Interactive High-Fidelity Biomolecular and Cellular Visualization with RTX Ray Tracing APIs

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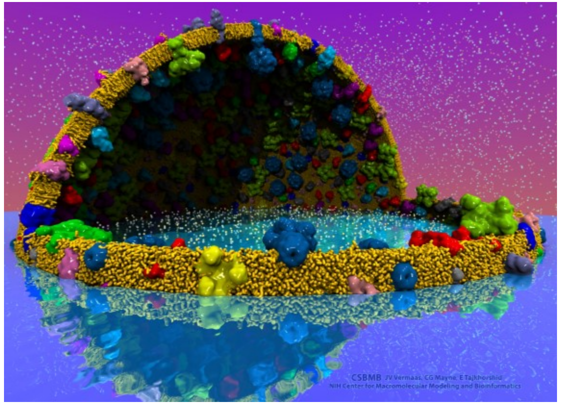
http://www.ks.uiuc.edu/Research/gpu/

15:00-15:50, Room 230B, San Jose Convention Center

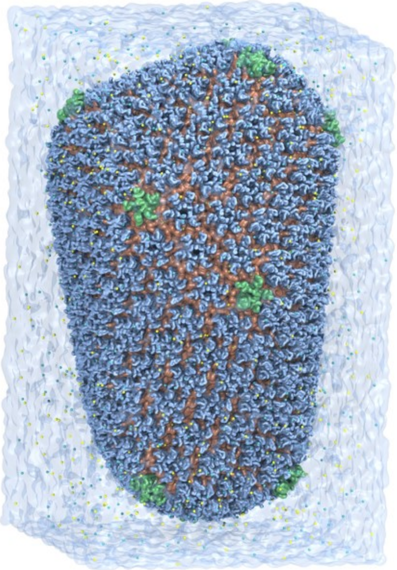
San Jose, CA, Wednesday March 20th, 2019

VMD – "Visual Molecular Dynamics"

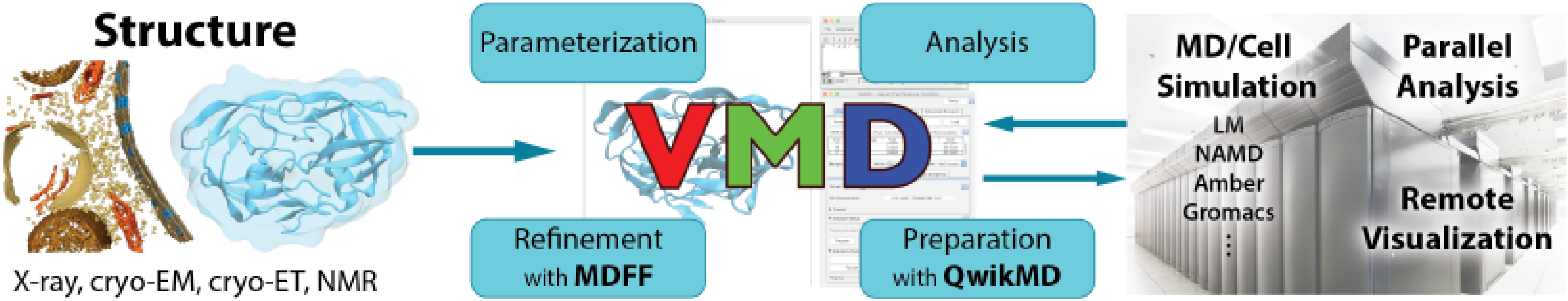
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
  - Sequence information
- User extensible scripting and plugins
- Over 100,000 users, 28,000 citations
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



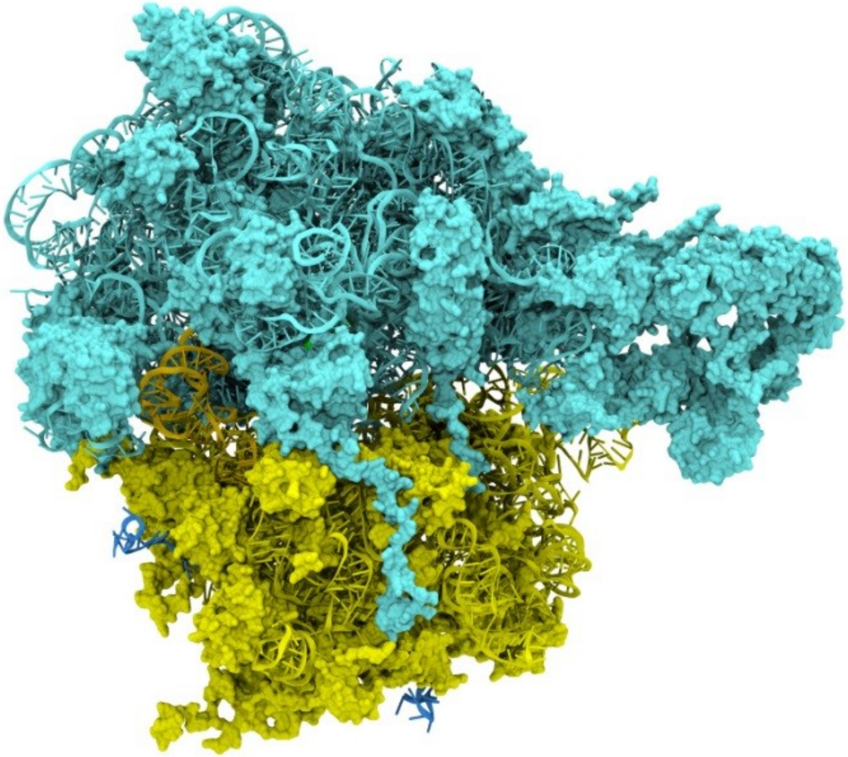
MD Simulation



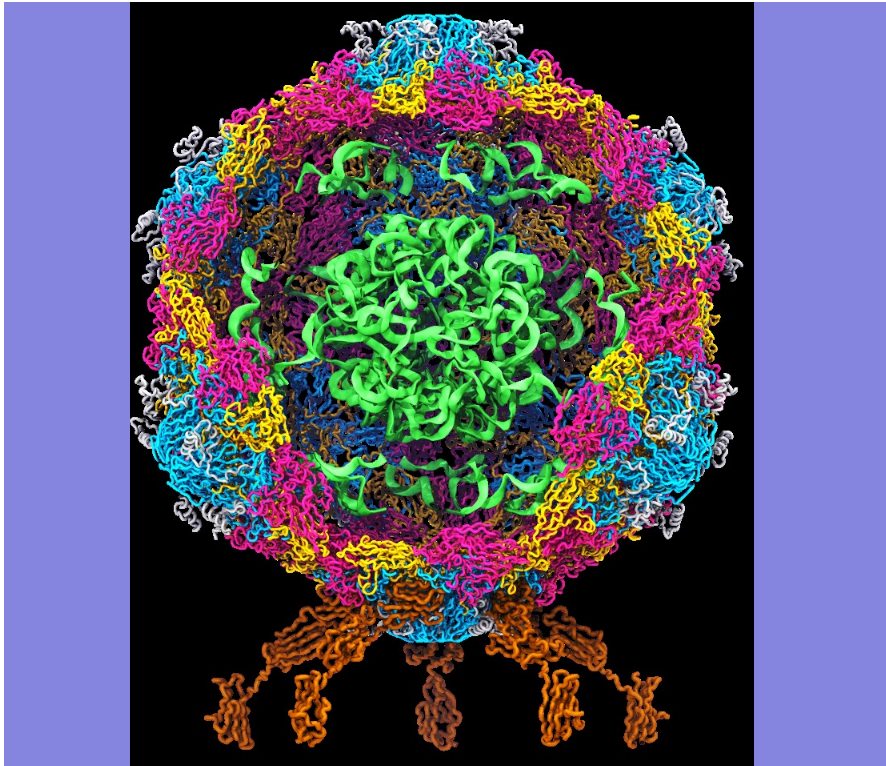
Goal: A Computational Microscope

Study the molecular machines in living cells

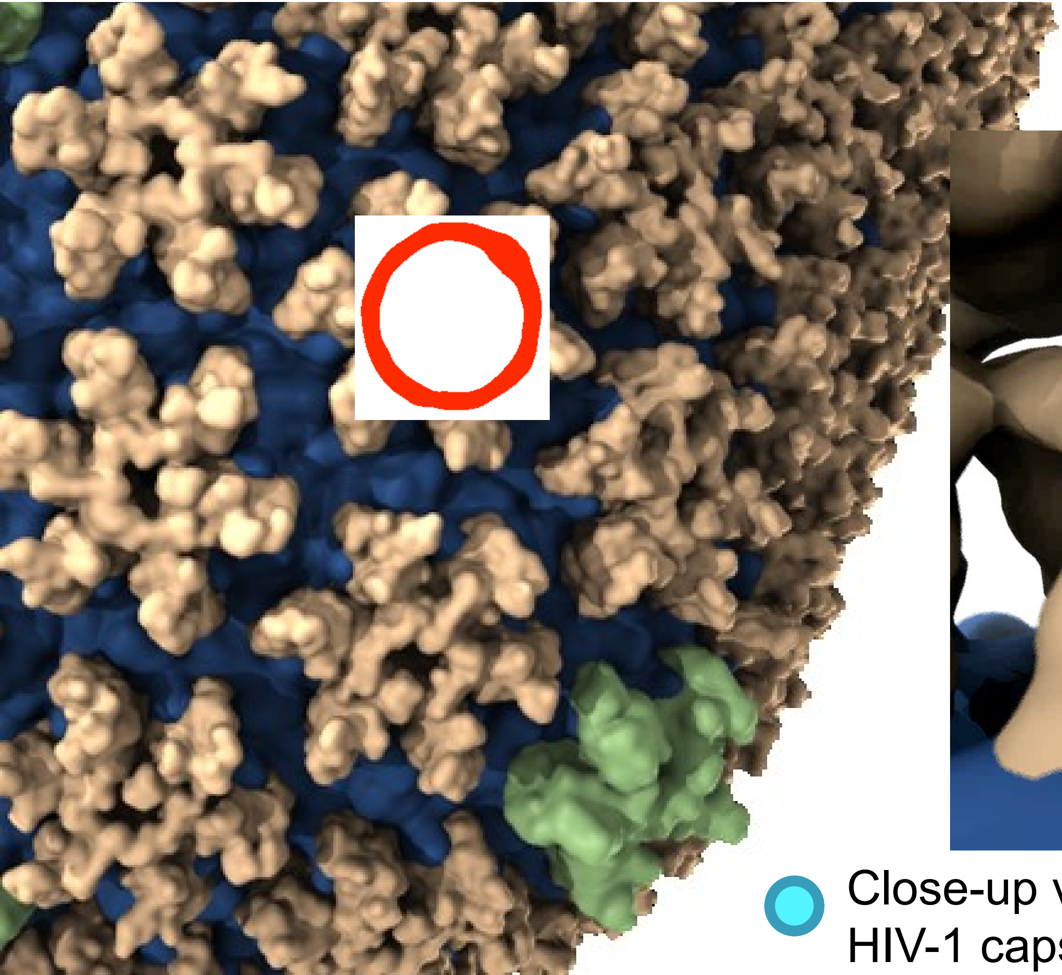
Ribosome: target for antibiotics



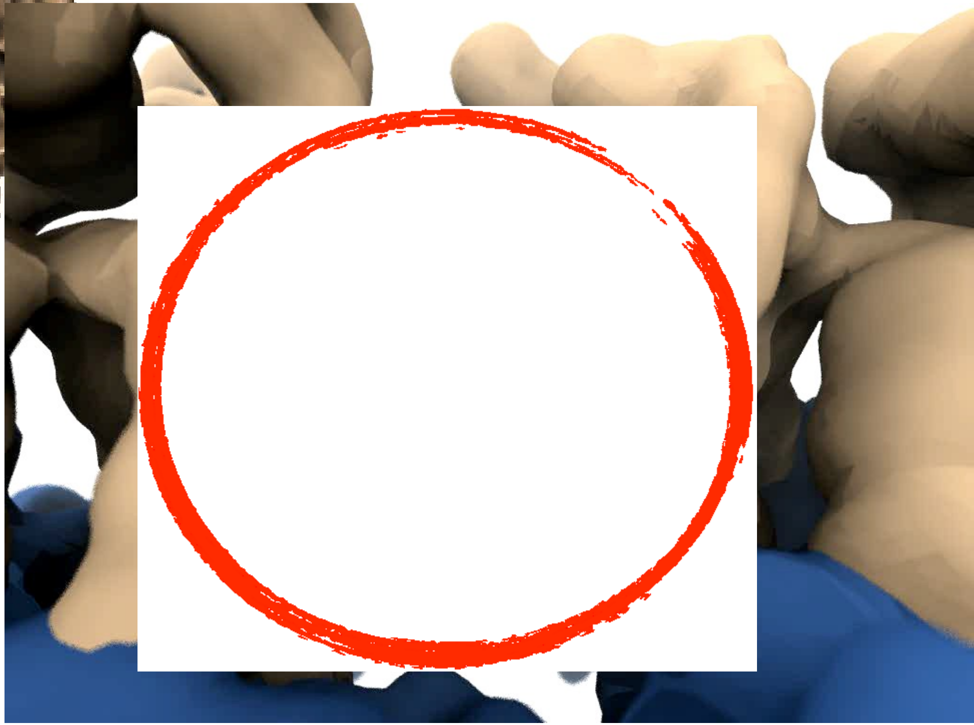
Poliovirus



Goal: Intuitive interactive viz. in crowded molecular complexes

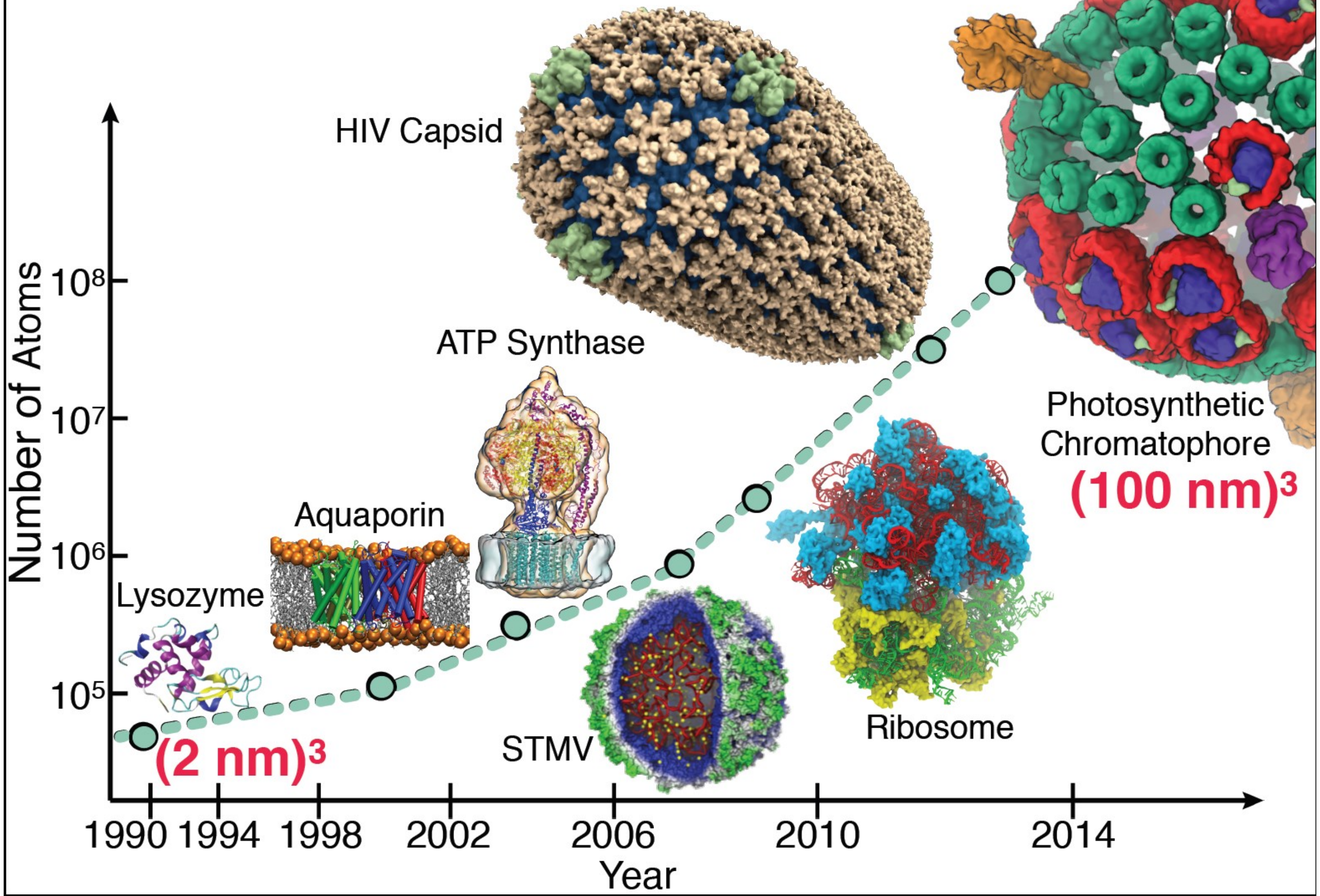


Results from 64M atom, 1 µs sim!



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

All-Atom Molecular Dynamics Today

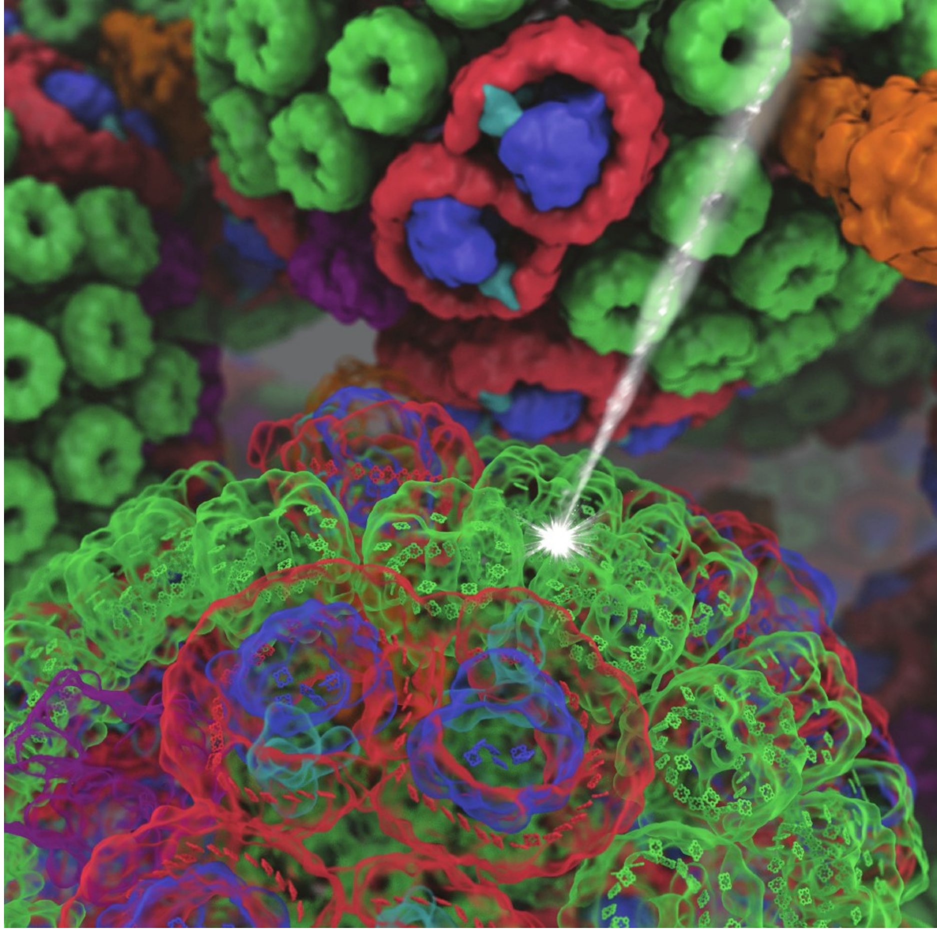


High Fidelity Ray Tracing with OptiX

- 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, and **remote supercomputers**
- Interactivity is critically important for scientists that need to obtain results without becoming a graphics expert

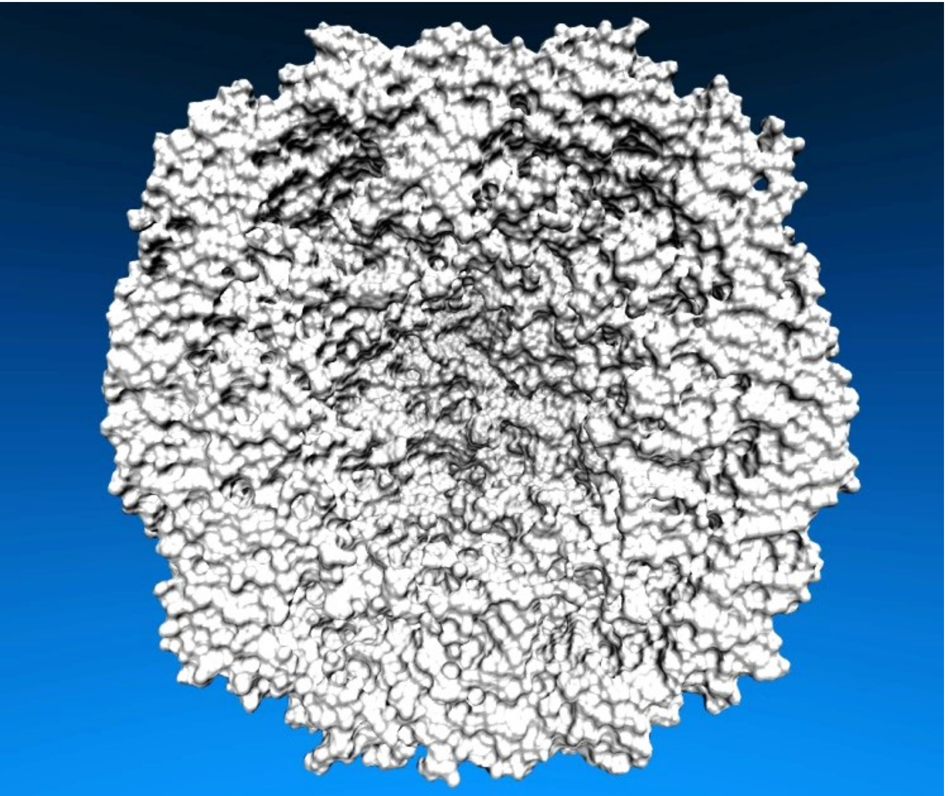
- Large-scale parallel rendering: in situ or post hoc visualization tasks
- **Stereoscopic panorama and full-dome projections**
- **Omnidirectional VR: YouTube, HMDs**



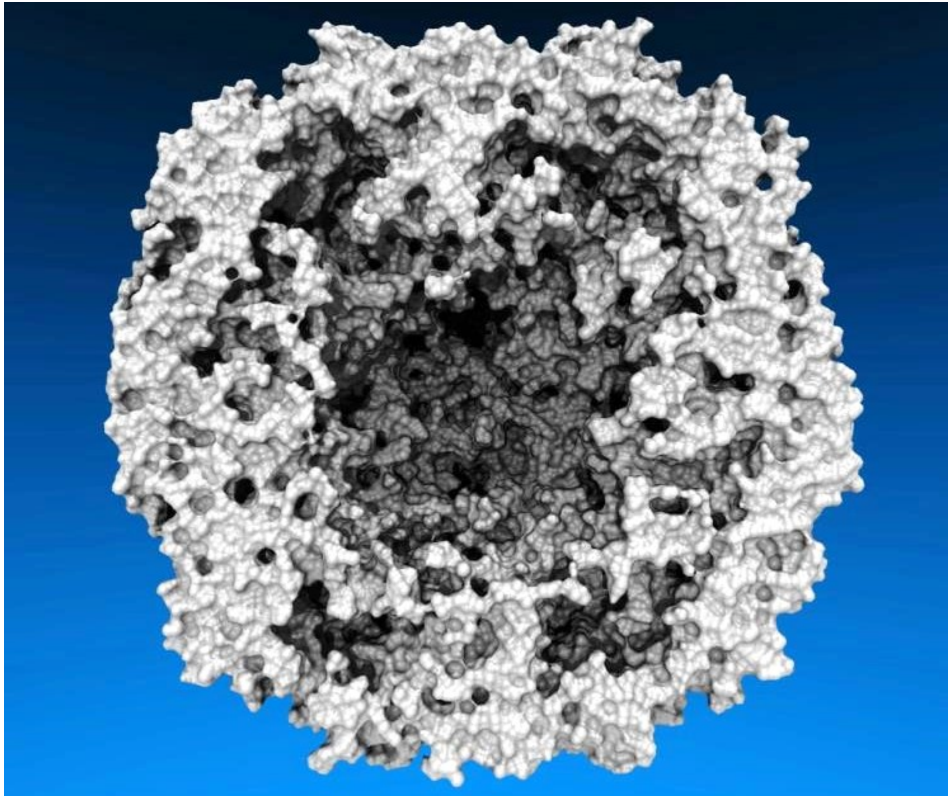
VMD/OptiX all-atom Chromatophore

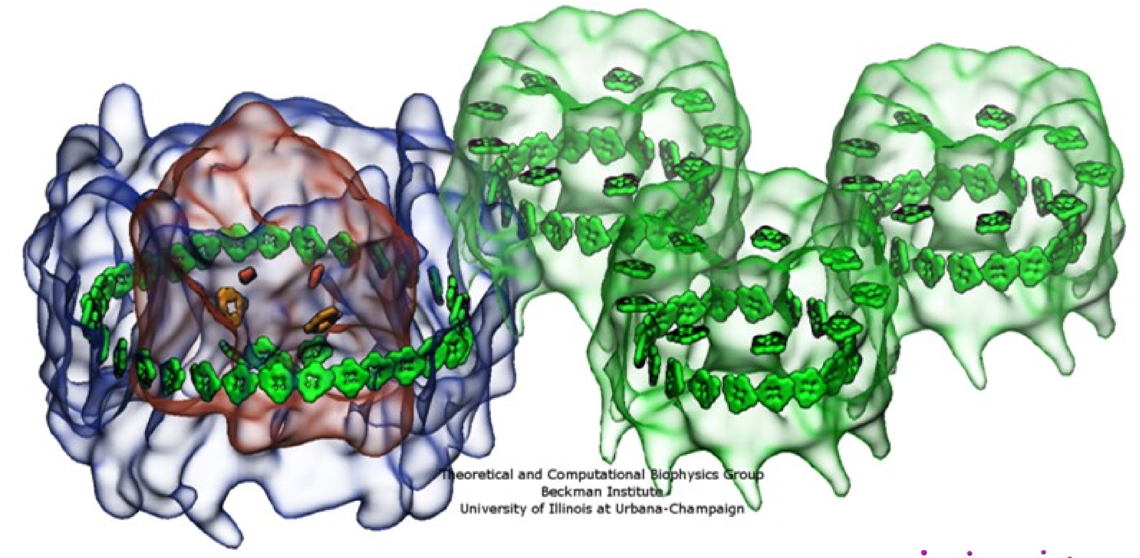
Lighting Comparison, STMV Capsid

Two lights, no shadows



Ambient occlusion + two lights, 144 AO rays/hit

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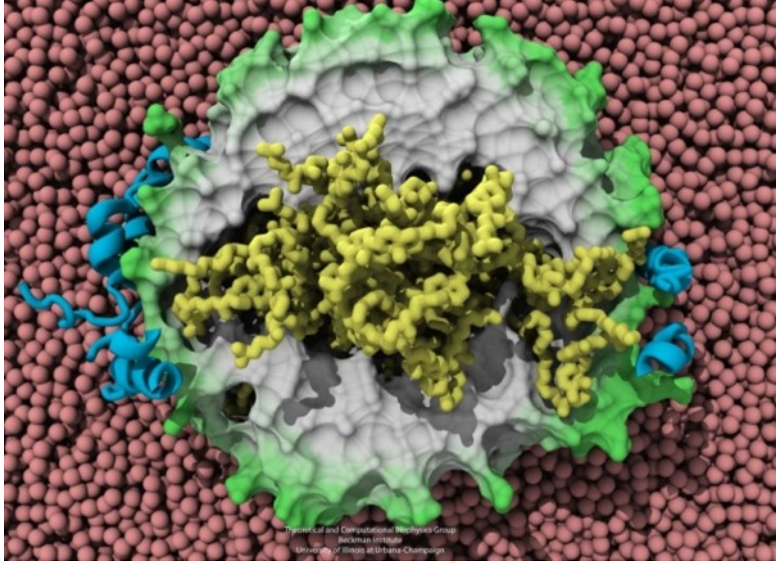
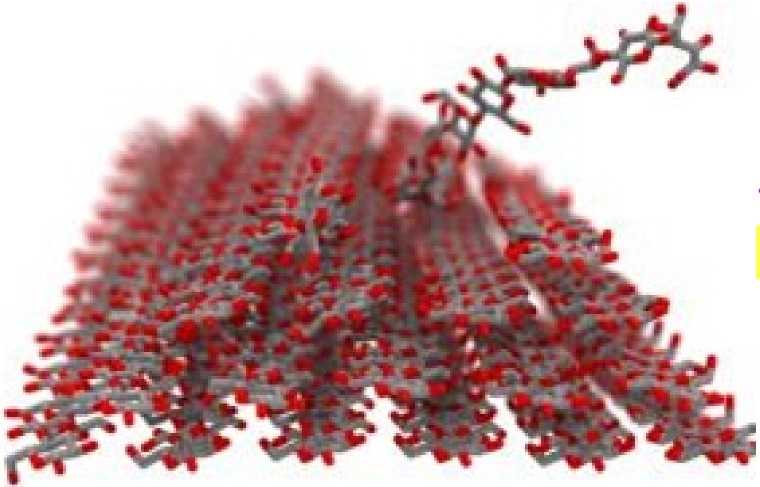
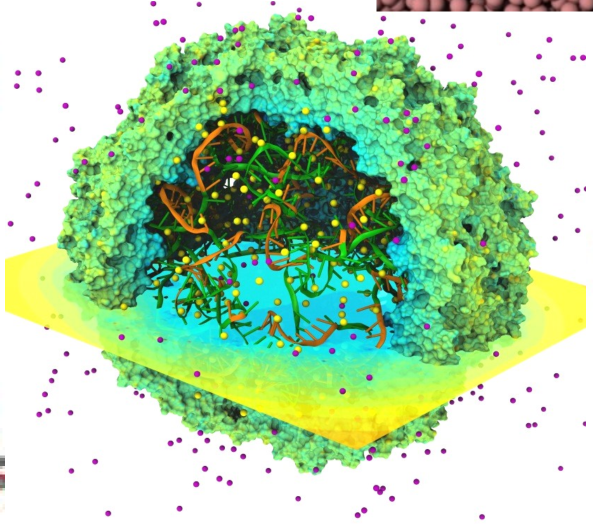
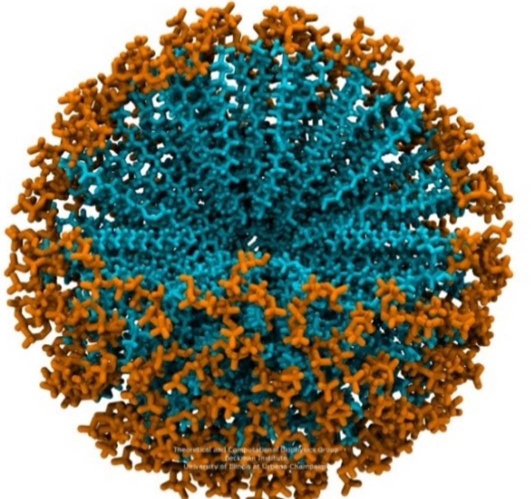




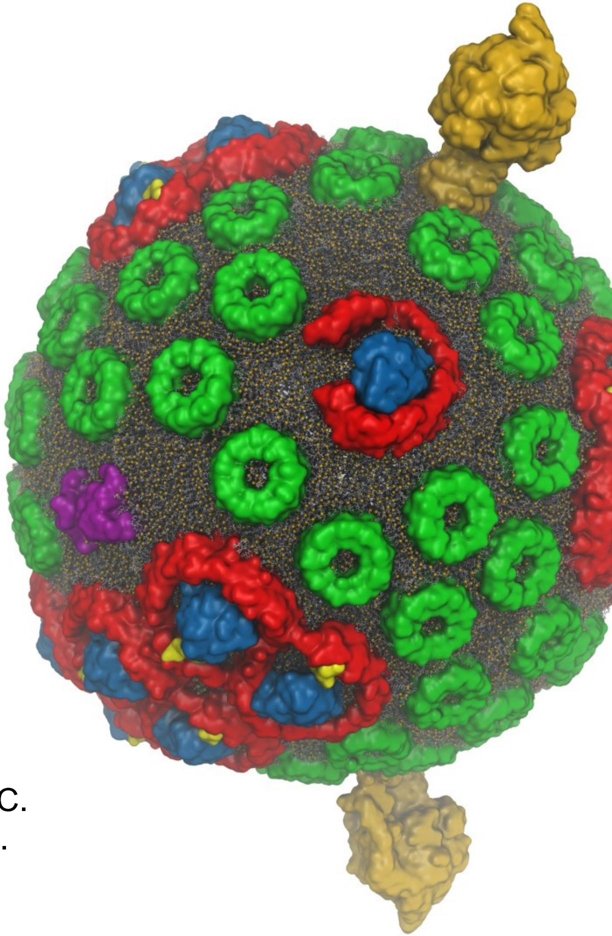




VMD w/ OptiX 6

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization
- **Remote ray tracing with NvPipe video streaming**
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- **VMD+OptiX NGC container: https://ngc.nvidia.com/registry/**
- **In-progress:**

  Denoising: faster 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.

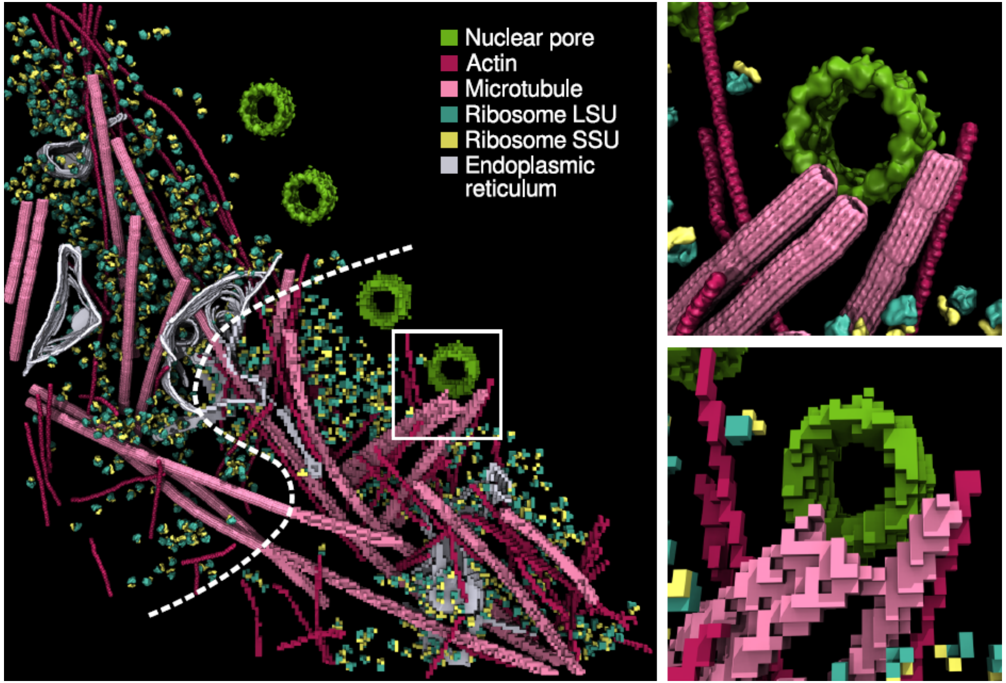
Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

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.

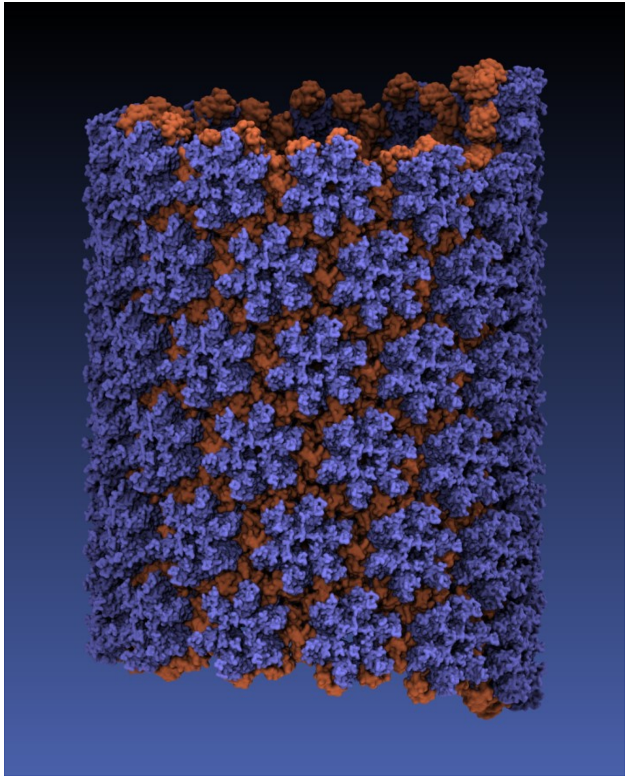
Interactive Ray Tracing of Tomograms

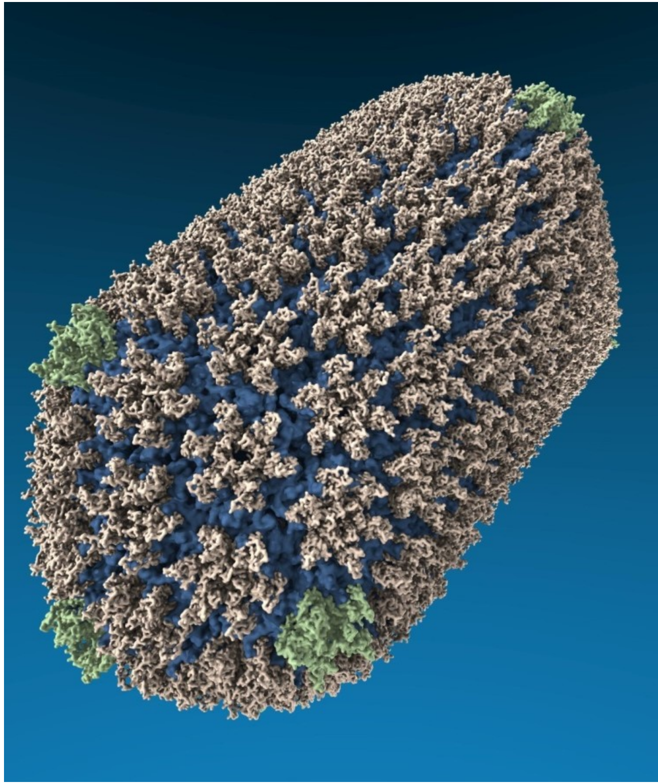
- High resolution cellular tomograms, **billions of voxels**
- Even isosurface or lattice site graphical representations involve ~100M geometric primitives
- >= 24GB GPUs allow interactive RT of large cellular tomograms



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

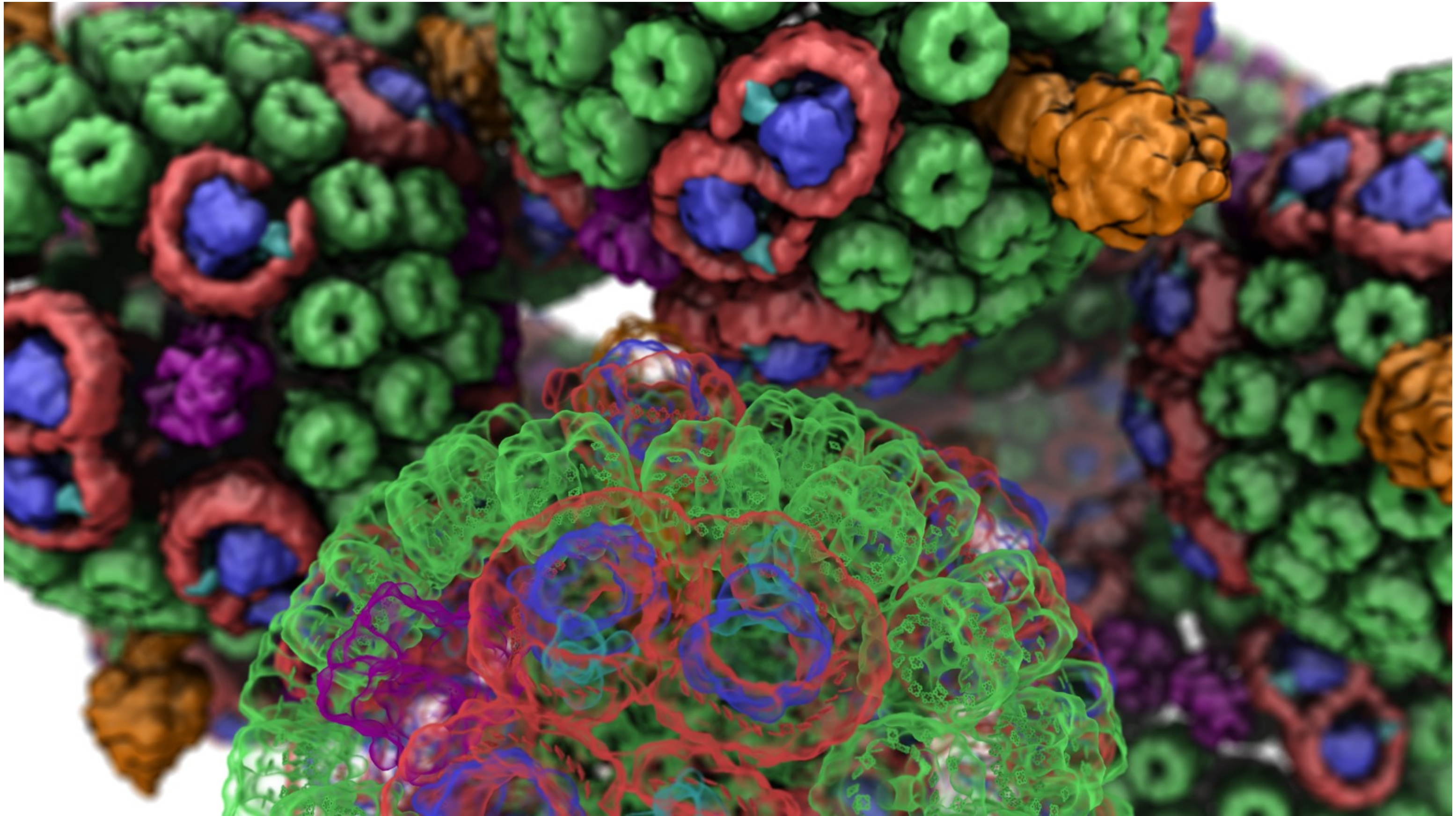
VMD "QuickSurf" Representation, Ray Tracing





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

VMD/OpiX RTX Acceleration



What is RTX Acceleration Doing?

- Hardware acceleration (Turing RT cores) of:
  - BVH AS traversal
  - Ray-triangle intersection
- BVH AS can embed triangle geometry
  - Triangle geometry buffer can then be ephemeral

Secondary Benefits and RTX Performance Observations

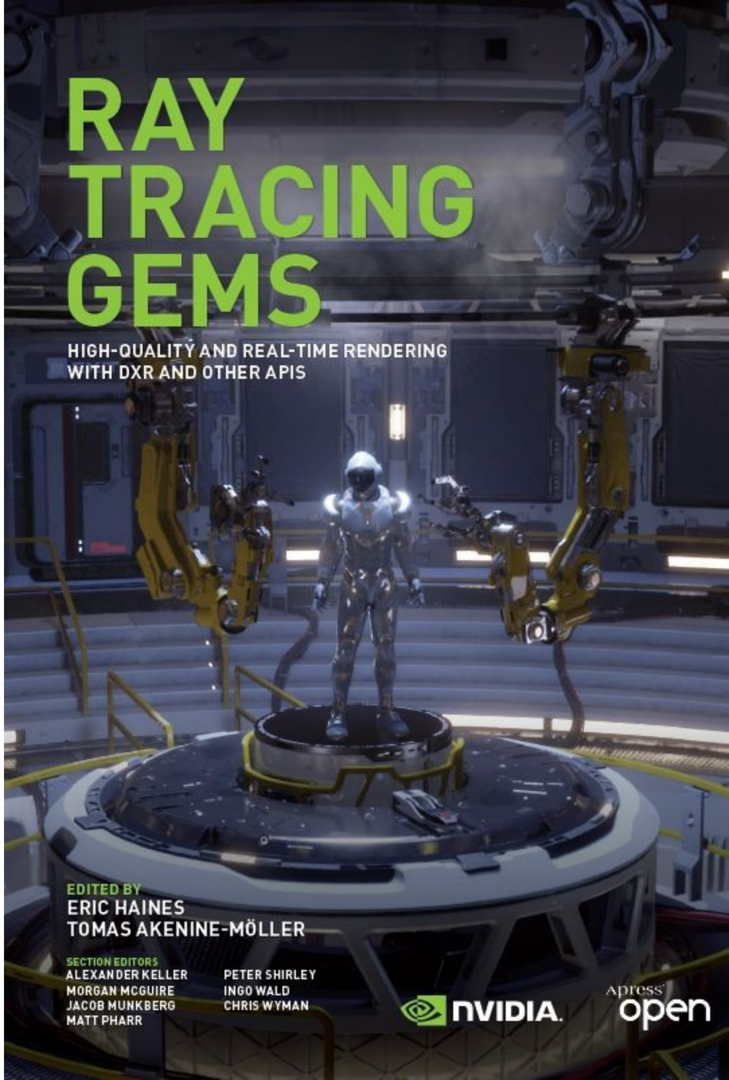
- Traversal and intersection work performed by RT cores vacates GPU SMs and makes them available for other RT work
- RTX hardware traversal performance approaches GPU memory bandwidth limits
- Future RTX hardware could end up being bandwidth bound in some cases
- Start adapting geometric data representations for minimum footprint, e.g. by using compressed or quantized data representations such as Octohedron Normal Vector encoding (replace 3x 32-bit floats with a single 32-bit int)

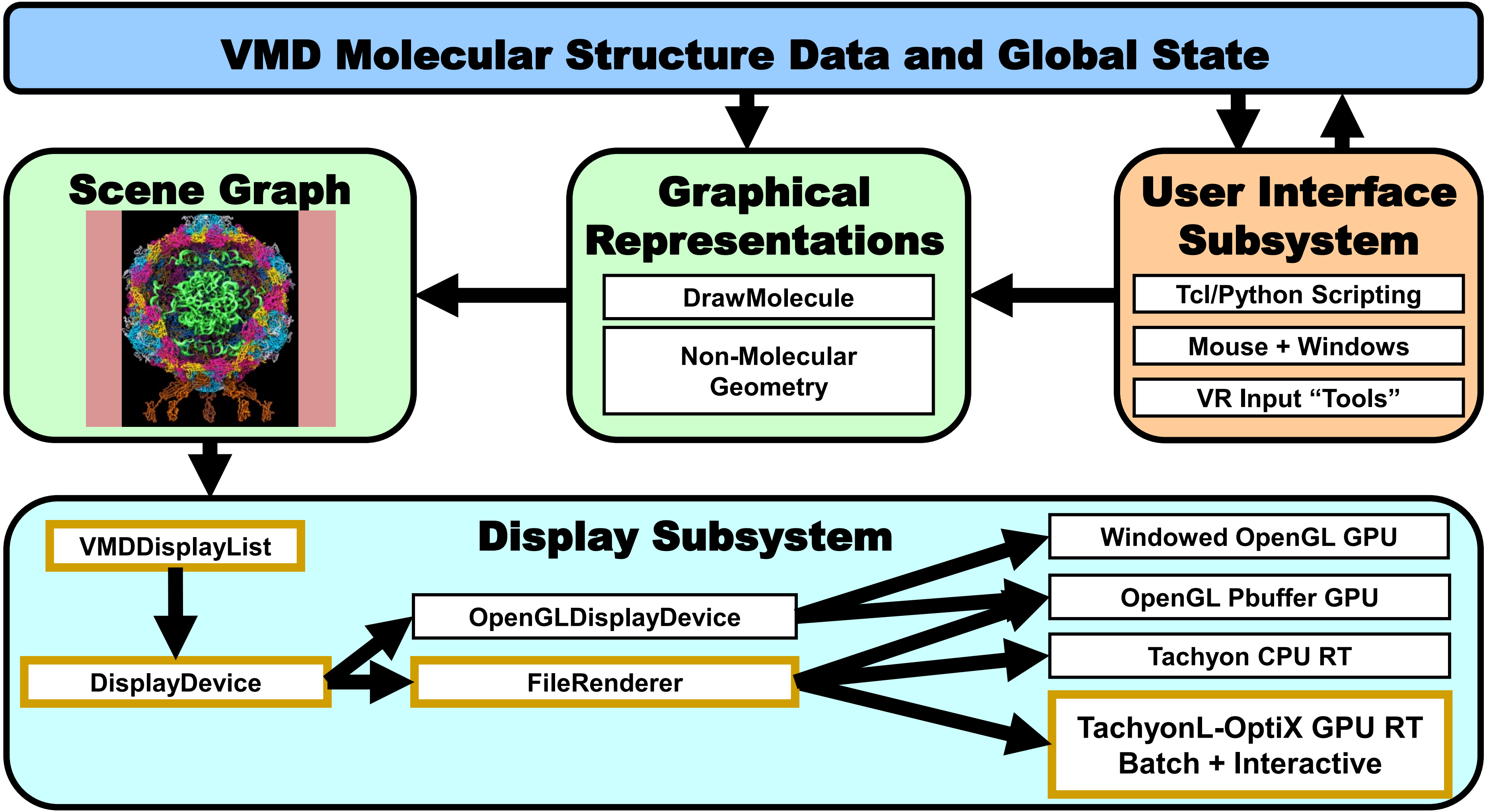
Ray Tracing Gems

- Ch. 4, “A Planetarium Dome Master Camera”
- Ch. 27, “Interactive Ray Tracing Techniques for High-Fidelity Scientific Visualization”
- Tons of great material and code samples!

- **See Eric Haines RTG GTC talk:**
  - **Room 230B (Concourse Level) on Thursday 2-3 PM**

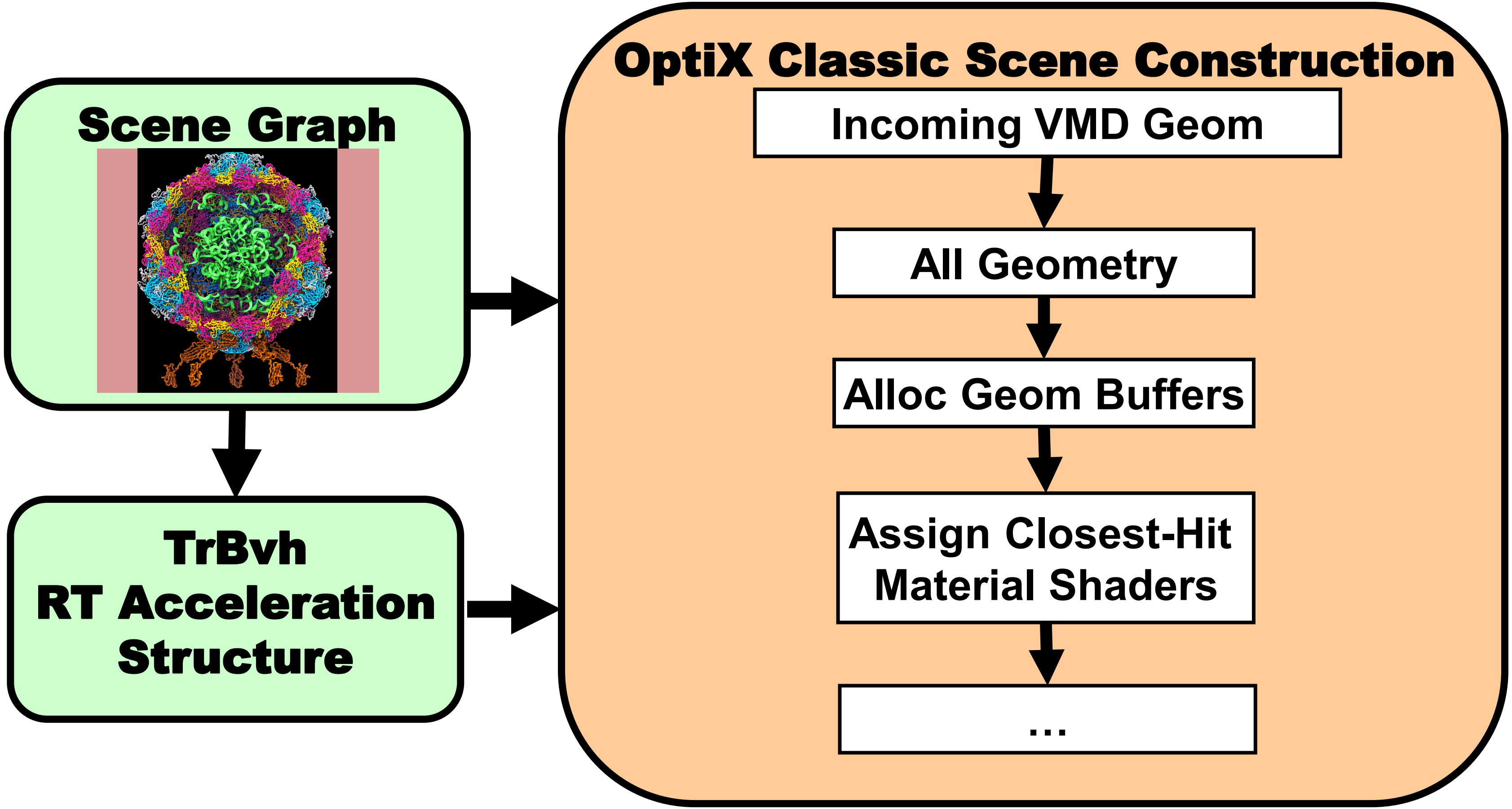
- **RTG book signings on Thursday, 3-4pm @ GTC book seller**



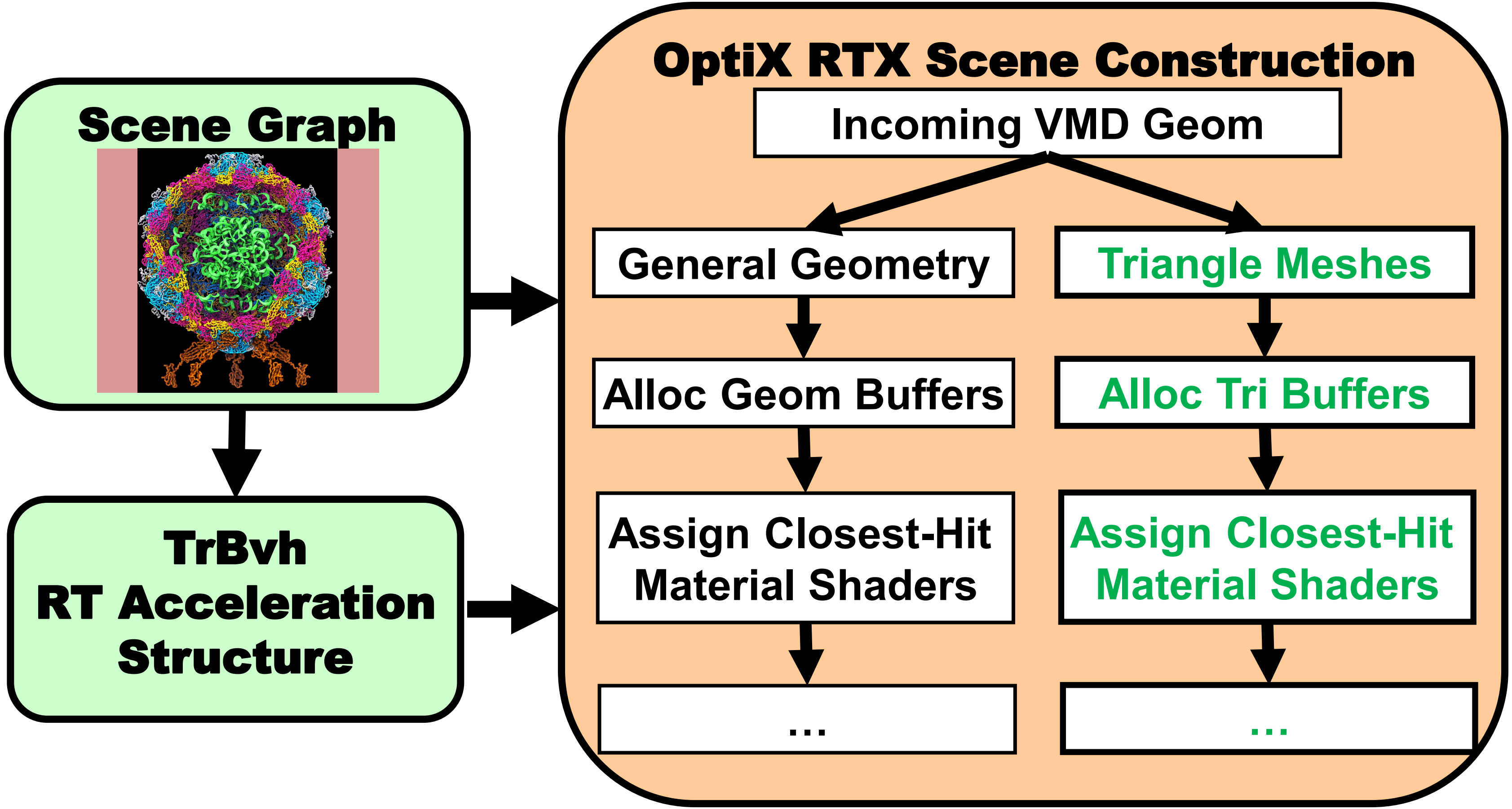


VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input “Tools”
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL Pbuffer GPU
Tachyon CPU RT
TachyonL-OptiX GPU RT
Batch + Interactive

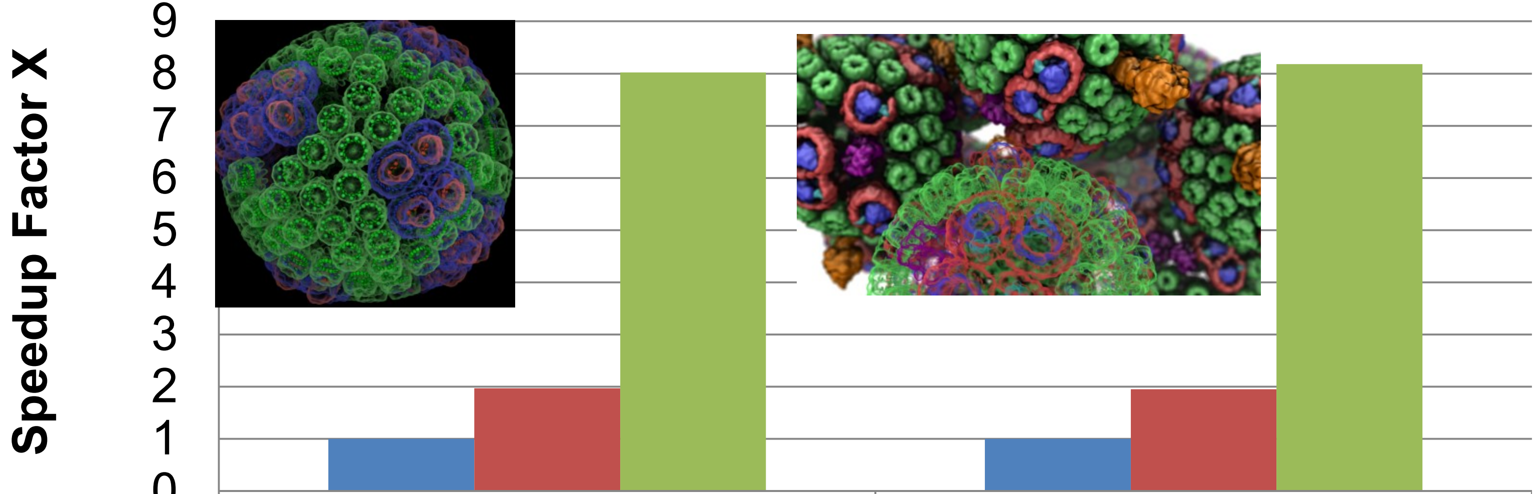
VMD Scene w/ OptiX Classic APIs



VMD Scene w/ OptiX RTX APIs



VMD OptiX RT performance on Quadro RTX 6000

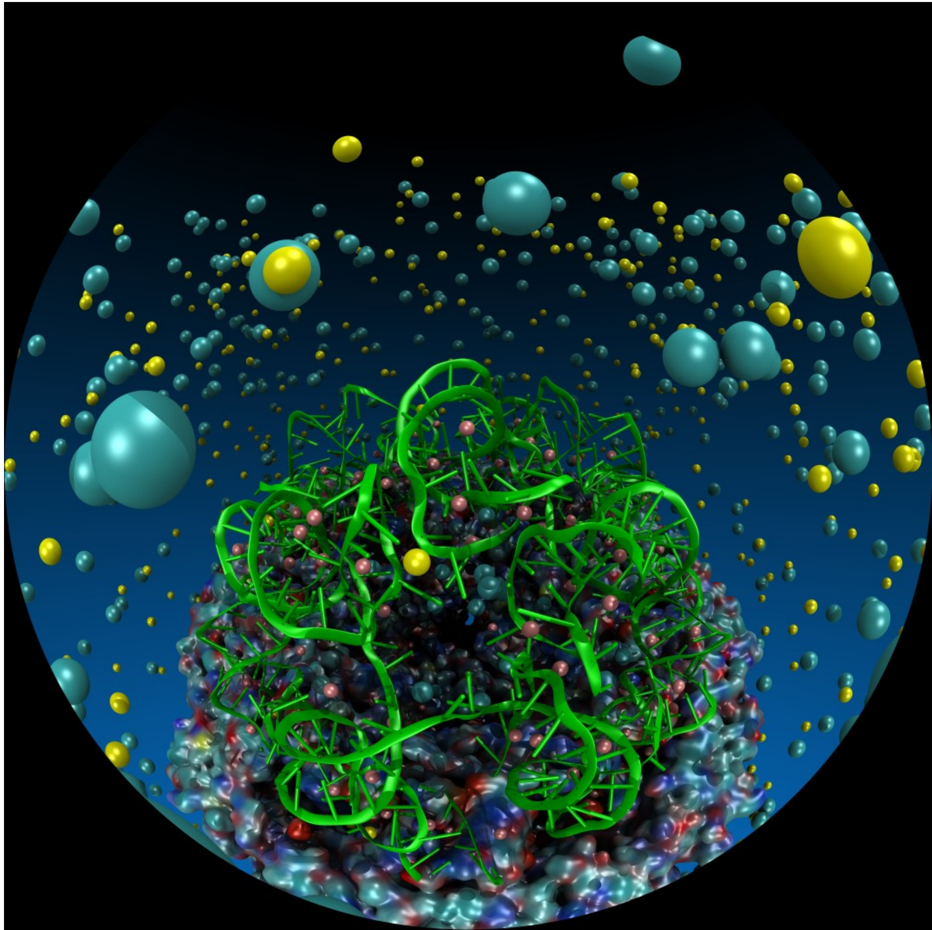


	Chromatophore @ 4Kx4K	Chrom Cell, 512x DoF @ 1080p
Quadro GV100	1	1
2x Quadro GV100	1.97	1.95
Quadro RTX 6000	8.02	8.18

VMD Planetarium Dome Master Camera

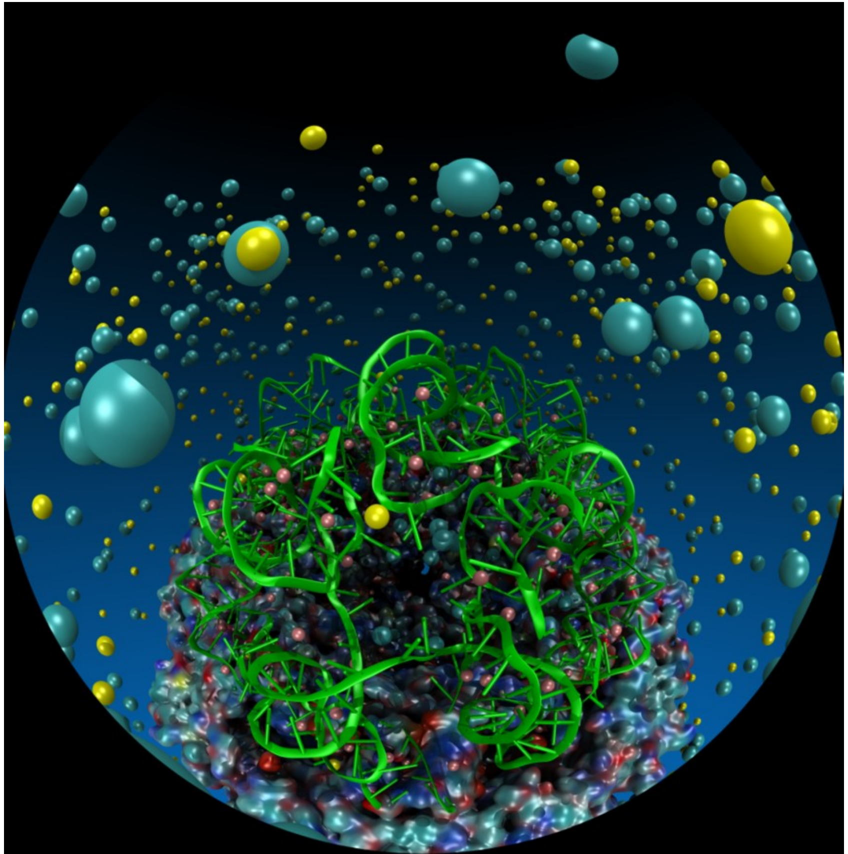
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, …
- Both mono and stereoscopic
- No post-processing required

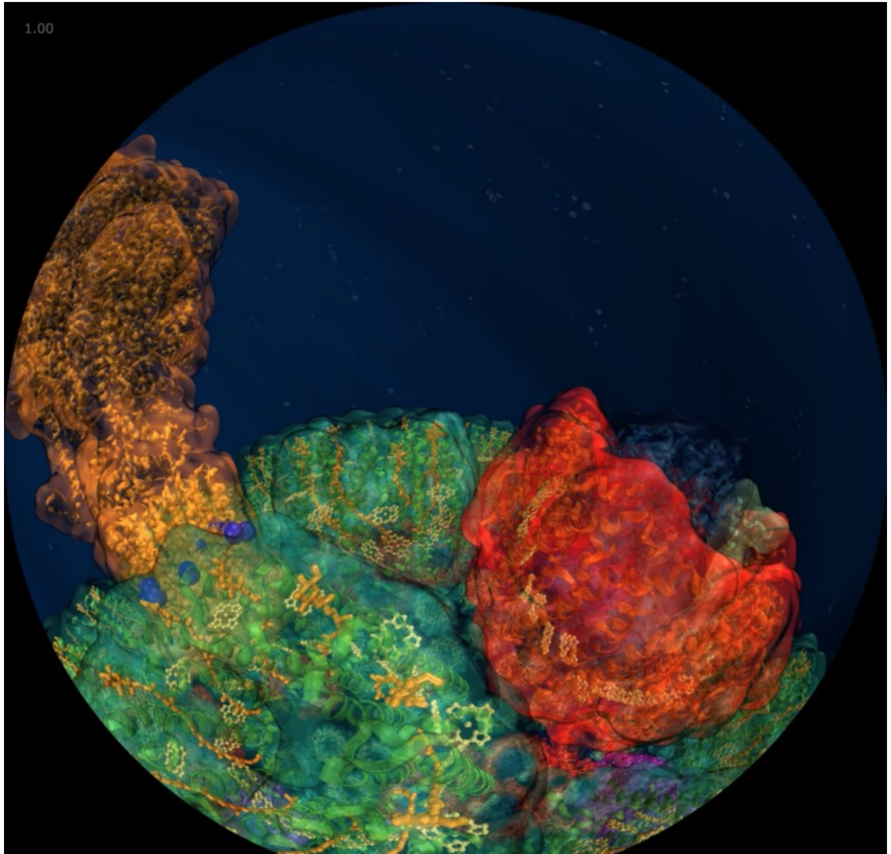
Ray Tracing Gems
Ch. 4



Planetarium Dome Master Projections

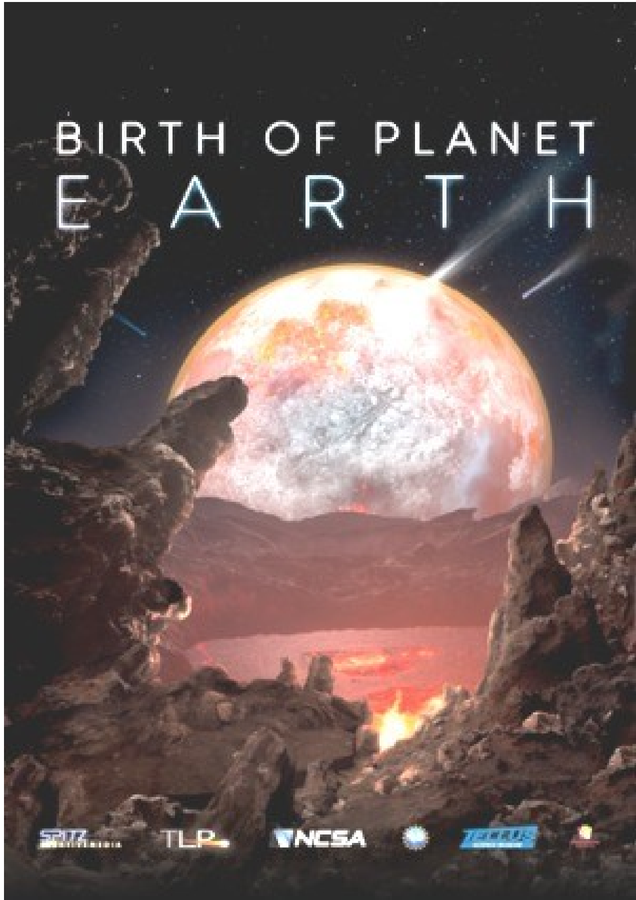
NSF CADENS Dome Show w/ NCSA AVL





Birth of Planet Earth Fulldome Show

- Premieres March 28, Zeiss Großplanetarium, Berlin, Germany
- First public showing on March 30, Das Planetarium am Insulaner, Berlin, Germany
- Joint project with:
  - Spitz Creative Media
  - NCSA Advanced Visualization Lab
  - Thomas Lucas Productions, Inc.
  - Tellus Science Museum
- NSF Support: CADENS award ACI-1445176



VMD Petascale Visualization and Analysis

- Analyze/visualize large trajectories too large to transfer off-site:
  - User-defined parallel analysis operations, data types
  - Parallel rendering, movie making
- Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis:
  - **GPU accelerated trajectory analysis w/ CUDA**
  - **OpenGL and GPU ray tracing for visualization and movie rendering**
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 nodes – can read in **231 TB in 15 minutes!**

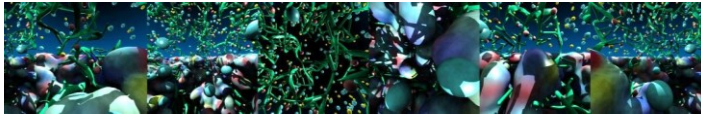
Parallel VMD currently available on:

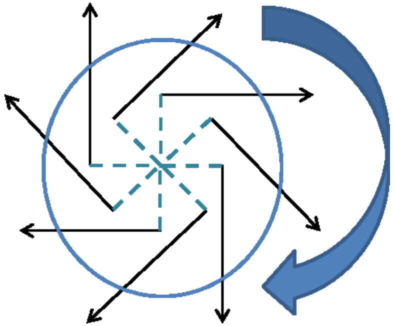
ORNL Titan, NCSA Blue Waters, Indiana Big Red II, CSCS Piz Daint, and similar systems

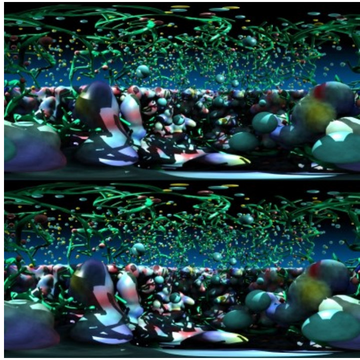
NCSA Blue Waters Hybrid Cray XE6 / XK7
22,640 XE6 dual-Opteron CPU nodes
4,224 XK7 nodes w/ Telsa K20X GPUs

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, …







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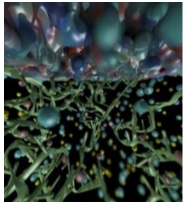
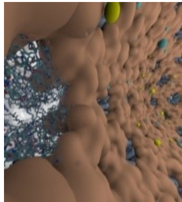
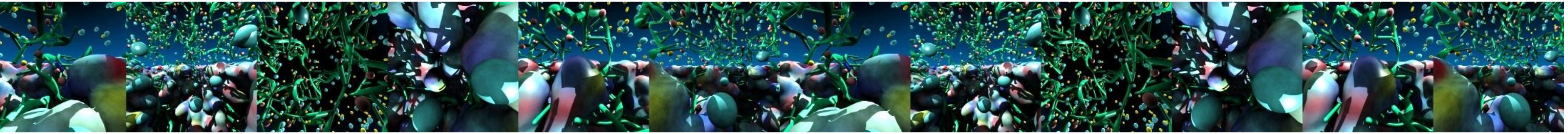




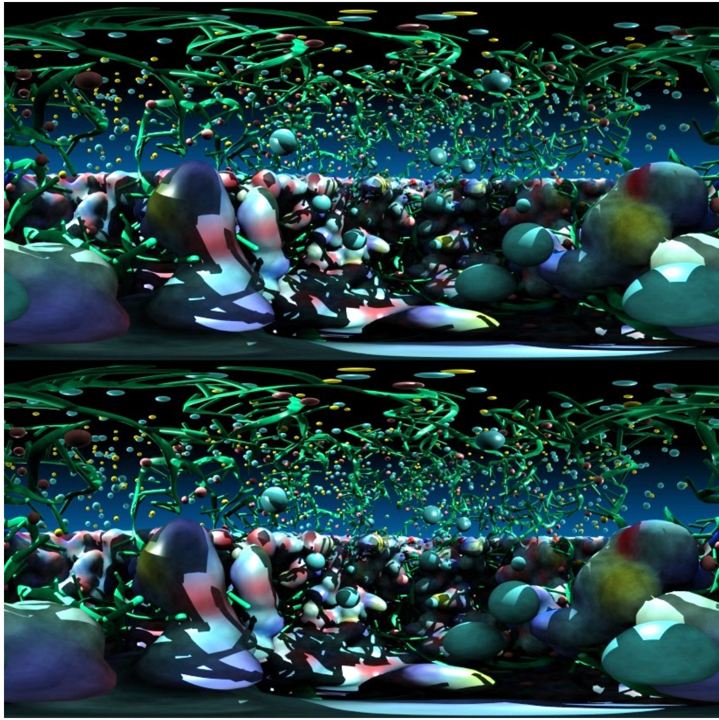
HMD Ray Tracing Challenges

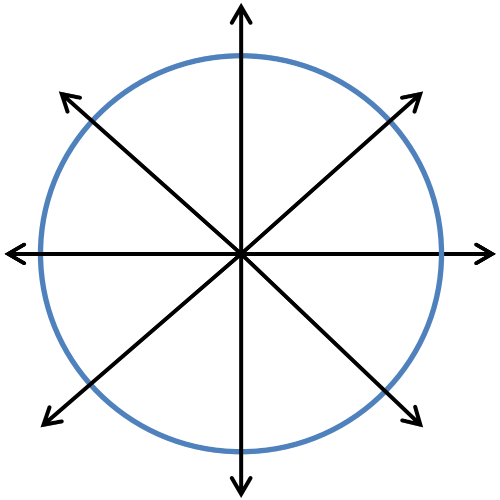
- HMDs require high frame rates **(90Hz or more)** and minimum latency between IMU sensor reads and presentation on the display
- Multi-GPU workstations fast enough to direct-drive HMDs at required frame rates for simple scenes with direct lighting, hard shadows
- Advanced RT effects such as AO lighting, depth of field, path tracing require **large sample counts**, difficult for direct-driving HMDs today
- **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**

Stereoscopic Panorama Ray Tracing w/ OptiX

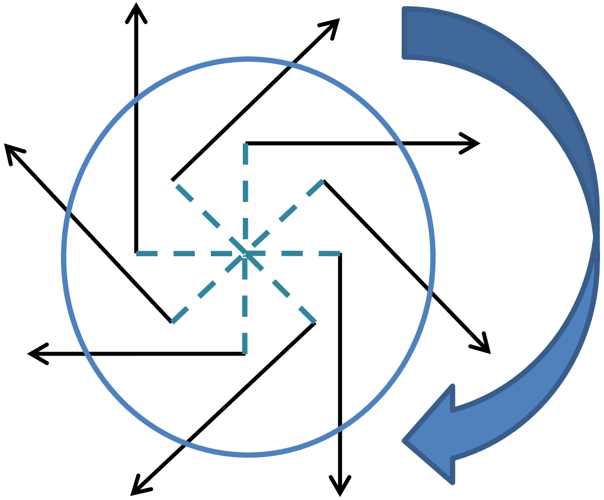


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple proxy geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**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



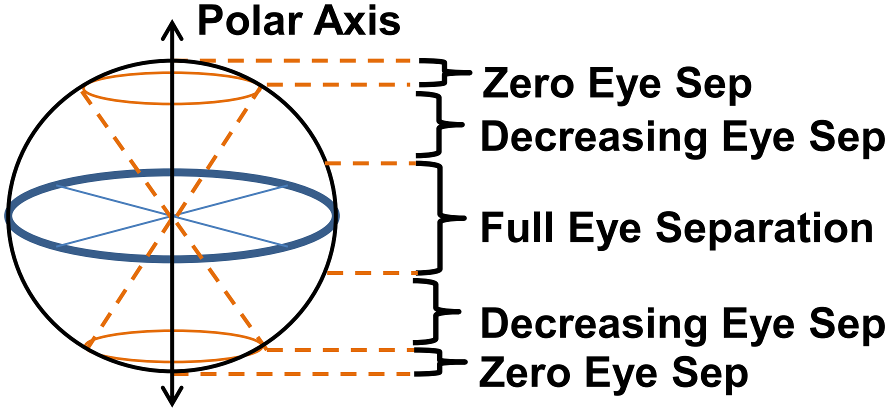


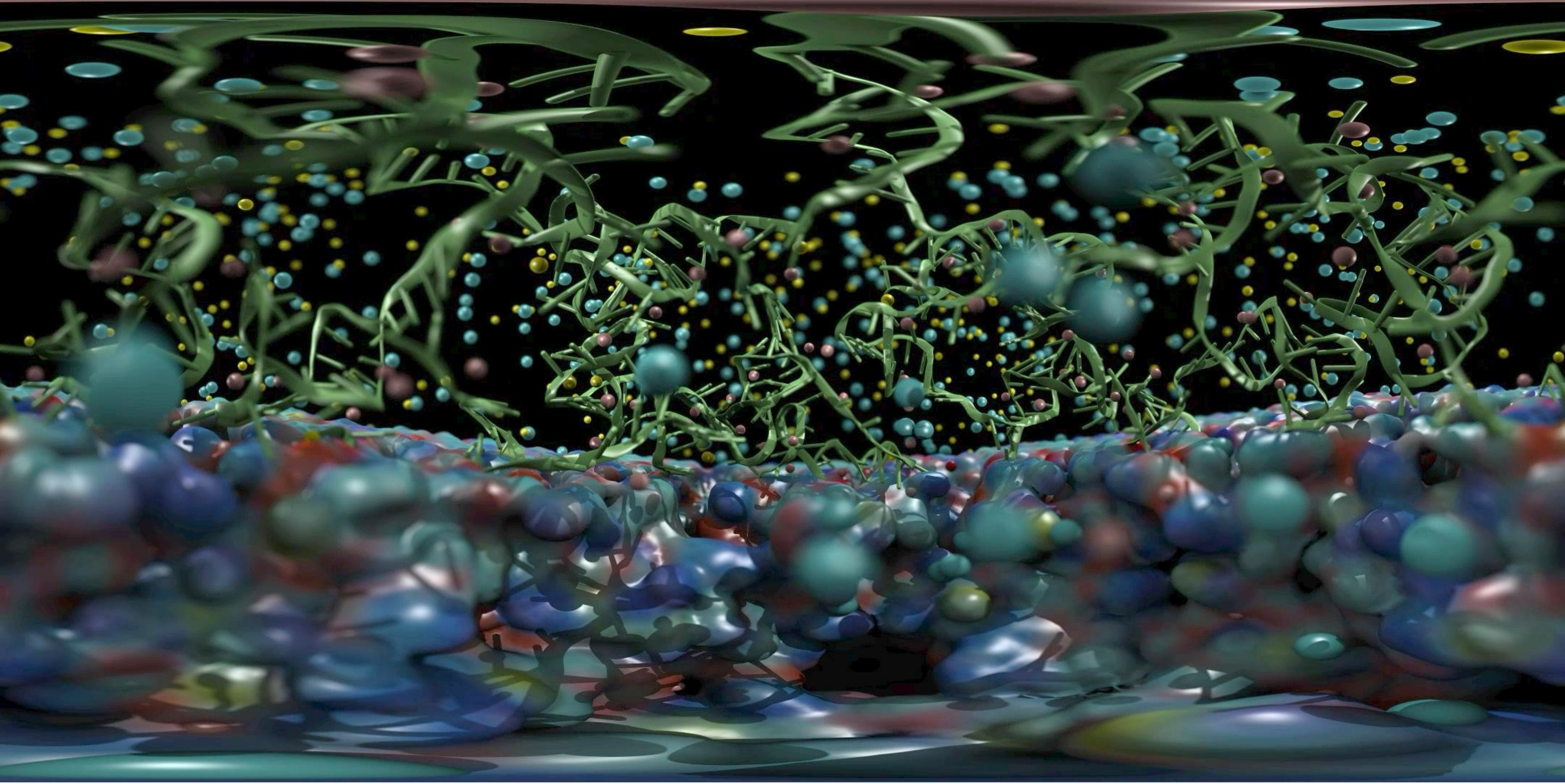
**A) Monoscopic circular projection.
Eye at center of projection (COP).**



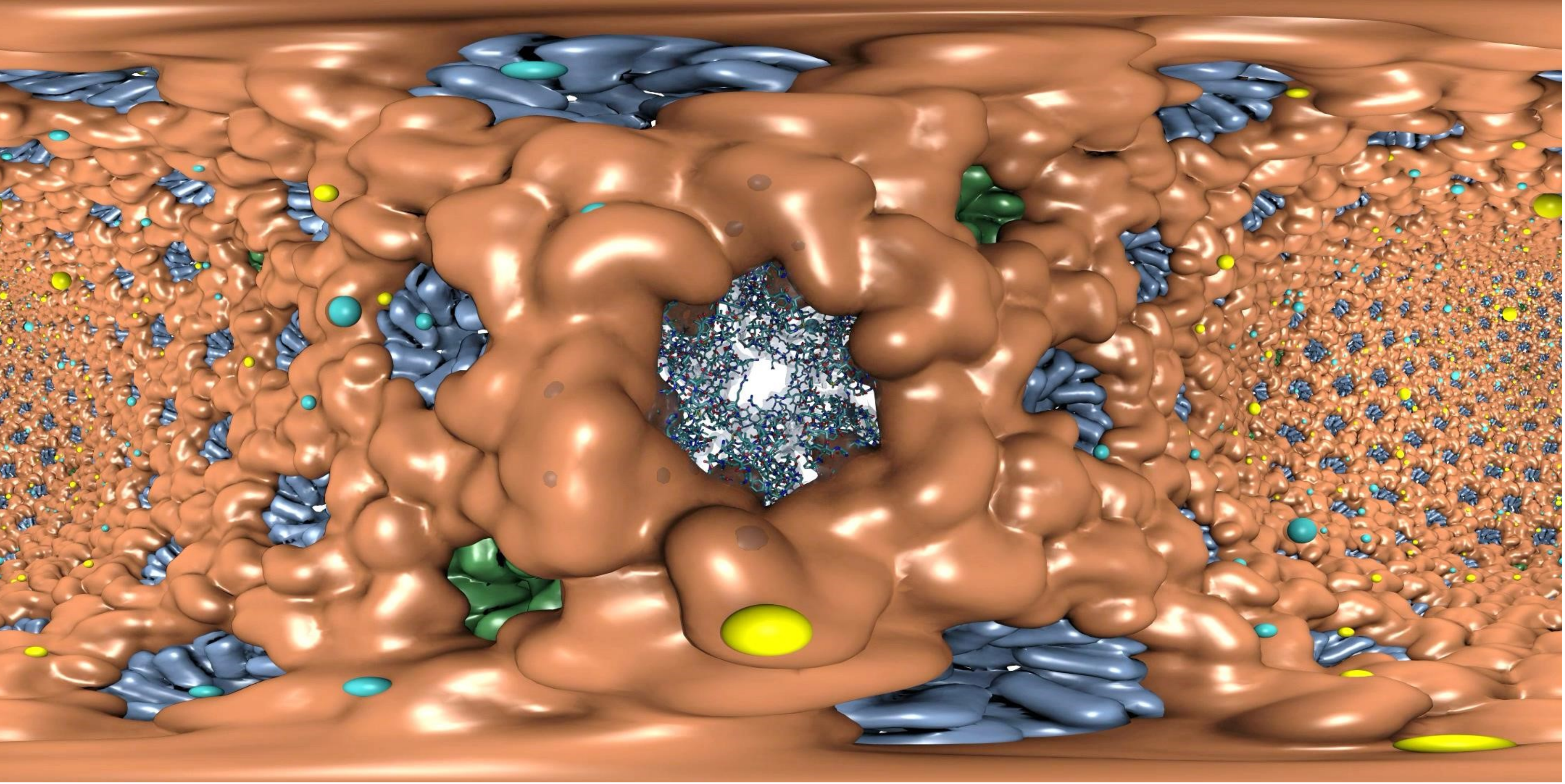
**B) Left eye stereo circular projection.
Eye offset from COP by half of interocular distance.**

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.



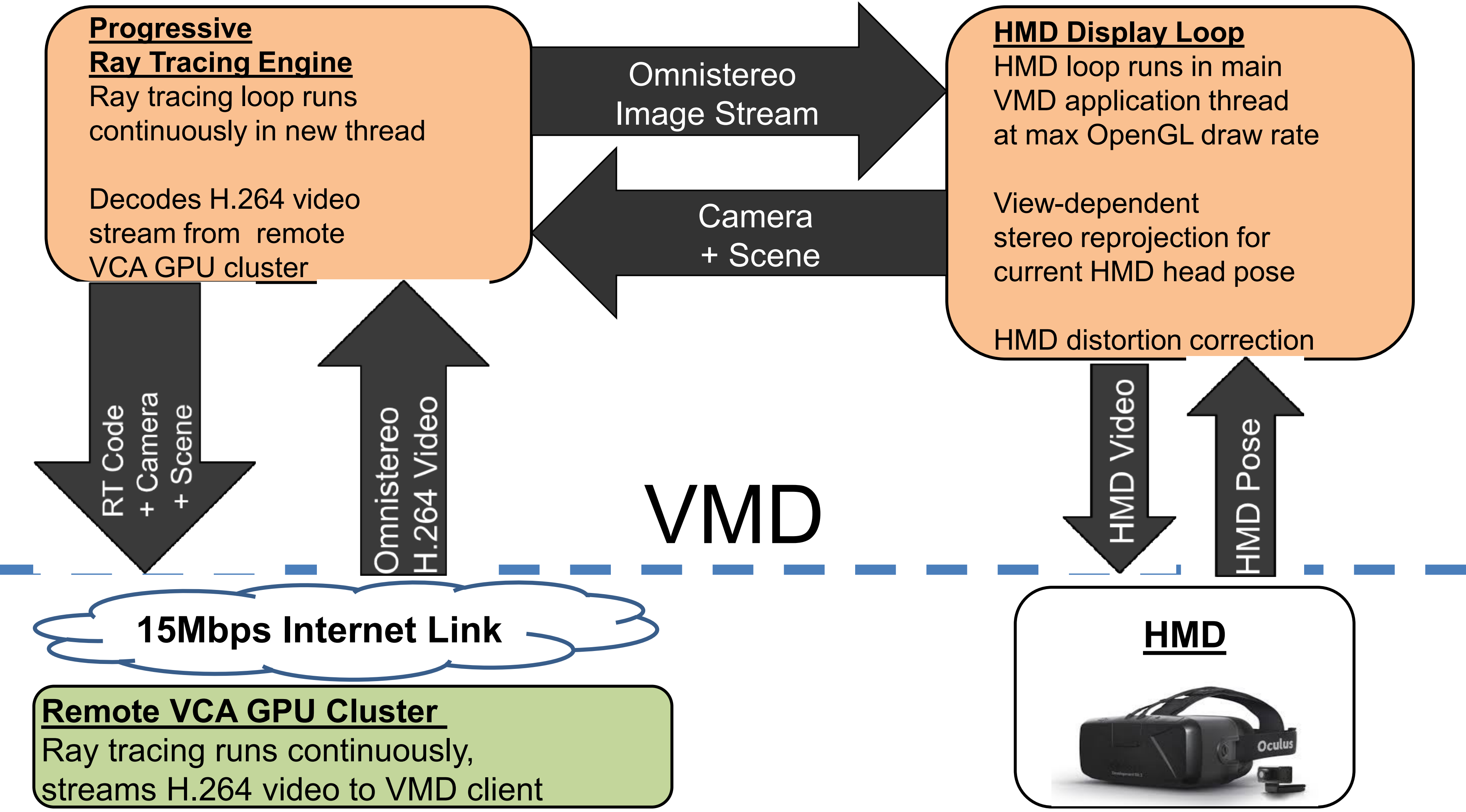


Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …



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

2016: 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

2019: Local RTX Omnidirectional Stereoscopic RT Performance @ 3072x1536 w/ 1-subframe

Scene	Per-subframe samples AA : AO (AO per-hit)	RT update rate (FPS)
STMV shadows	1:0 2:0 4:0	75.0 37.5 18.3
STMV Shadows+AO	1:1 1:2 1:4 1:8	65.8 57.5 37.5 25.2
STMV Shadows+AO+DoF	1:1 2:1 2:2	61.5 22.1 18.5
HIV-1 Shadows	1:0 2:0 4:0	75..0 74.2 37.5
HIV-1 Shadows+AO	1:1 1:2 1:4 1:8	72.0 61.0 37.5 23.1

HMD View-Dependent Reprojection with OpenGL

- Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface (sphere for equirectangular, cube for cube map)
- 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
- **Enables low-latency, high-frame-rate redraw** as HMD head pose changes **(150Hz or more)**

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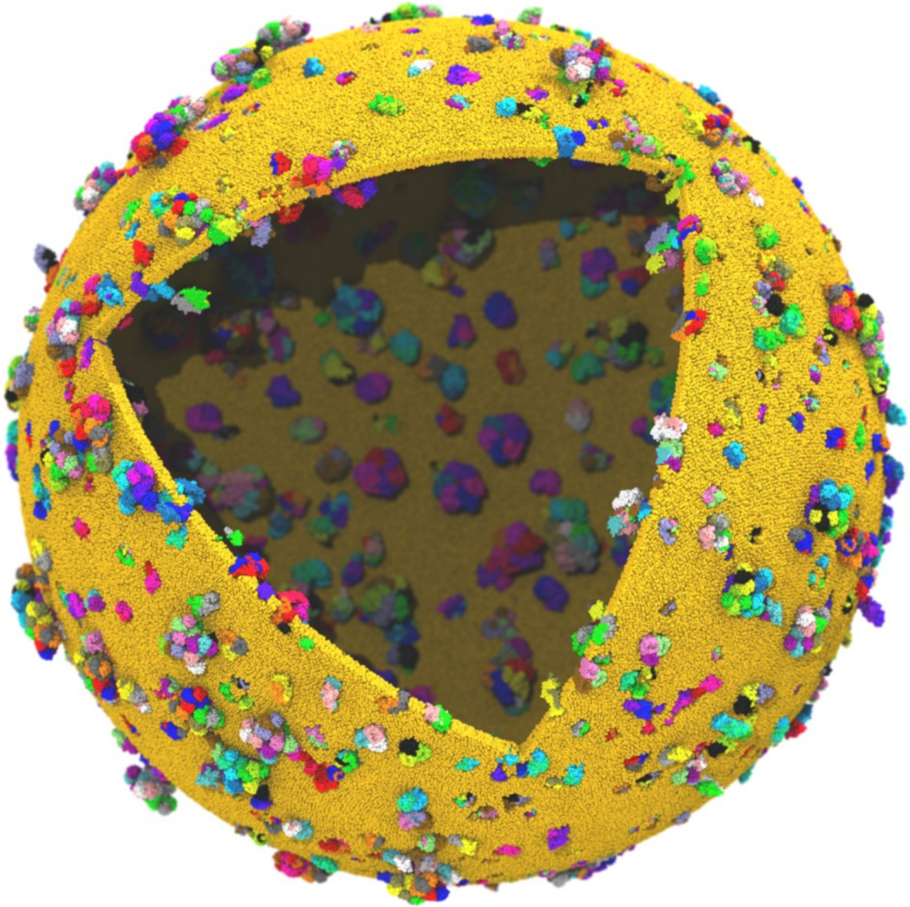
Ongoing Ray Traced VR Work

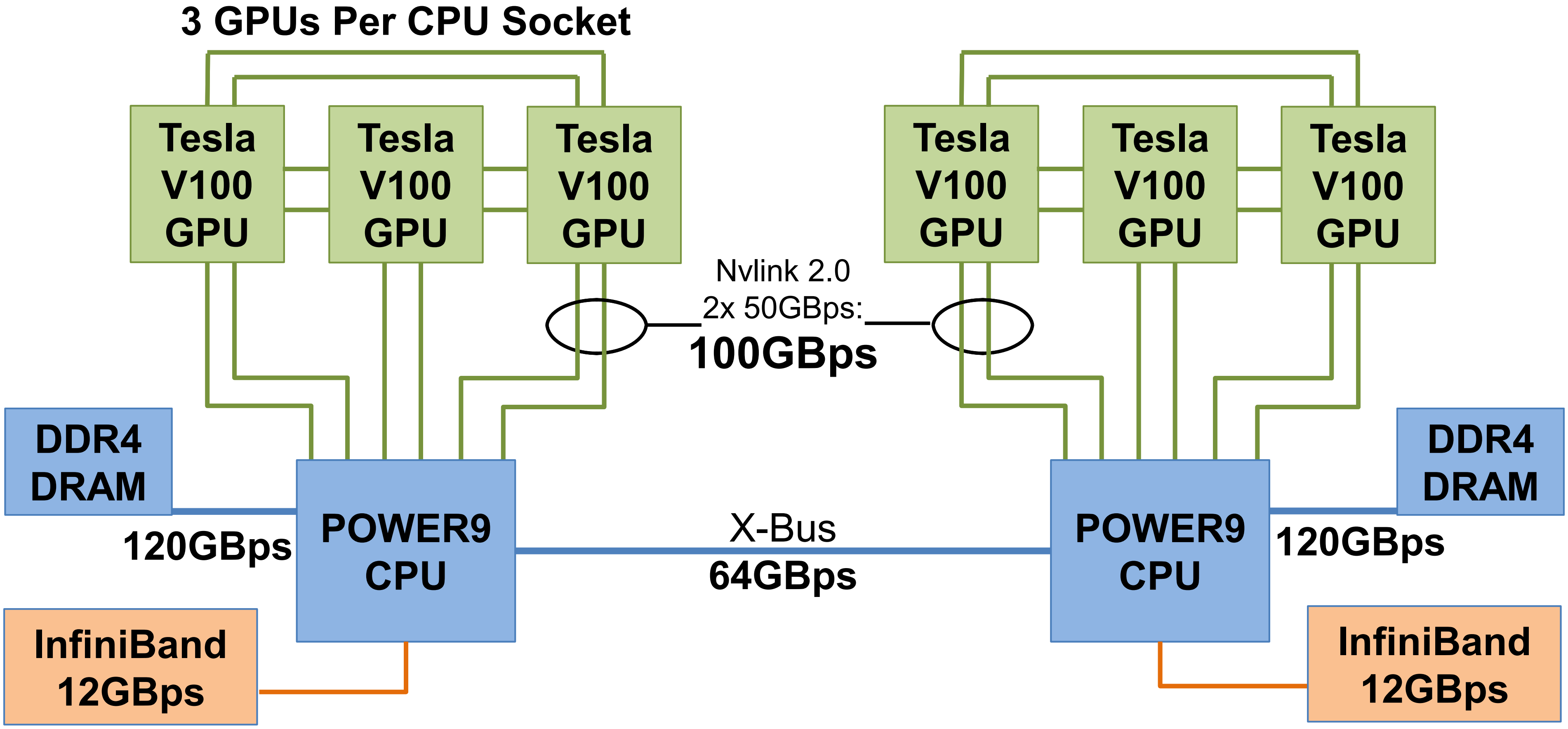
- OpenXR – cross platform muti-vendor HMD support
- VMD RTX ray tracing engine and optimizations:
  - **AI denoising for better average quality**
  - Interactive RT stochastic sampling strategies to improve interactivity
  - Improved omnidirectional cubemap/spheremap sampling approaches
  - **AI multi-view warping to allow rapid in-between view generation amid multiple HMD head locations**
  - **H.265 for high-res omnidirectional video streaming**
  - **Multi-node parallel RT and remote viz. on general clusters and supercomputers, e.g. NCSA Blue Waters, ORNL Titan**
- Tons of work to do on VR user interfaces, multi-user collaborative visualization, …

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



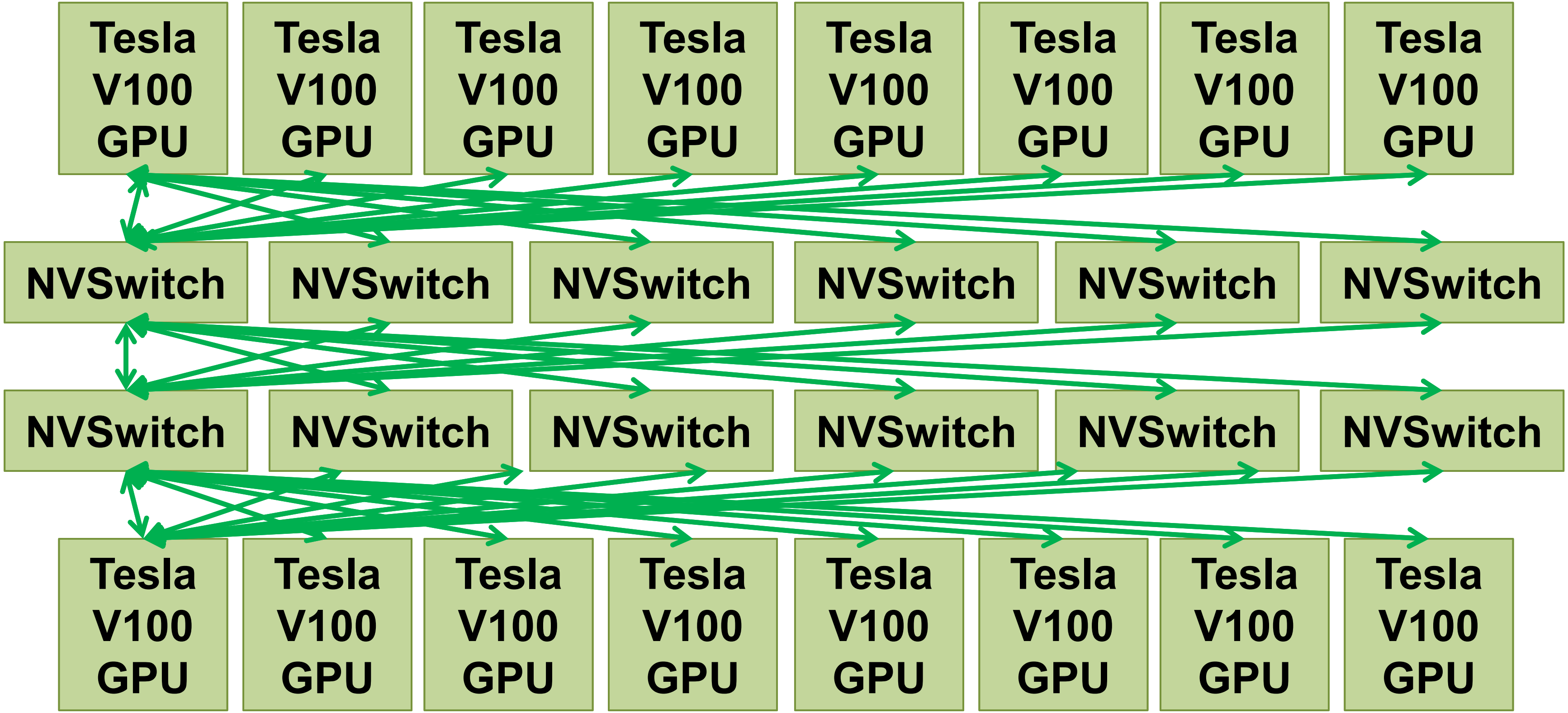
IBM AC922, ORNL Summit Node



NVIDIA DGX-2

16x 32GB Tesla V100 GPUs w/ 300GB/s NVLink, fully switched

512GB HBM2 RAM w/ **2.4TB/s Bisection Bandwidth, 2 PFLOPS**



RT Opportunities and Challenges Posed by Future DGX-2-Like Node/System Designs

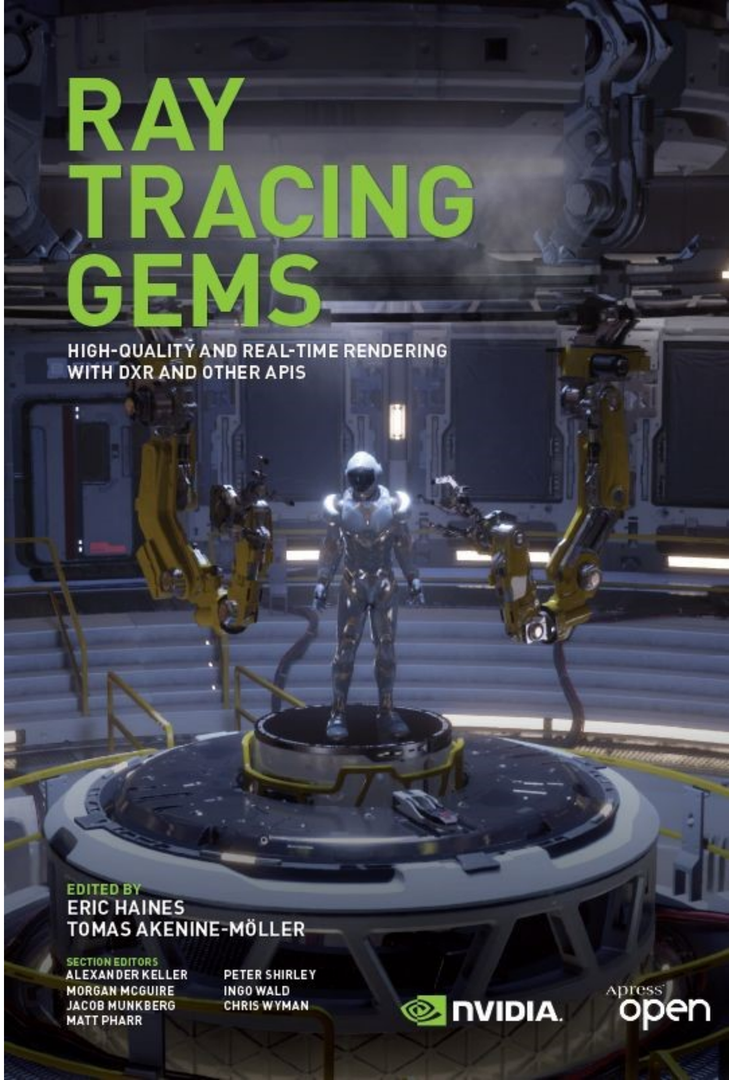
- **512GB of fast HBM2 RAM w/ 2.4TB/sec bisection bandwidth!!!**
- **CPUs "oversubscribed" by GPUs**
- GPU RT must dis-involve CPUs to greatest possible extent
- **Fully-switched NVLink**-connected memory systems permit fine-grained multi-GPU RT algorithms via direct peer memory load/stores
- **Throughput oriented GPU RT work scheduling can hide both local and remote memory latencies gracefully**
- Application control of the distribution of scene geometry among GPUs, replication or distribution of RT acceleration structures
- Permit both "capacity" oriented distributed memory RT approaches and "performance" focused RT approaches heavy on data replication.

Ray Tracing Gems

- Ch. 4, "A Planetarium Dome Master Camera"
- Ch. 27, "Interactive Ray Tracing Techniques for High-Fidelity Scientific Visualization"
- Tons of great material and code samples!

- **See Eric Haines RTG GTC talk:**
  - **Room 230B (Concourse Level) on Thursday 2-3 PM**

- **RTG book signings on Thursday, 3-4pm @ GTC book seller**



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:

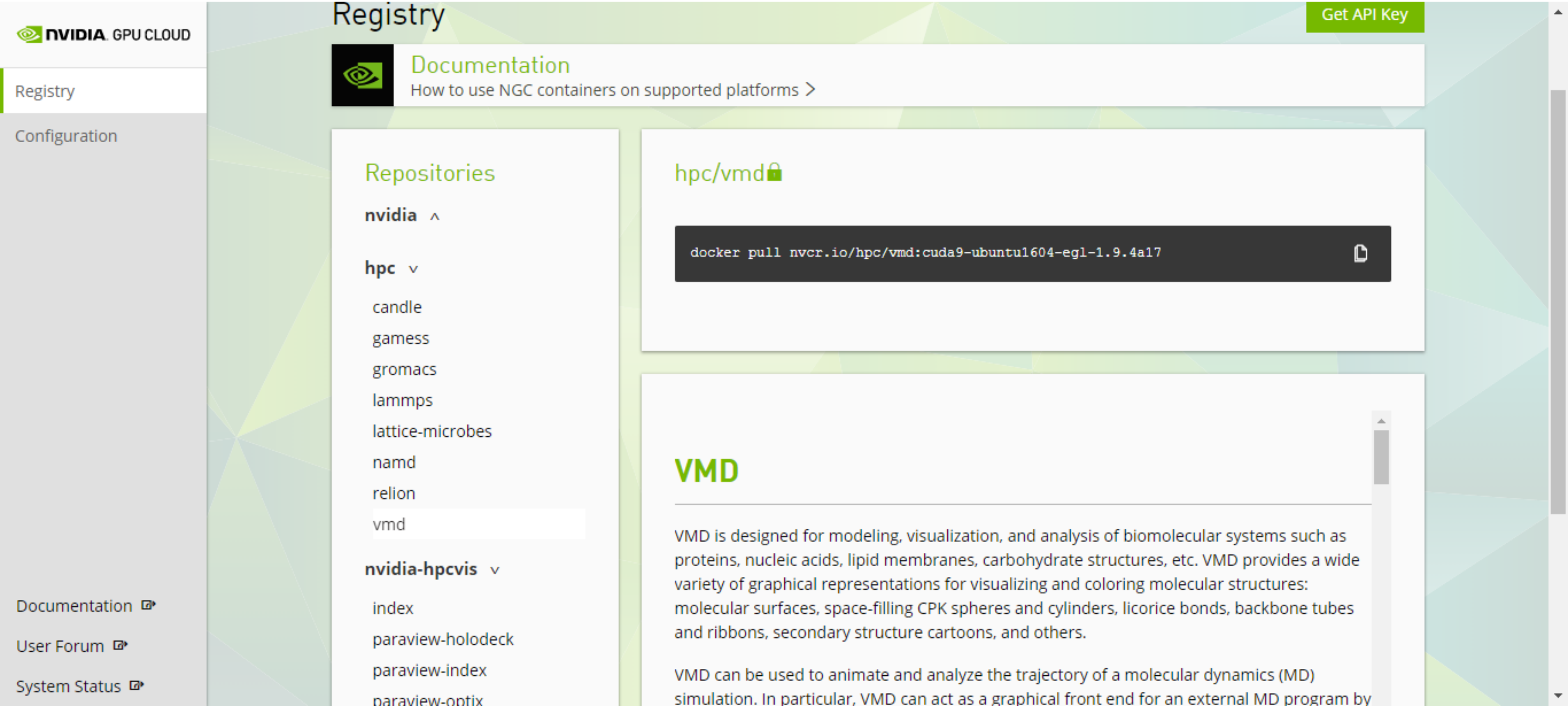
    http://www.ks.uiuc.edu/Research/cloud/

Clusters, Supercomputers

Workstations,
Servers,
Cloud

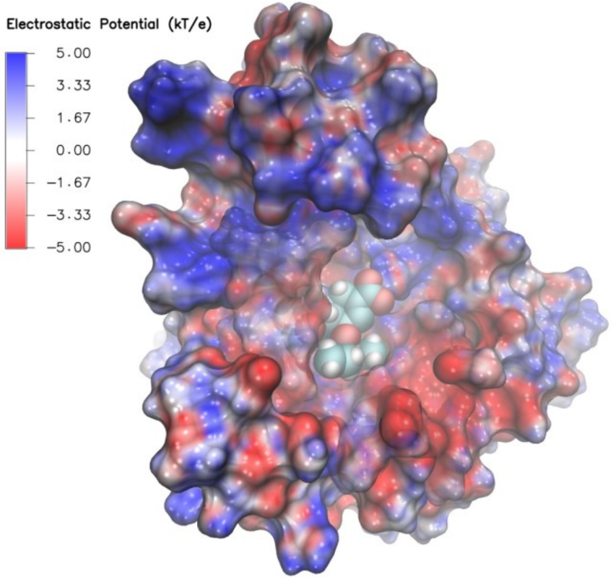
Molecular dynamics-based refinement and validation for sub-5 Å cryo-electron microscopy maps. Abhishek Singharoy, Ivan Teo, Ryan McGreevy, John E. Stone, Jianhua Zhao, and Klaus Schulten. *eLife*, 10.7554/eLife.16105, 2016. (66 pages).
QwikMD-integrative molecular dynamics toolkit for novices and experts. 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



VMD OptiX/EGL NGC Container

- **https://ngc.nvidia.com/registry/**
- **CUDA-accelerated** viz+analysis
- **EGL off-screen rendering** – no windowing system needed
- **OptiX high-fidelity GPU ray tracing** engine built in
- All dependencies included
- **Easy to deploy on a wide range of GPU accelerated platforms**



High performance molecular visualization: In-situ and parallel rendering with EGL. J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014-1023, 2016.

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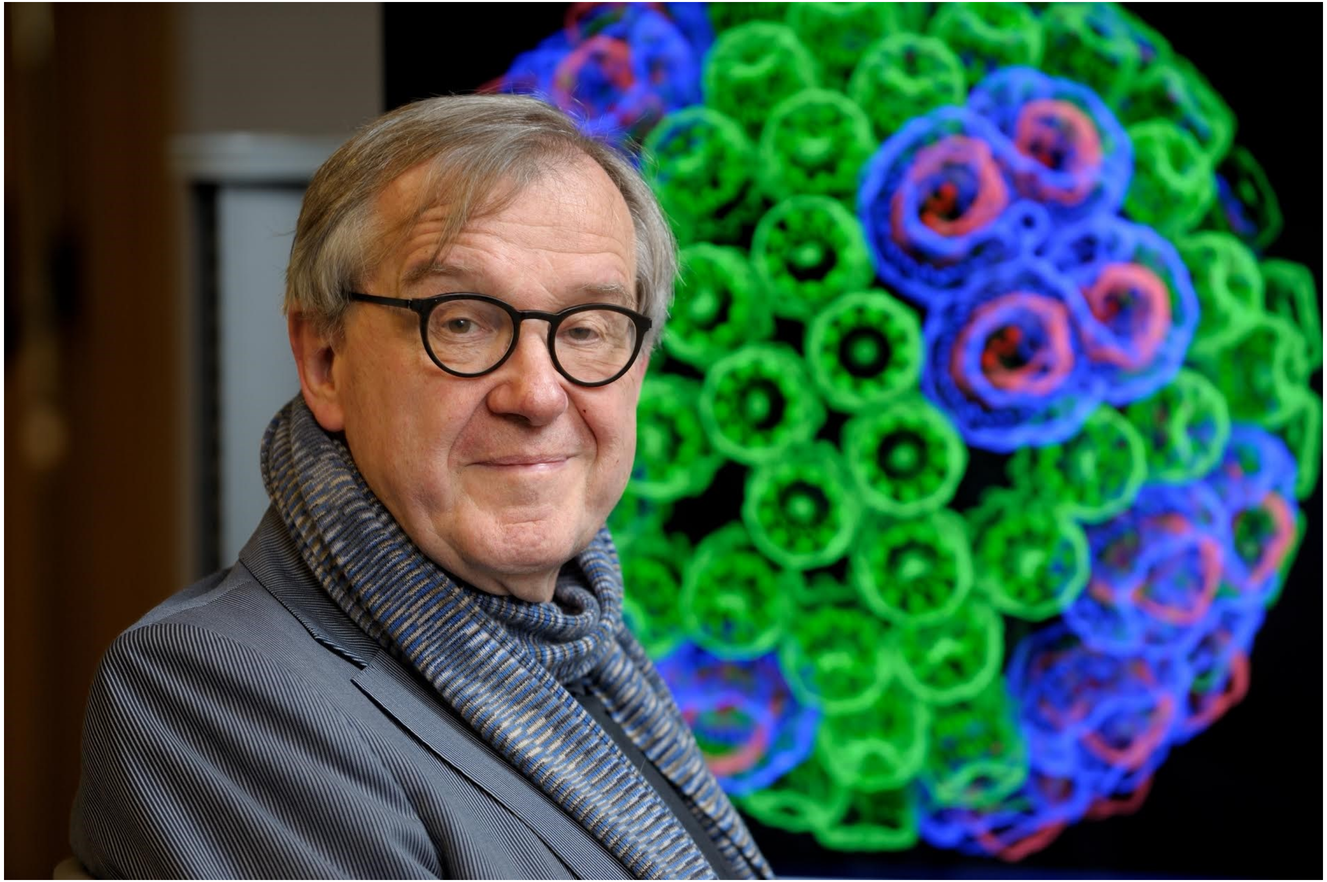
  - NSF Blue Waters:
    NSF OCI 07-25070, PRAC "The Computational Microscope",
    ACI-1238993, ACI-1440026



“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.

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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.
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- **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.

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- **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.

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- **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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- **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.
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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.

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- **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.

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