

S5386—Publication-Quality Ray Tracing of Molecular Graphics with OptiX

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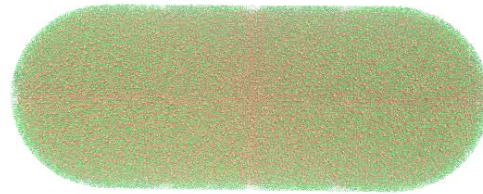
S5386, GPU Technology Conference

9:00-9:25, Room LL21E, San Jose Convention Center,
San Jose, CA, Thursday March 19, 2015

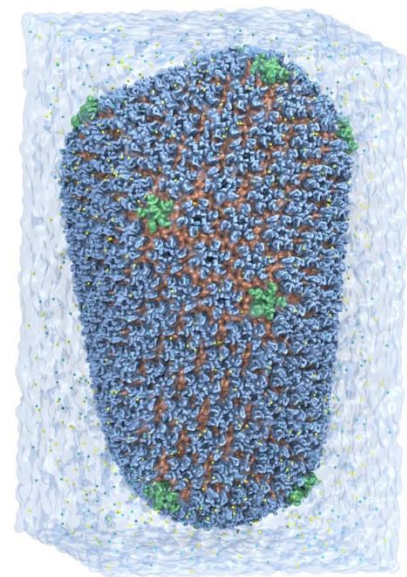


VMD – “Visual Molecular Dynamics”

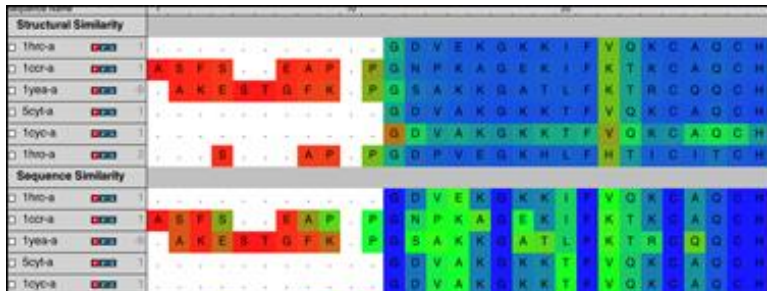
- Visualization and analysis of:
 - molecular dynamics simulations
 - particle systems and whole cells
 - cryoEM densities, volumetric data
 - quantum chemistry calculations
 - sequence information
- User extensible w/ scripting and plugins
- <http://www.ks.uiuc.edu/Research/vmd/>



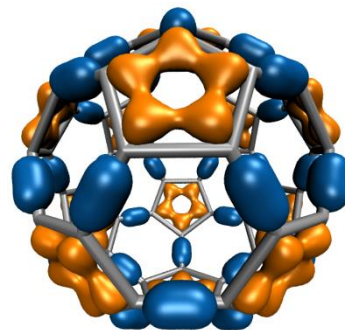
Whole Cell Simulation



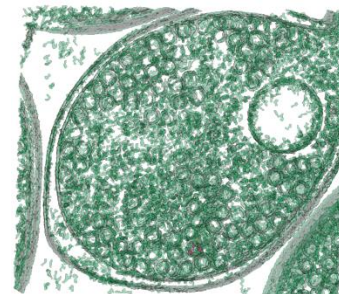
MD Simulations



Sequence Data



Quantum Chemistry

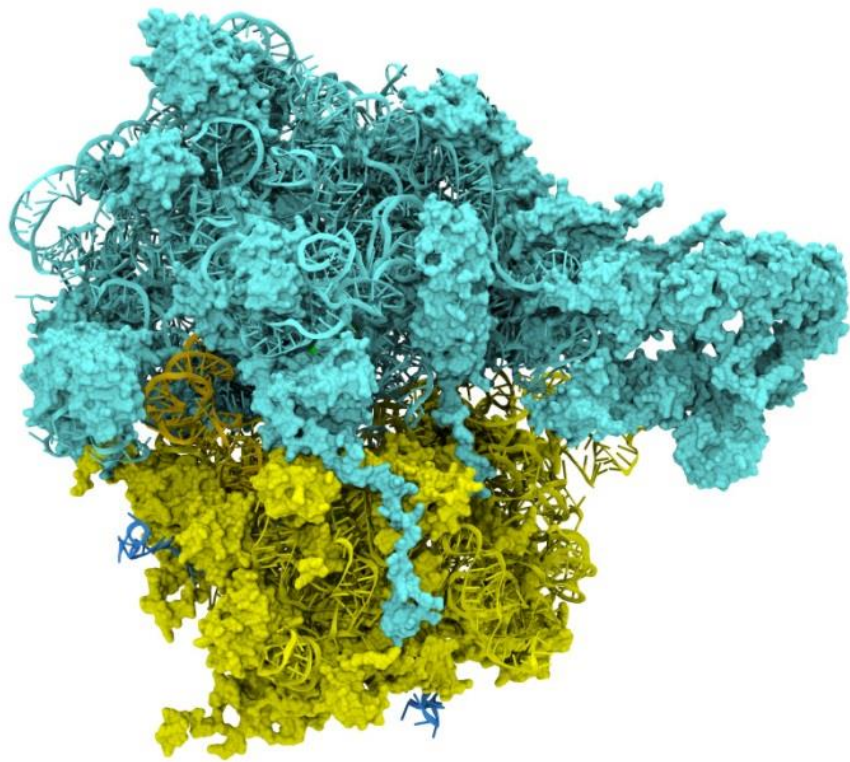


CryoEM, Cellular Tomography

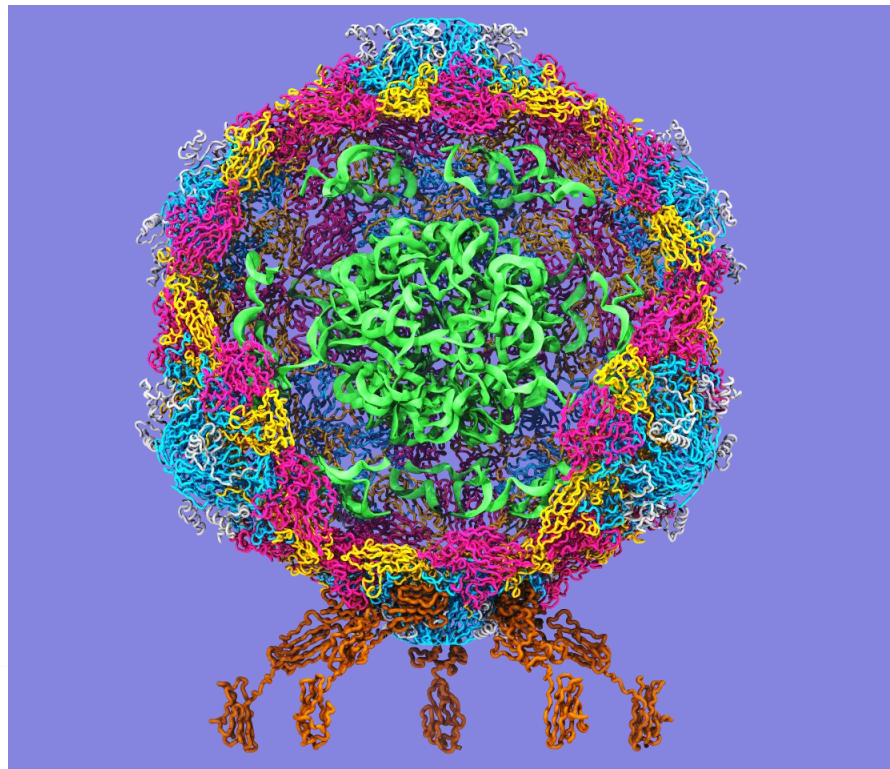
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

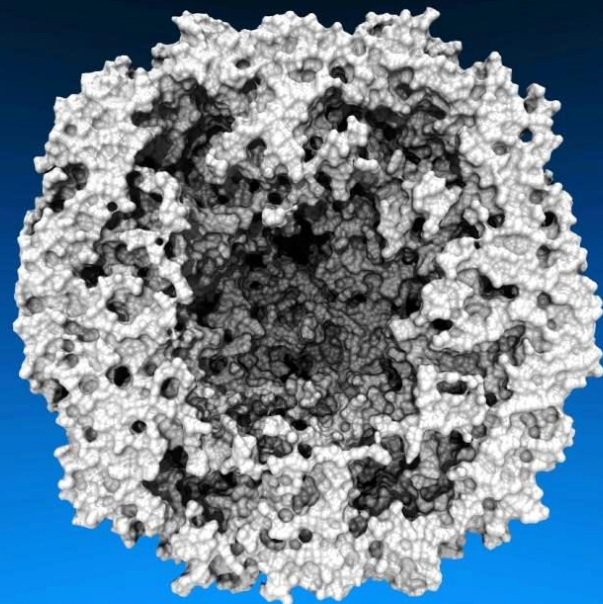
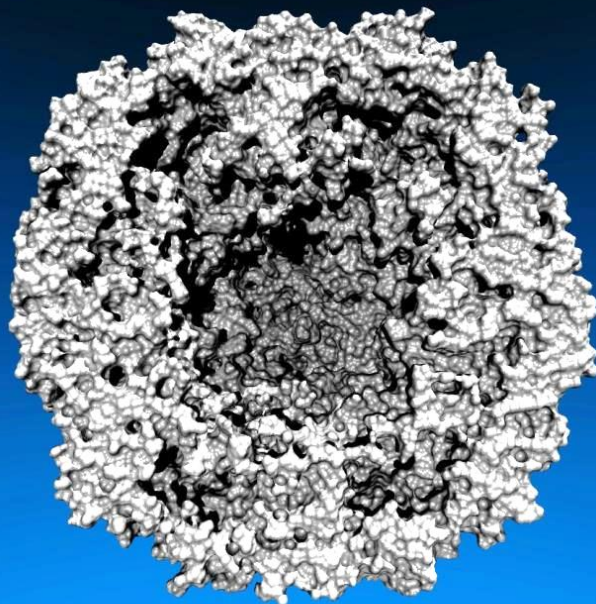
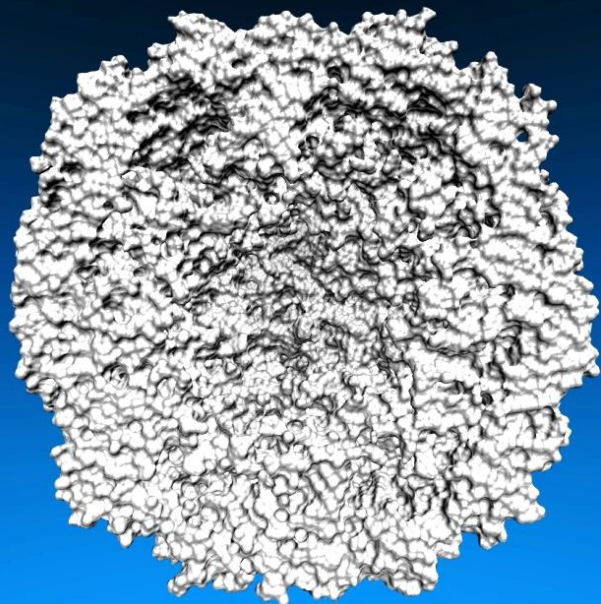


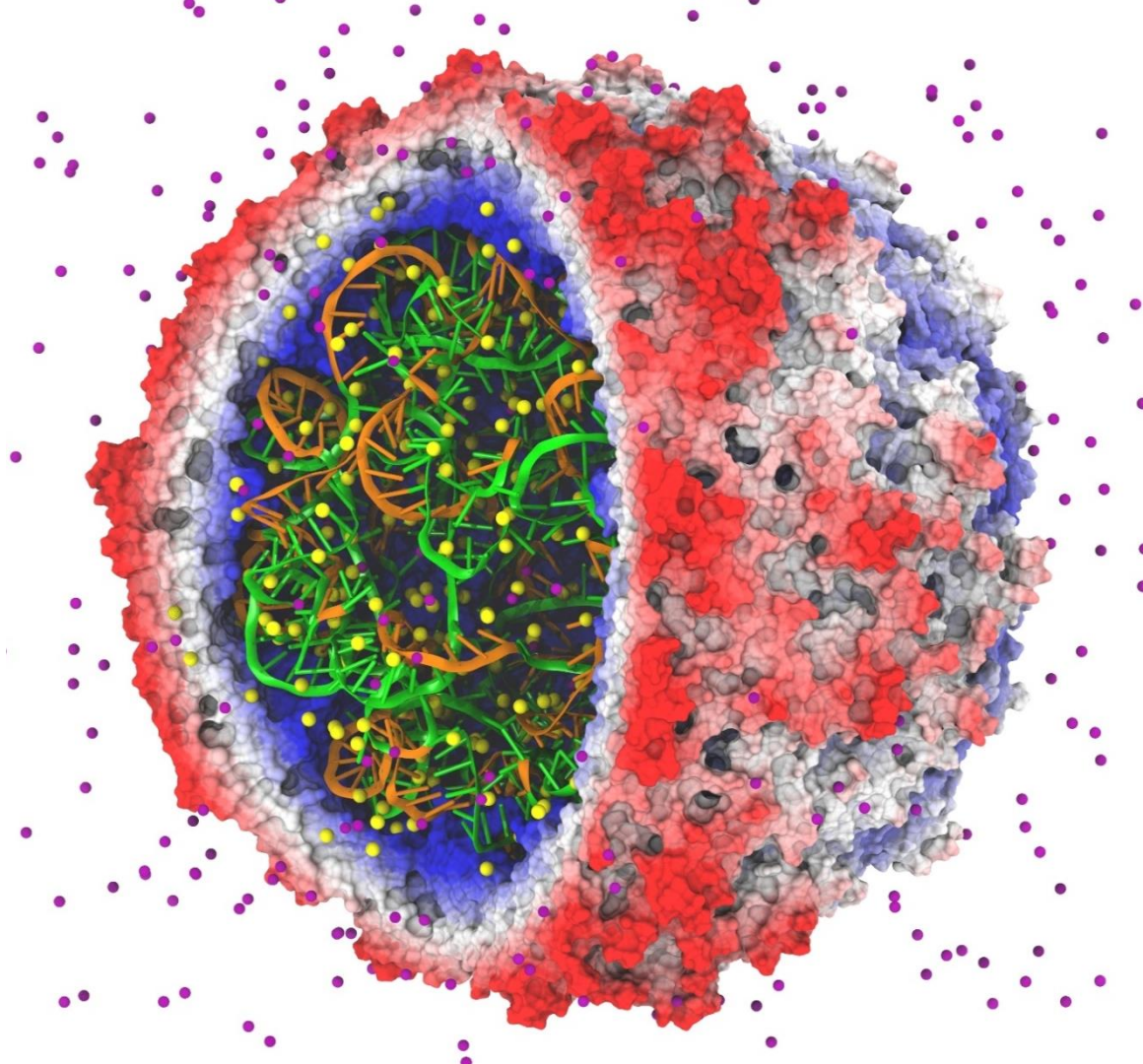
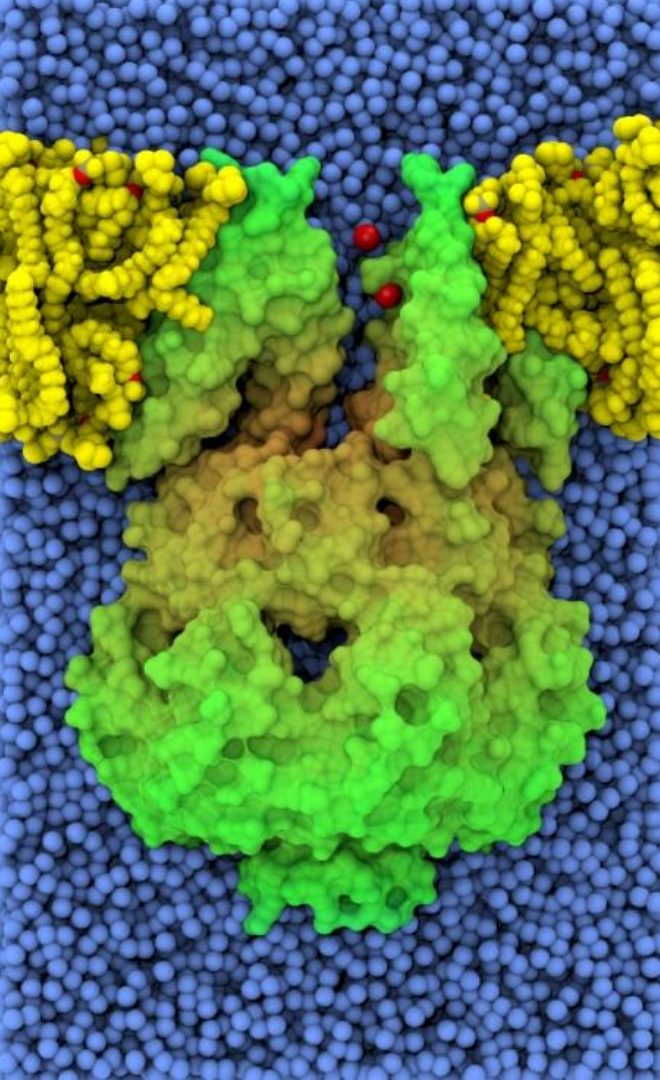
Lighting Comparison

Two lights, no shadows

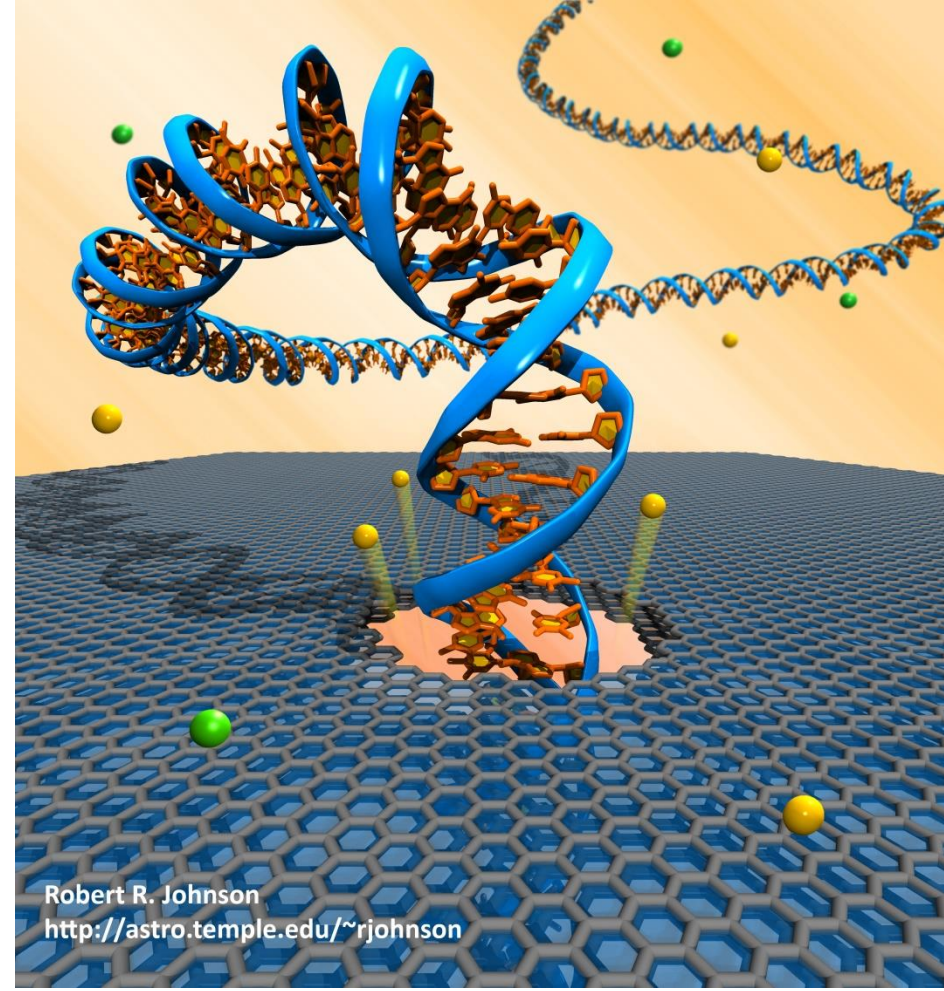
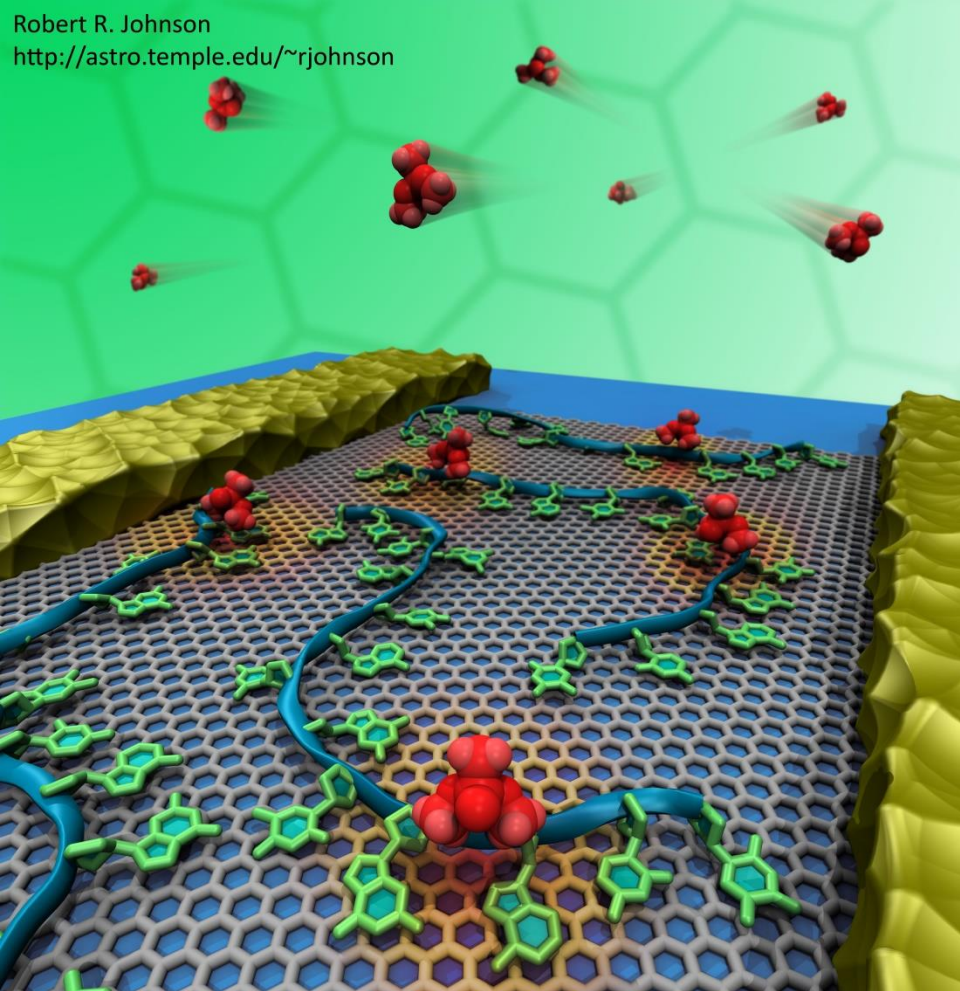
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit

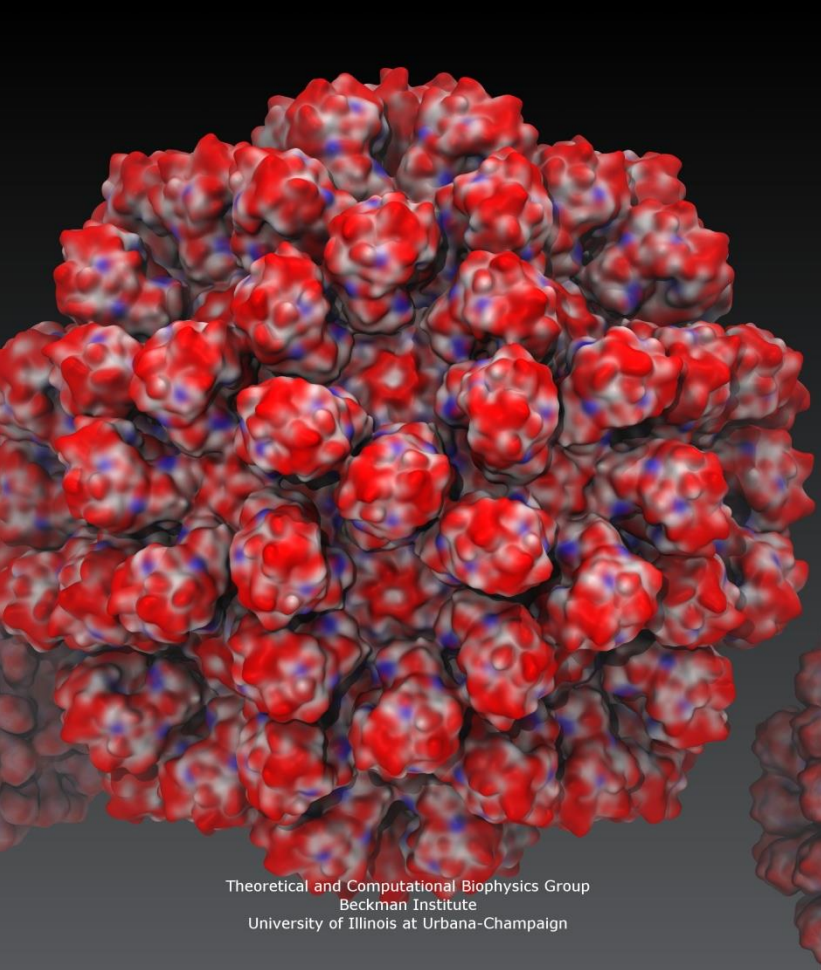




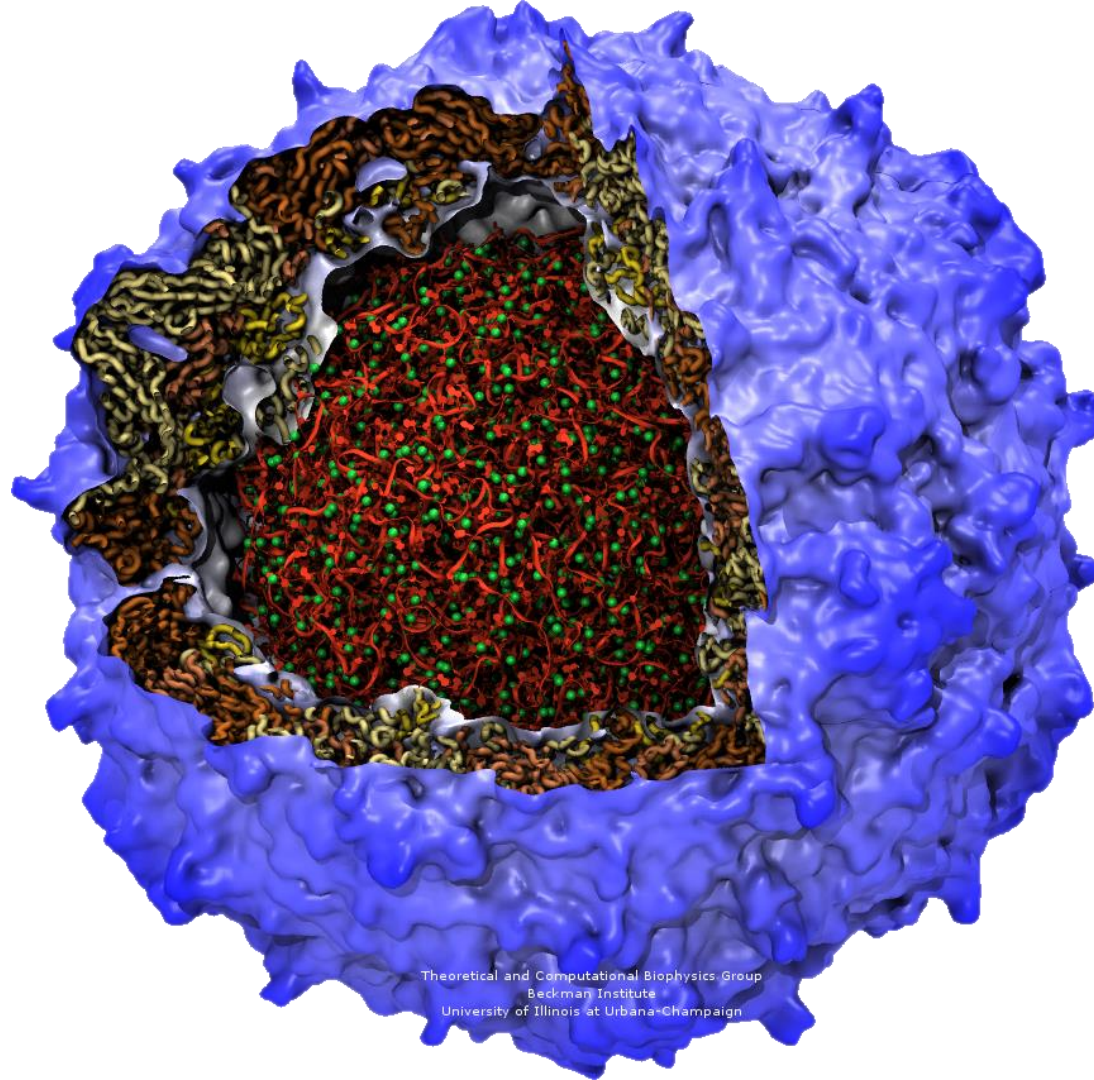
Robert R. Johnson
<http://astro.temple.edu/~rjohnson>



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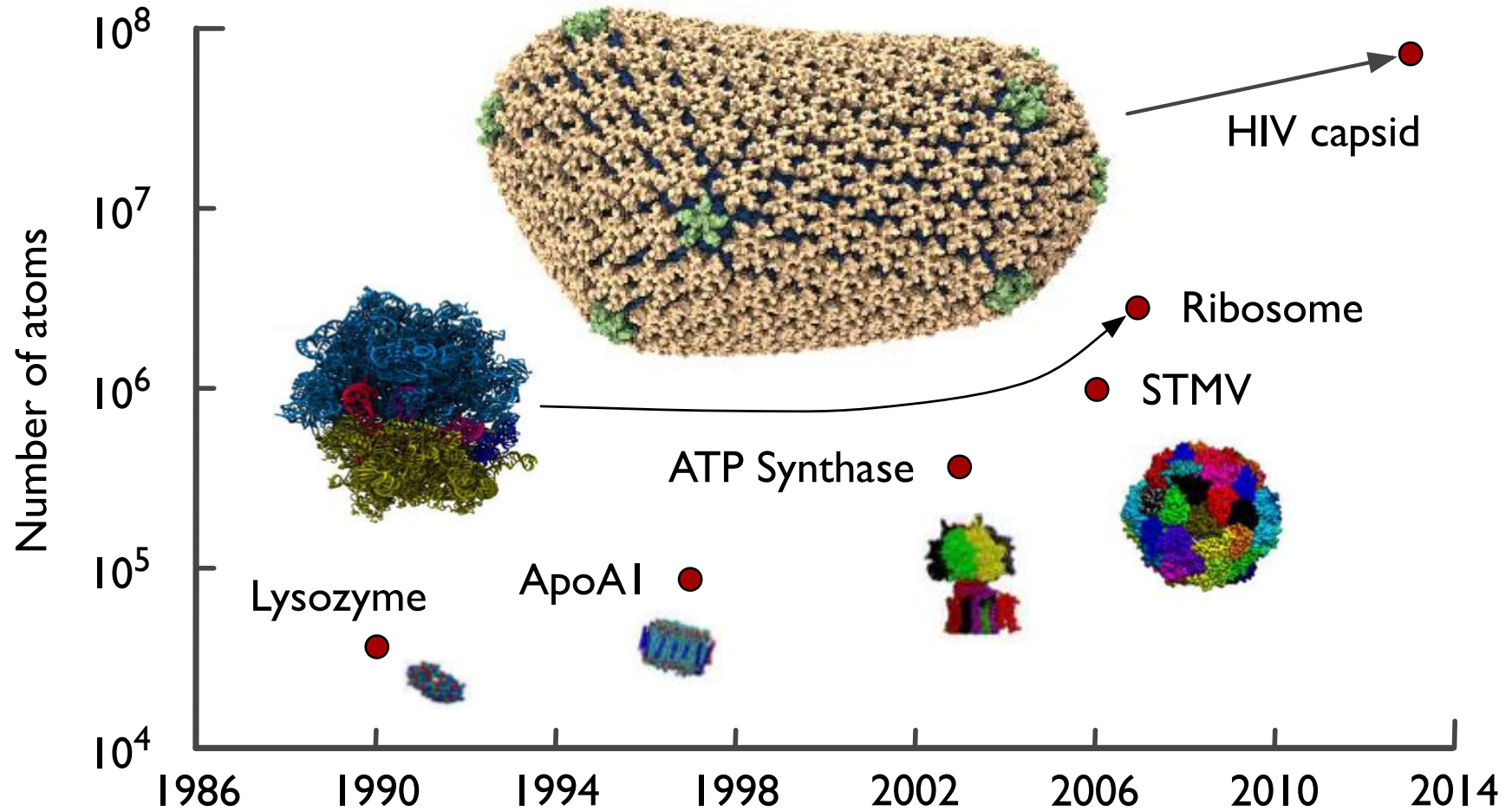


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Computational Biology's Insatiable Demand for Processing Power



Visualization Goals, Challenges

- Increased GPU acceleration for visualization of **petascale molecular dynamics trajectories**
- **Overcome GPU memory capacity limits**, enable high quality visualization of >100M atom systems
- Use GPU to accelerate not only interactive-rate visualizations, but also photorealistic ray tracing with **artifact-free ambient occlusion lighting**, etc.
- Maintain **ease-of-use**, intimate link to VMD analytical features, atom selection language, etc.



VMD GPU-Accelerated Ray Tracing Engine

- Complementary to VMD OpenGL GLSL renderer that uses fast, low-cost, interactivity-oriented rendering techniques
- Key ray tracing benefits:
 - Ambient occlusion lighting and hard shadows
 - High quality transparent surfaces
 - Depth of field focal blur and similar optical effects
 - Mirror reflection
 - Single-pass stereoscopic rendering
 - Special cameras: planetarium dome master format



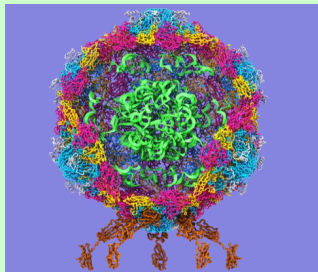
Why Built-In VMD Ray Tracing Engines?

- **No disk I/O** or communication to outboard renderers
- **Eliminate unnecessary data replication and host-GPU memory transfers**
- Directly operate on VMD internal molecular scene, **quantized/compressed data formats**
- Implement all **curved surface primitives**, volume rendering, texturing, shading features required by VMD
- **Same scripting, analysis, atom selection**, and rendering features are available on all platforms, **graceful CPU fallback**



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

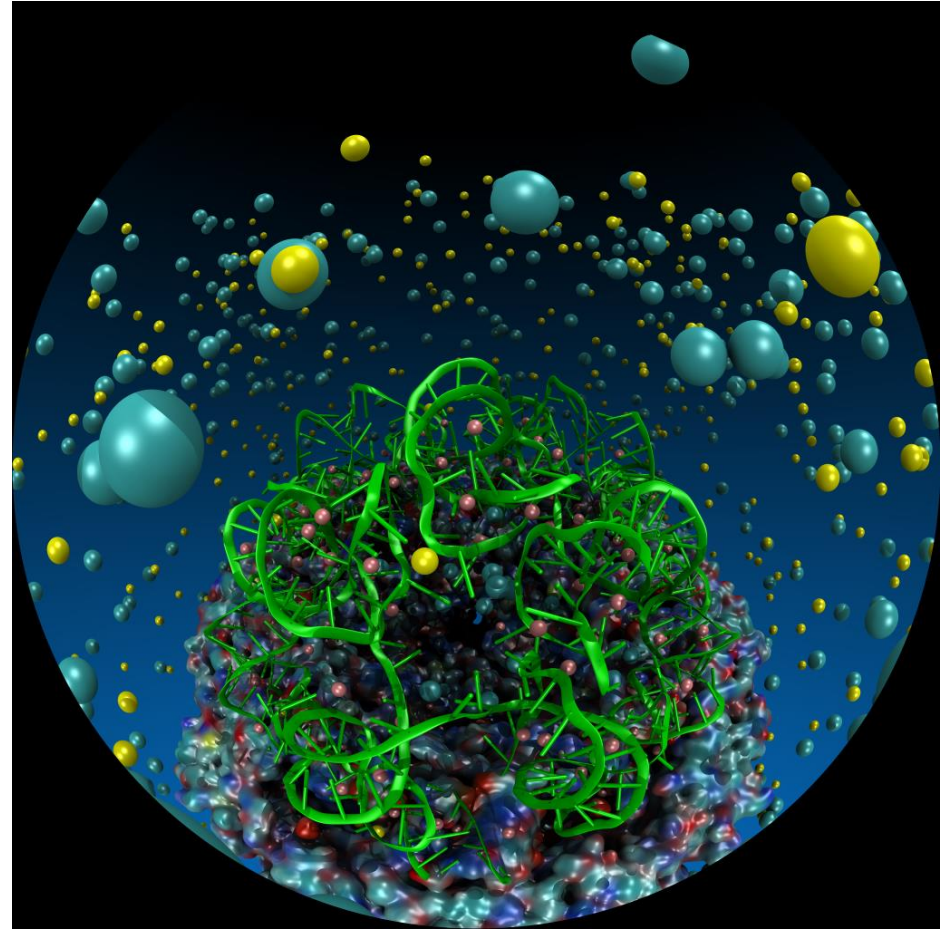
OpenGL Pbuffer GPU

Tachyon CPU RT

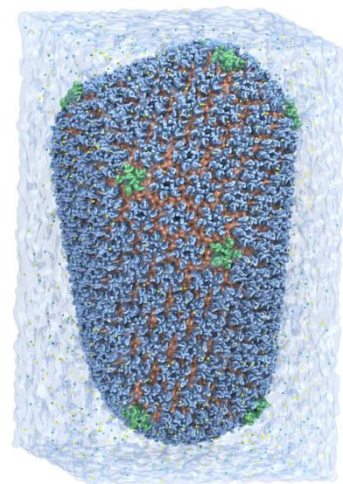
TachyonL-OptiX GPU RT
Batch + Interactive

VMD Planetarium Dome Master Camera

- Trivial to implement in OptiX
- 40 lines of CUDA code including antialiasing and handling corner cases for transcendental fctns
- Try implementing this in OpenGL . . . (yuck)
- Stereoscopic cameras and other special purpose projections are similarly easy



HIV-1 Parallel HD Movie Rendering on Blue Waters Cray XE6/XK7

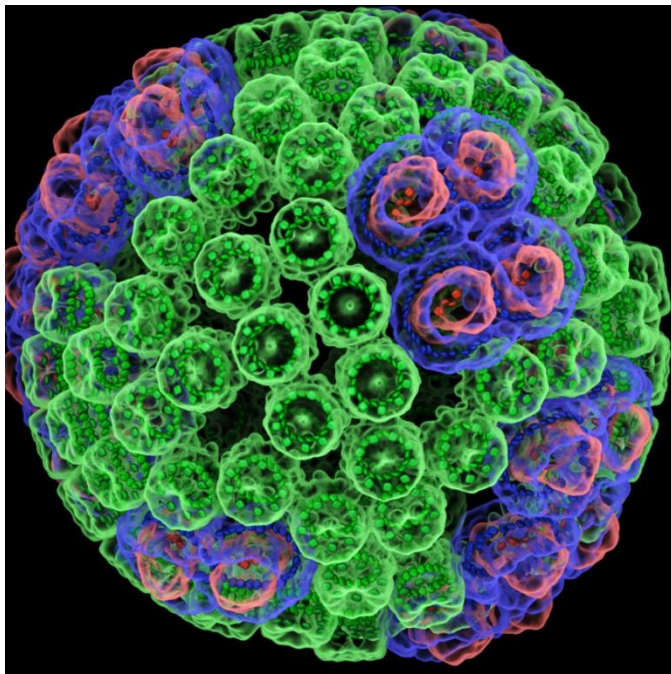


New “TachyonL-OptiX” on XK7 vs. Tachyon on XE6:
K20X GPUs yield **up to eight times** geom+ray tracing speedup

Node Type and Count	Script Load Time	State Load Time	Geometry + Ray Tracing	Total Time
256 XE6 CPUs	7 s	160 s	1,374 s	1,541 s
512 XE6 CPUs	13 s	211 s	808 s	1,032 s
64 XK7 Tesla K20X GPUs	2 s	38 s	655 s	695 s
128 XK7 Tesla K20X GPUs	4 s	74 s	331 s	410 s
256 XK7 Tesla K20X GPUs	7 s	110 s	171 s	288 s

VMD Chromatophore Rendering on Blue Waters

- New representations, GPU-accelerated molecular surface calculations, memory-efficient algorithms for huge complexes
- VMD GPU-accelerated ray tracing engine w/ OptiX+CUDA+MPI+Pthreads
- ***Each revision:*** 7,500 frames render on ~96 Cray XK7 nodes in 290 node-hours, 45GB of images prior to editing



GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.

J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

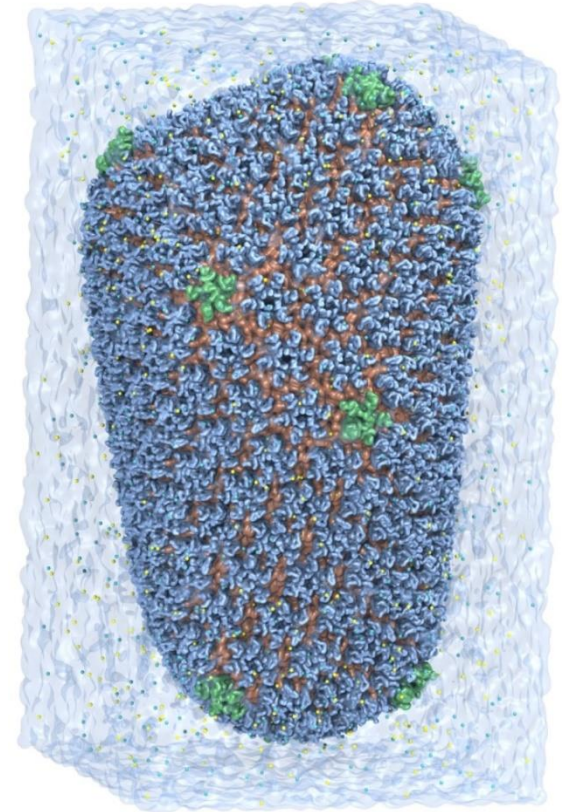
Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.

M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.

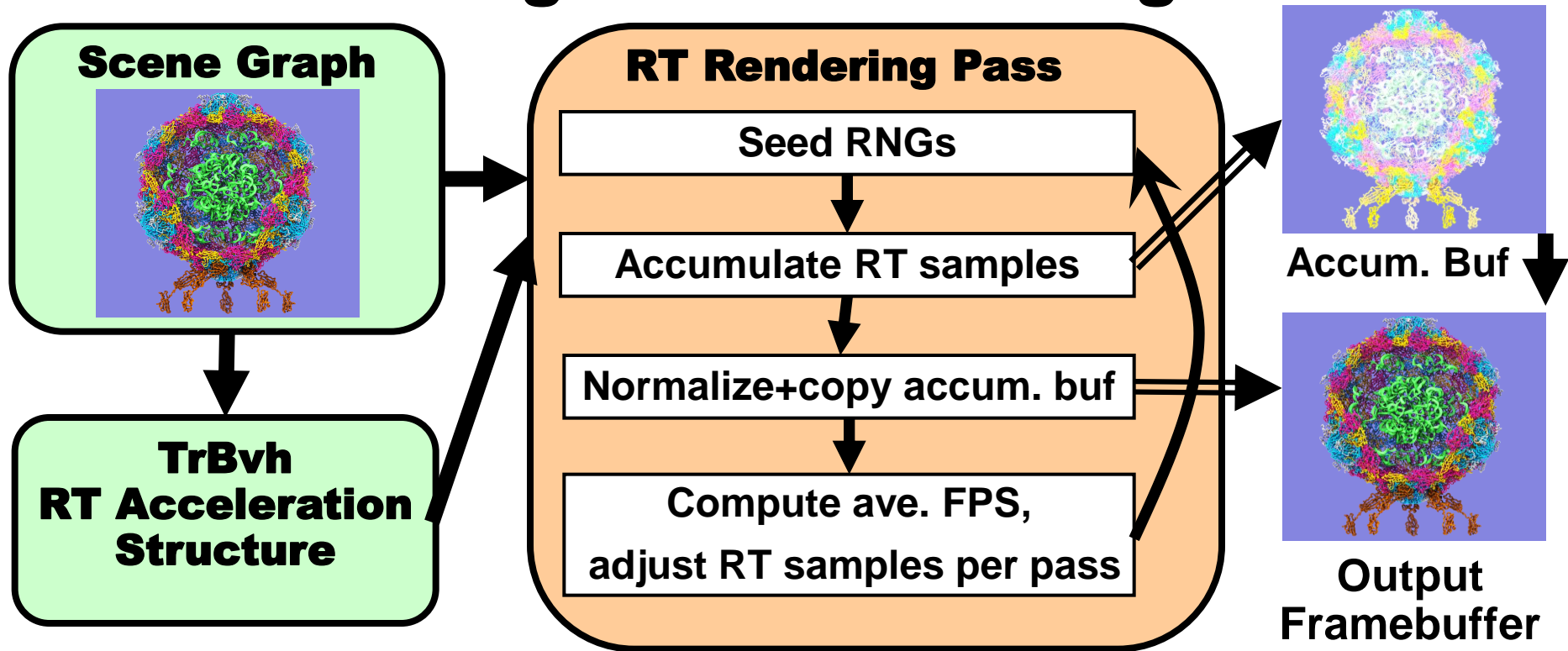
*****Winner of the SC'14 Visualization and Data Analytics Showcase**

VMD 1.9.2 Interactive GPU Ray Tracing

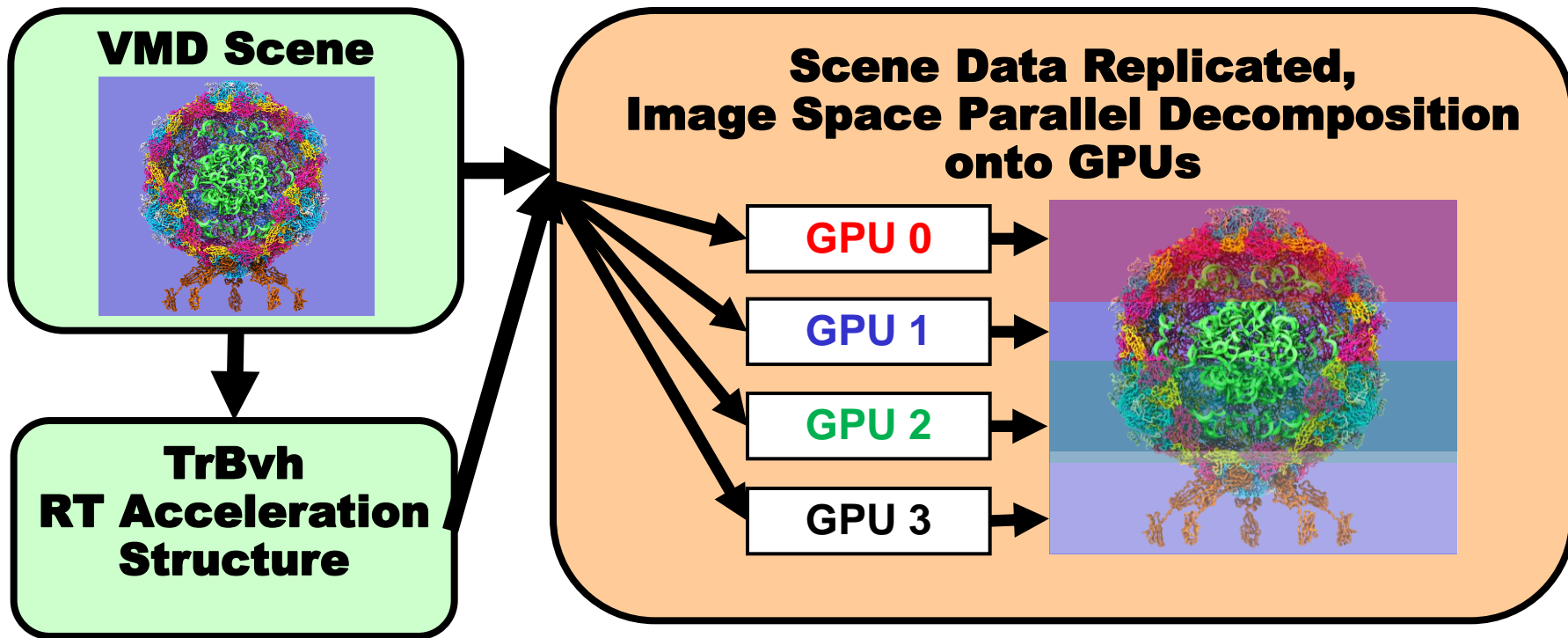
- Ray tracing heavily used for VMD publication-quality images/movies
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides ~~–*interactive*–~~ ray tracing on laptops, desktops, and *remote* visual supercomputers



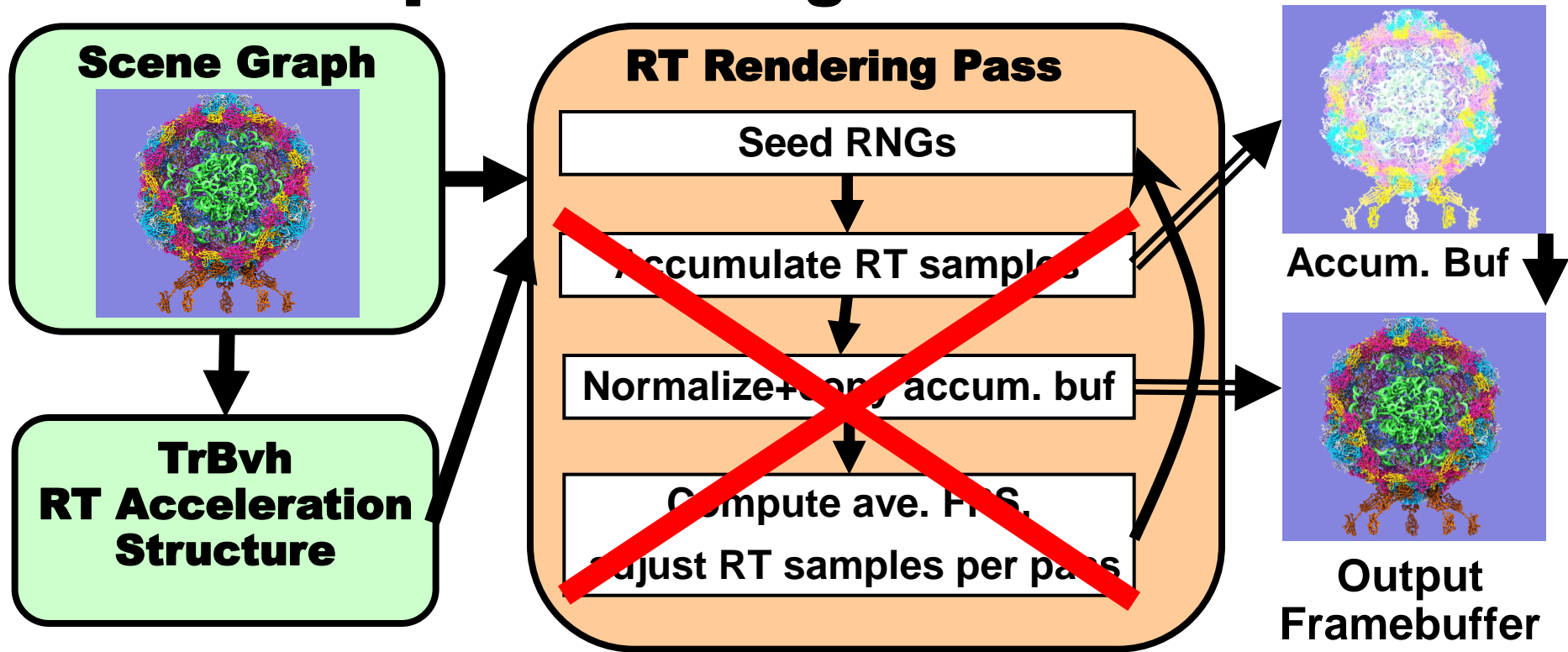
VMD TachyonL-OptiX Interactive RT w/ Progressive Rendering



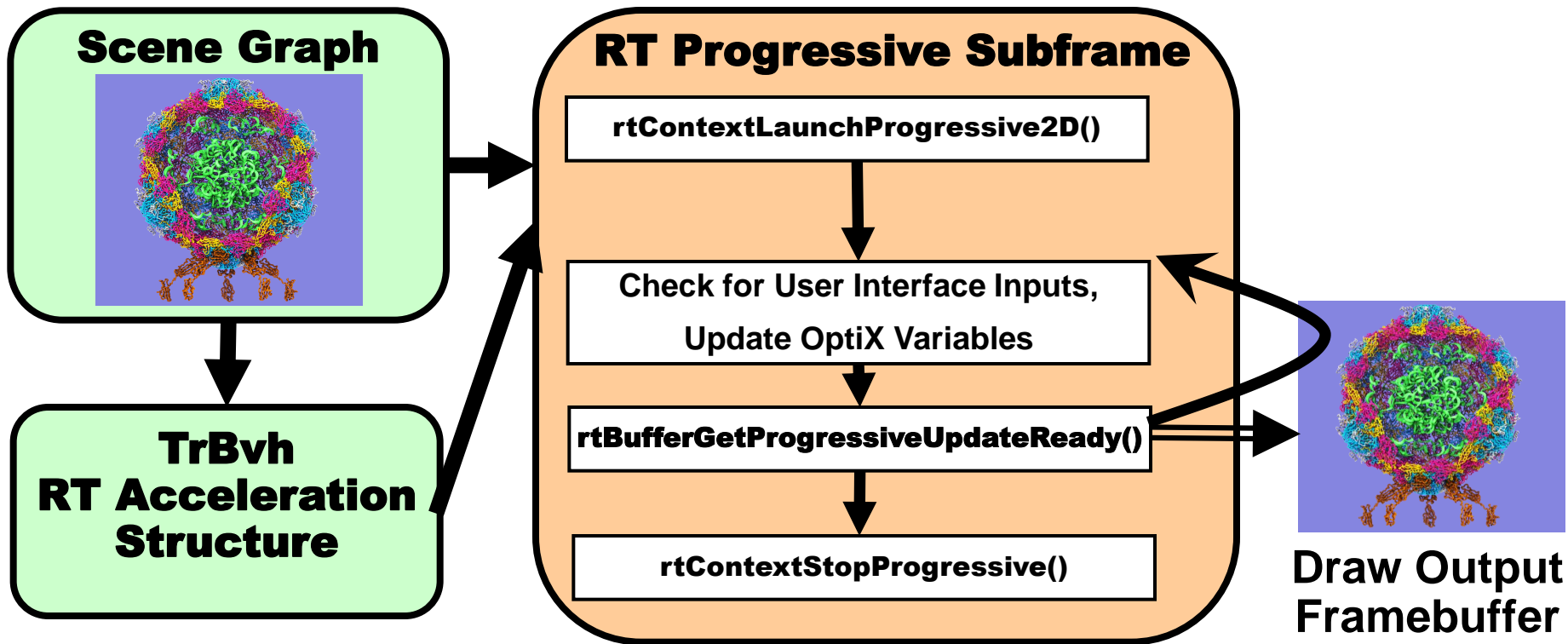
VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node



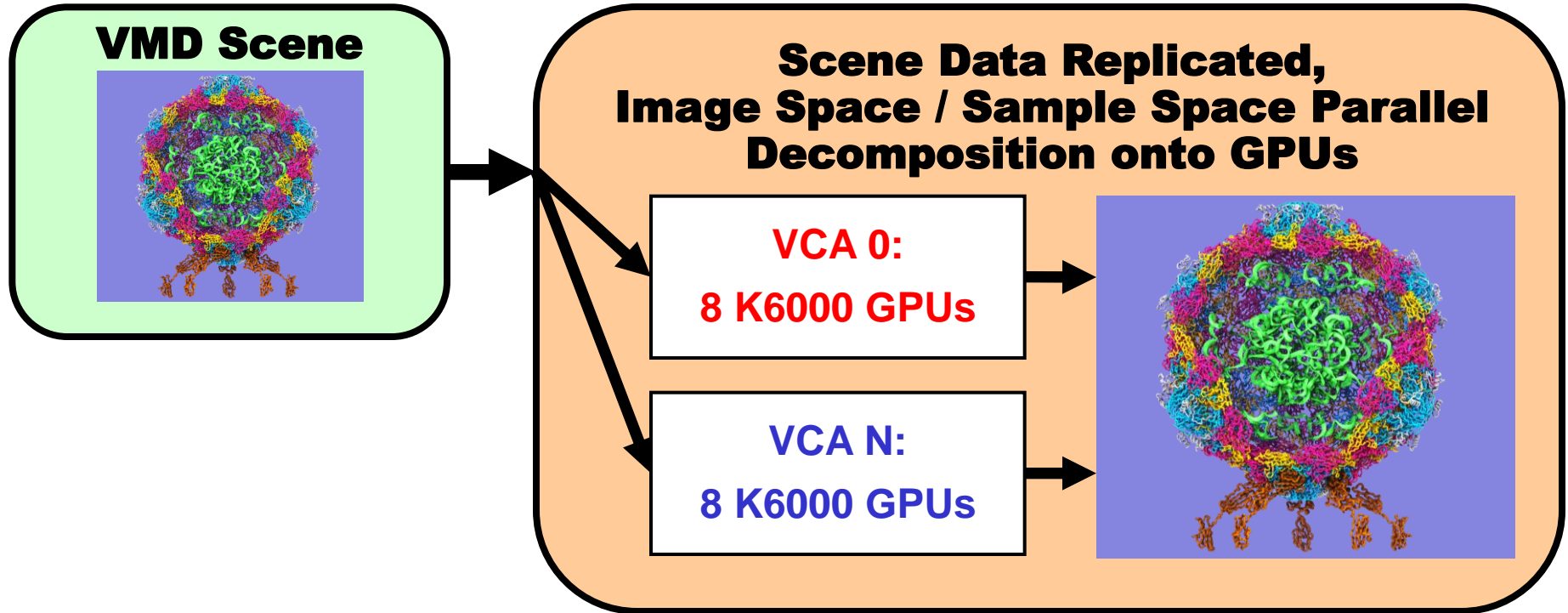
VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



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

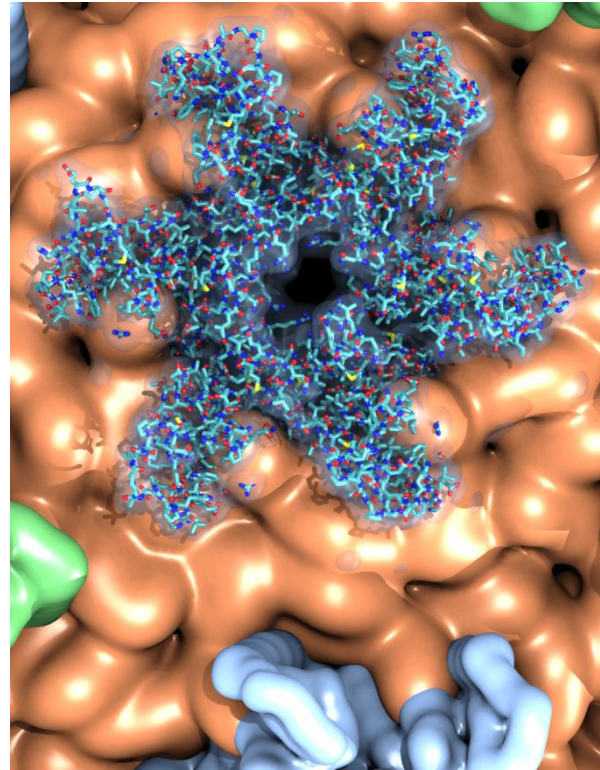


VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster



VMD-Next: Coming Soon

- Further integration of interactive ray tracing into VMD
 - Seamless interactive RT in main VMD display window
 - Support trajectory playback in interactive RT
 - Enable multi-node interactive RT on HPC systems
- Improved movie making tools, off-screen OpenGL movie rendering, parallel movie rendering:
 - EGL for parallel graphics w/o X11 server
 - Built-in (basic) interactive remote visualization on HPC clusters and supercomputers
- Improved structure building tools
- Many new and updated user-contributed plugins:



GPU Ray Tracing of
HIV-1 Capsid Detail

Future Work

- Improved performance / quality trade-offs in interactive RT stochastic sampling strategies
- Optimize GPU scene DMA and BVH regen speed for time-varying geometry, e.g. MD trajectories
- Continue tuning of GPU-specific RT intersection routines, memory layout
- GPU-accelerated movie encoder back-end
- Interactive RT combined with remote viz on HPC systems, much larger data sizes



Acknowledgements

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





NIH BTRC for Macromolecular Modeling and Bioinformatics

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GPU Computing 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.



GPU Computing 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.



GPU Computing Publications

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- **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.



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- **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.



GPU Computing 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.
- **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.

