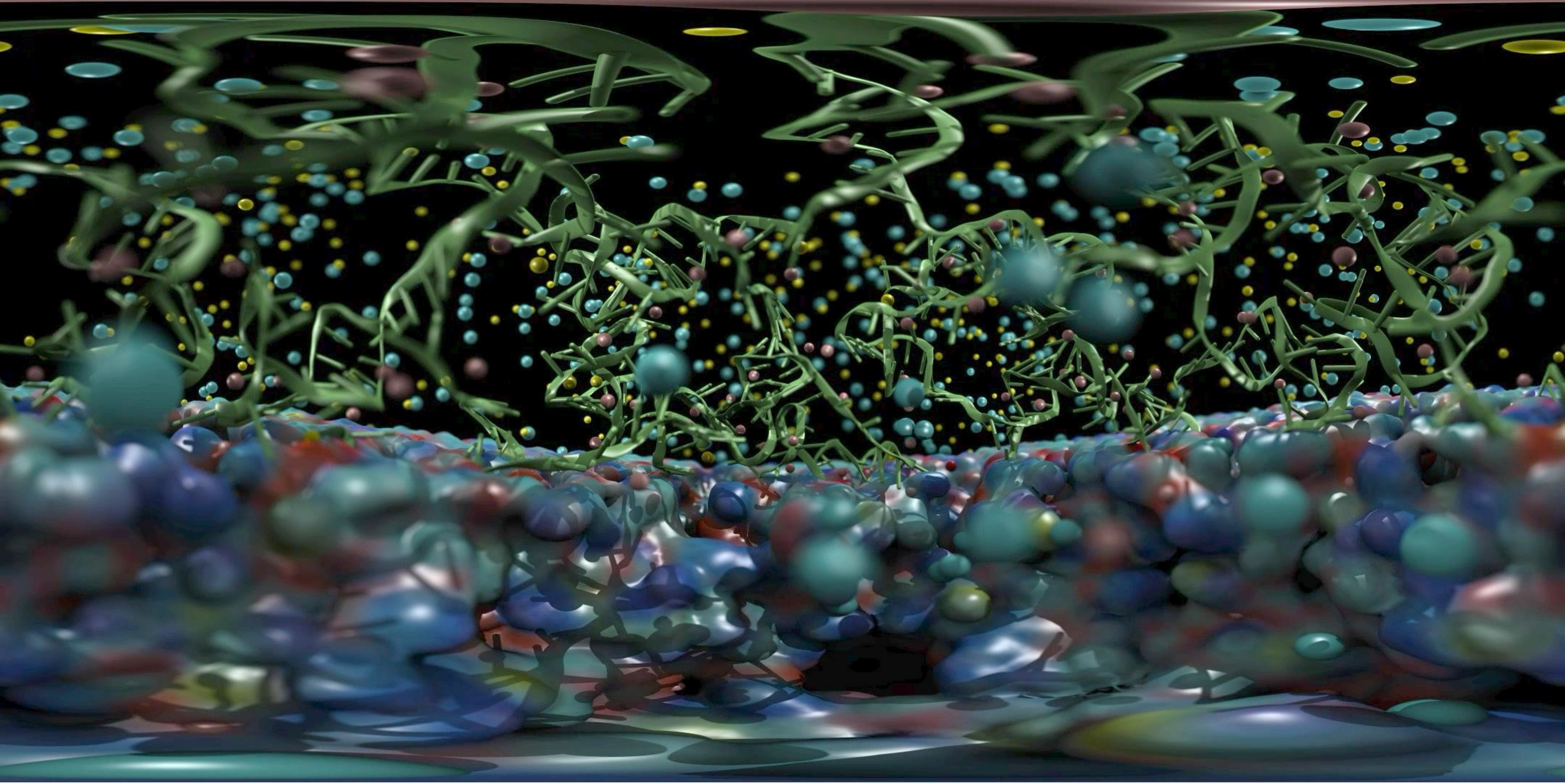


Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone, et al. J. Parallel Computing, 55:17-27, 2016.

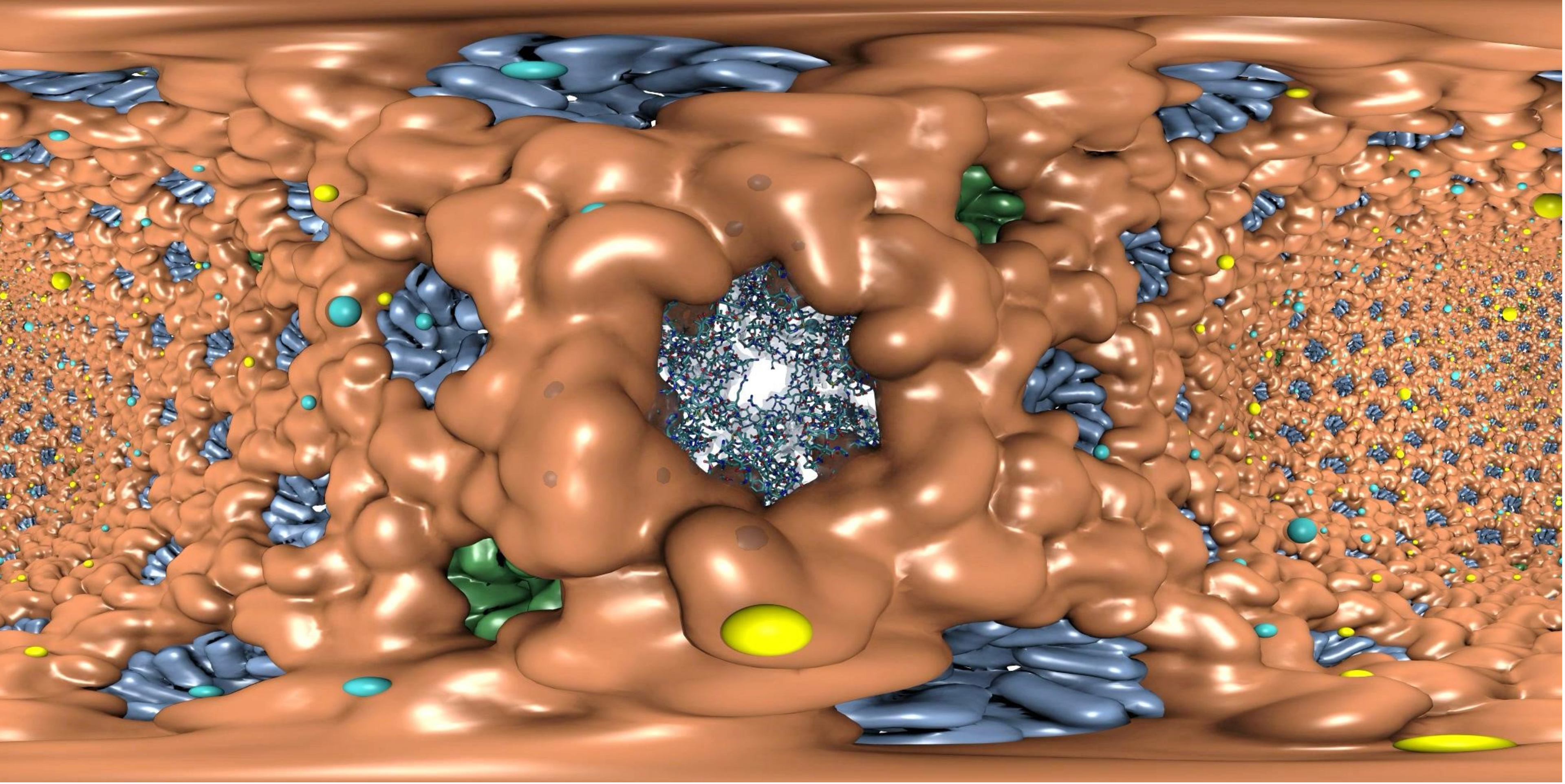
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), pp. 1048-1057, 2016.



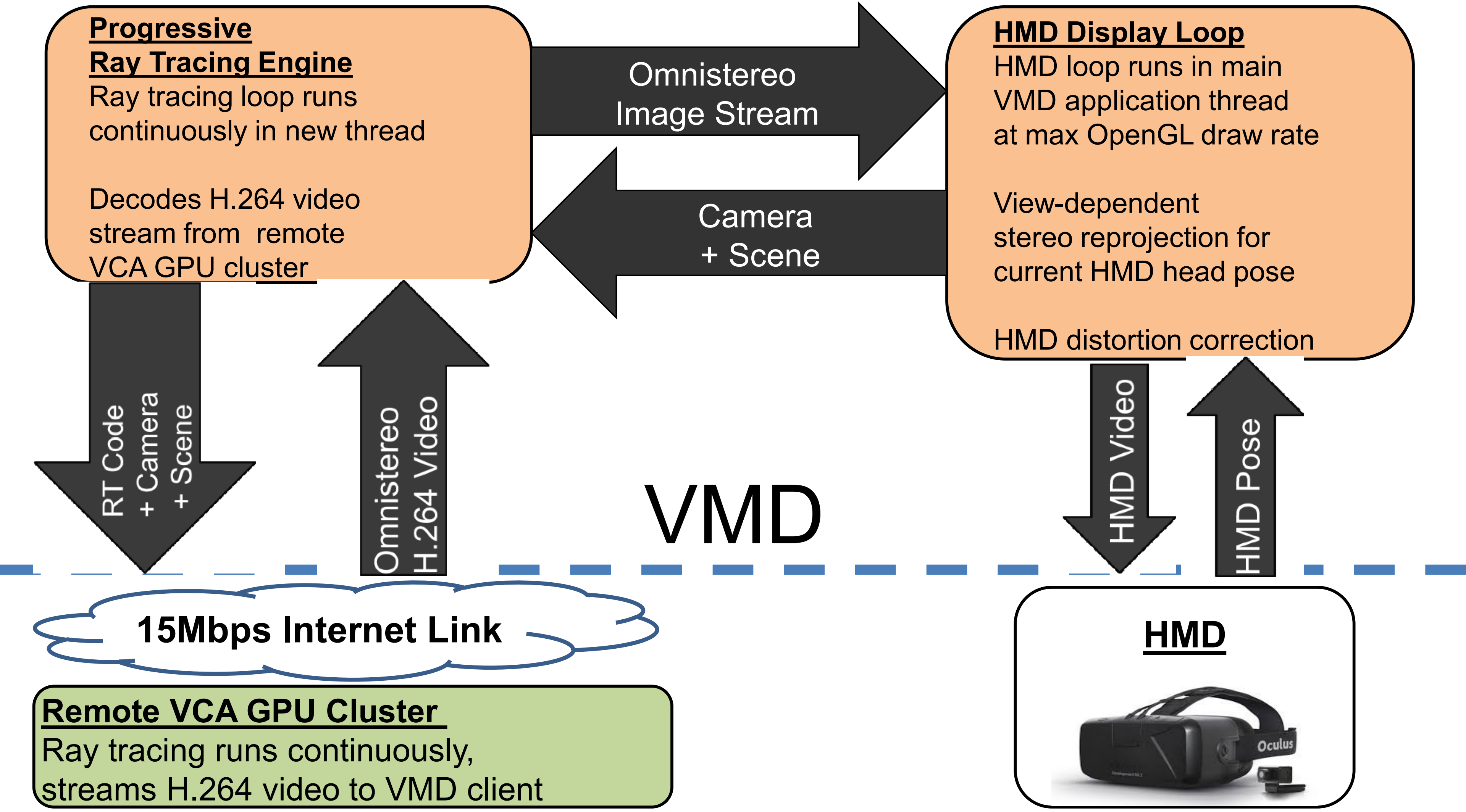




Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …



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

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 Workshops (IPDPSW), pp. 1048-1057, 2016.

Making Our Research Tools Easily Accessible

- Docker "container" images available in NVIDIA NGC registry
  - Users obtain Docker images via registry, download and run on the laptop, workstation, cloud, or supercomputer of their choosing
  - **https://ngc.nvidia.com/registry/**
  - **https://ngc.nvidia.com/registry/hpc-vmd**

- Cloud based deployment
  - Full virtual machines (known as "AMI" in Amazon terminology)
  - Amazon AWS EC2 GPU-accelerated instances:

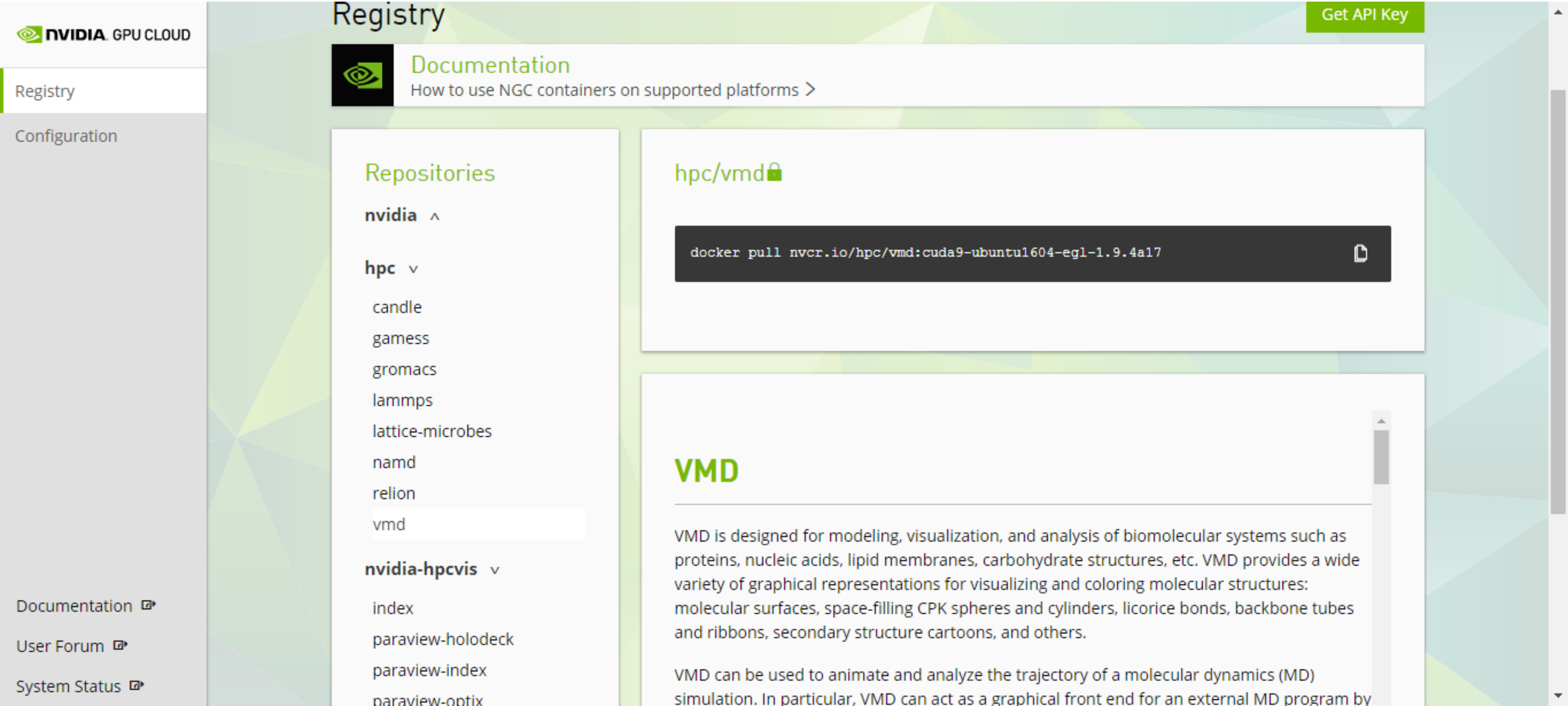
  http://www.ks.uiuc.edu/Research/cloud/

Clusters, Supercomputers

Workstations,
Servers,
Cloud

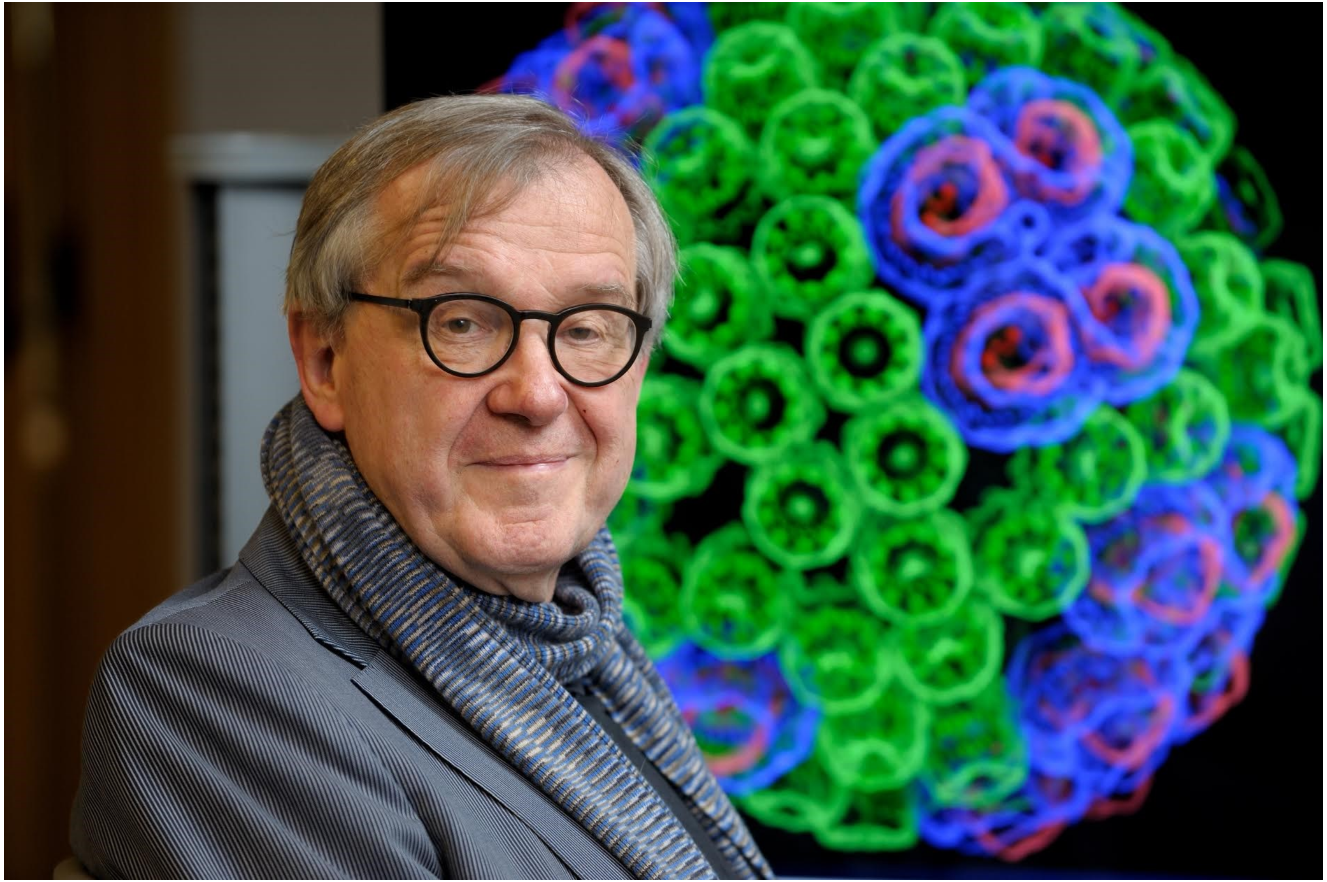
Molecular dynamics-based refinement and validation for sub-5 Å cryo-electron microscopy maps. Abhishek Singharoy, Ivan Teo, Ryan McGreevy, John E. Stone, Jianhua Zhao, and Klaus Schulten. *eLife*, 10.7554/eLife.16105, 2016. (66 pages).
QwikMD-integrative molecular dynamics toolkit for novices and experts. Joao V. Ribeiro, Rafael C. Bernardi, Till Rudack, John E. Stone, James C. Phillips, Peter L. Freddolino, and Klaus Schulten. *Scientific Reports*, 6:26536, 2016.
High performance molecular visualization: In-situ and parallel rendering with EGL. John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014-1023, 2016.

VMD / NAMD / LM, NGC Containers



Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- NVIDIA CUDA and OptiX teams
- Funding:
  - NIH support: P41GM104601
  - DOE INCITE, ORNL Titan: DE-AC05-00OR22725
  - NSF Blue Waters:
    NSF OCI 07-25070, PRAC "The Computational Microscope", ACI-1238993, ACI-1440026



“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

Related Publications
http://www.ks.uiuc.edu/Research/gpu/

- **NAMD goes quantum: An integrative suite for hybrid simulations.** Melo, M. C. R.; Bernardi, R. C.; Rudack T.; Scheurer, M.; Riplinger, C.; Phillips, J. C.; Maia, J. D. C.; Rocha, G. D.; Ribeiro, J. V.; Stone, J. E.; Neese, F.; Schulten, K.; Luthey-Schulten, Z.; Nature Methods, 2018. (**In press)**
- **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.

Related Publications

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

- **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.
- **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.
- **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.

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. E. 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.
- **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.

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. E. 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.
- **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.