S8665—VMD: Biomolecular Visualization from Atoms to Cells Using Ray Tracing, Rasterization, and VR

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

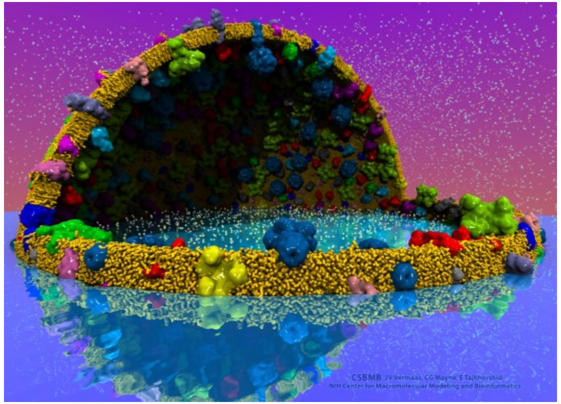
S8665, GPU Technology Conference

11:00-11:50, Hilton Almaden 2,

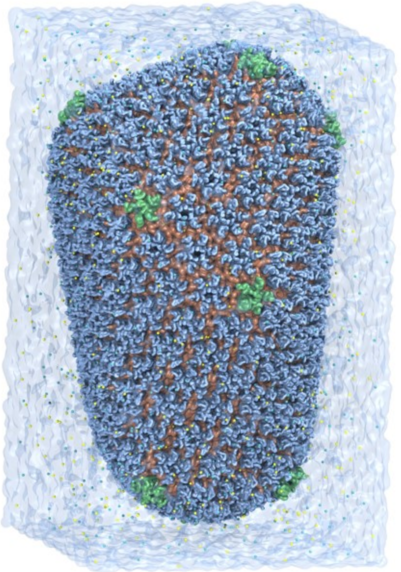
San Jose, CA, Thursday March 29th, 2018

VMD – “Visual Molecular Dynamics”

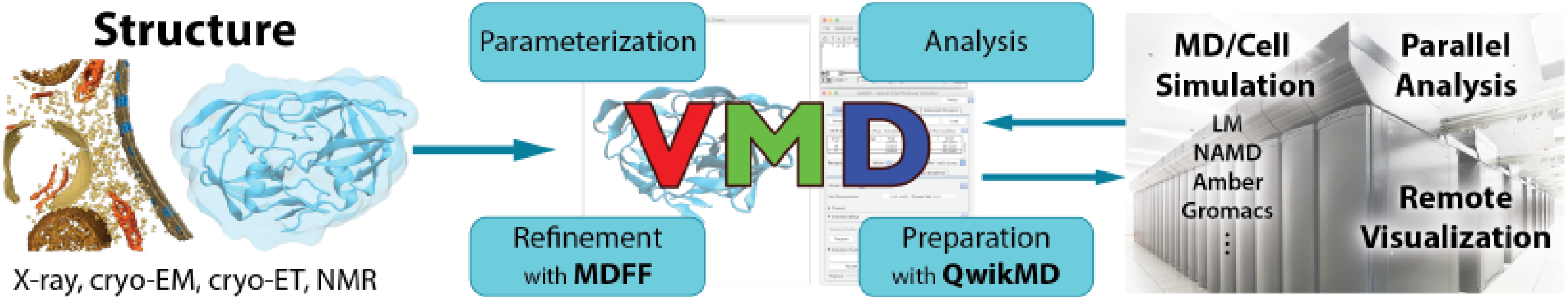
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
  - Sequence information
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



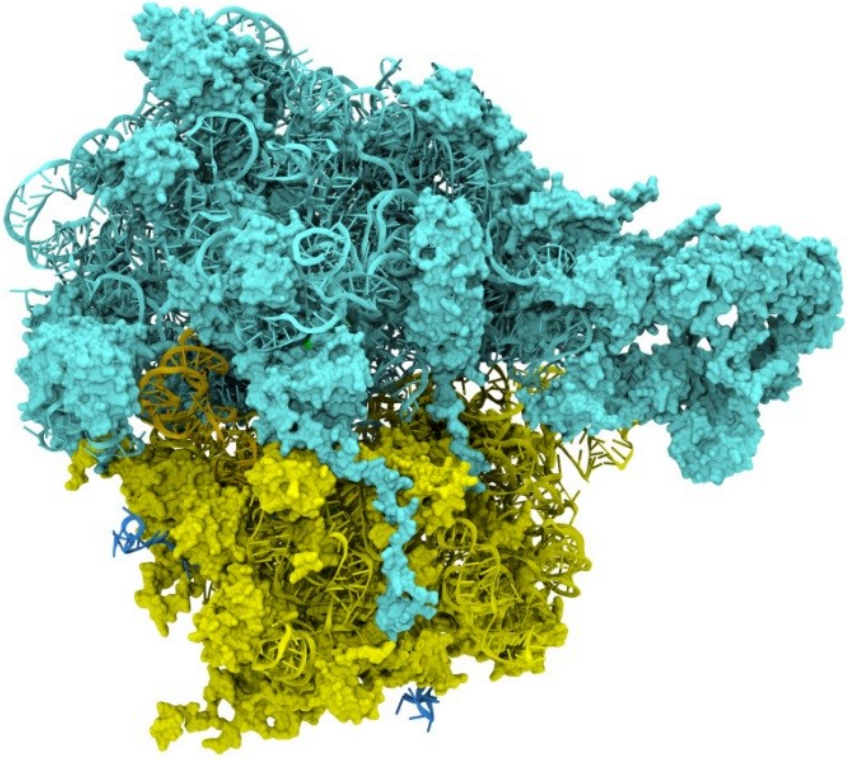
MD Simulation



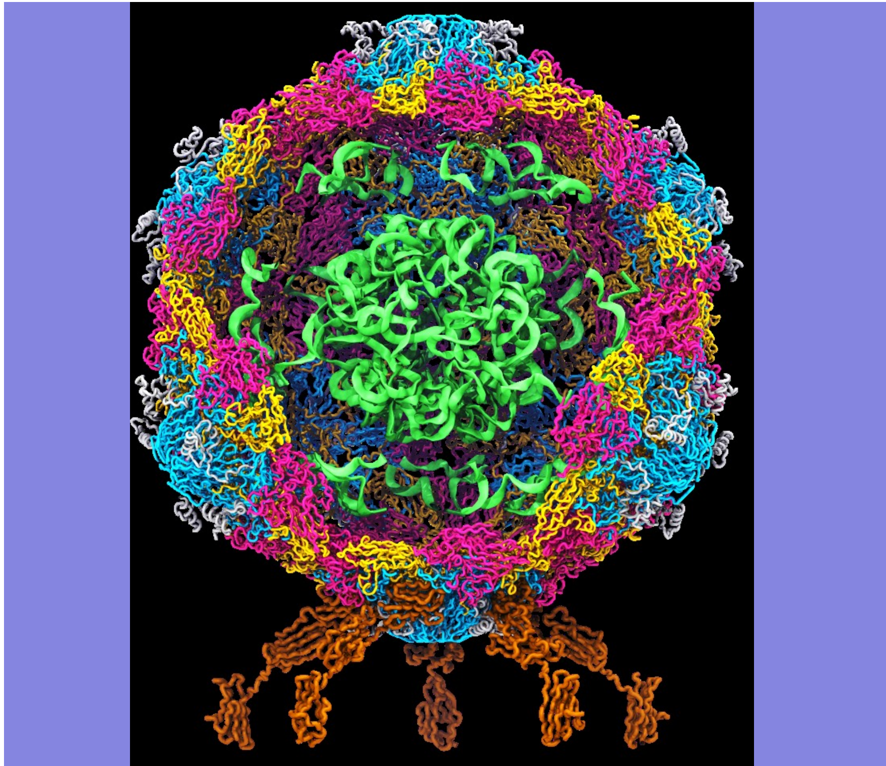
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



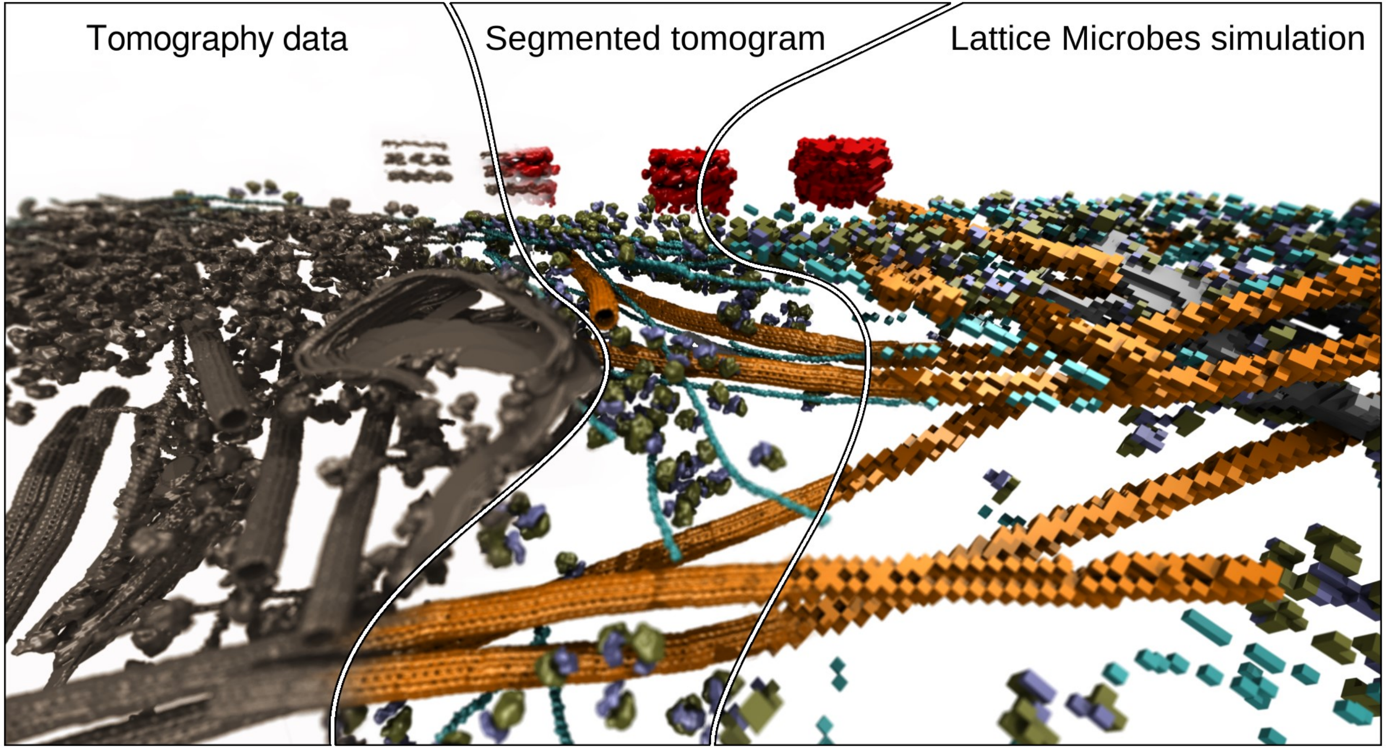
Poliovirus



Cryo-EM / Cryo-ET Image Segmentation

Evaluate 3-D volumetric electron density maps and segment them, to identify key structural components

Index/label components so they can be referred to, colored, analyzed, and simulated…



Cryo-EM Density Map Segmentation Approach, goals

Goals:

- **Reach interactive performance rates (under 1 second)** for common density map sizes between 128^3 to 256^3 voxels
- Handle **next-generation problem sizes (768^3 to 2048^3)** smoothly with only a brief wait

Key methods:

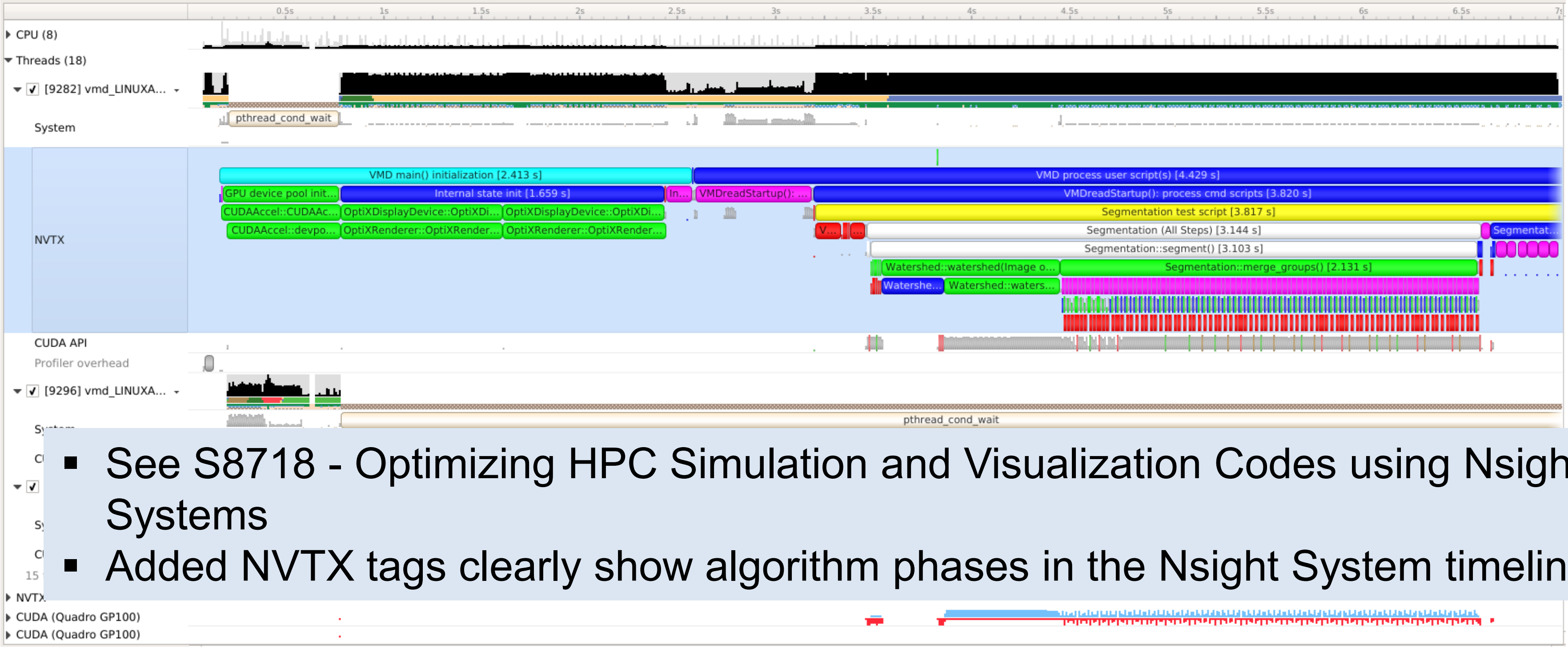
- **Tile-based early-exit schemes** pervasively used for all iterative segmentation update/merge kernels
- **Privatization, shared memory atomic counters** for segmentation group index kernels
- **Significantly faster than published algorithm designs we are aware of**

Watershed segmentation:

- Smooth/denoise image (e.g. blur)
- Find local minima of image/gradients
- Connect minimum voxels with neighbors of similar intensity, marking them with the same "group" number
- "Grow" each group (merging groups where rules allow) until no more updates occur

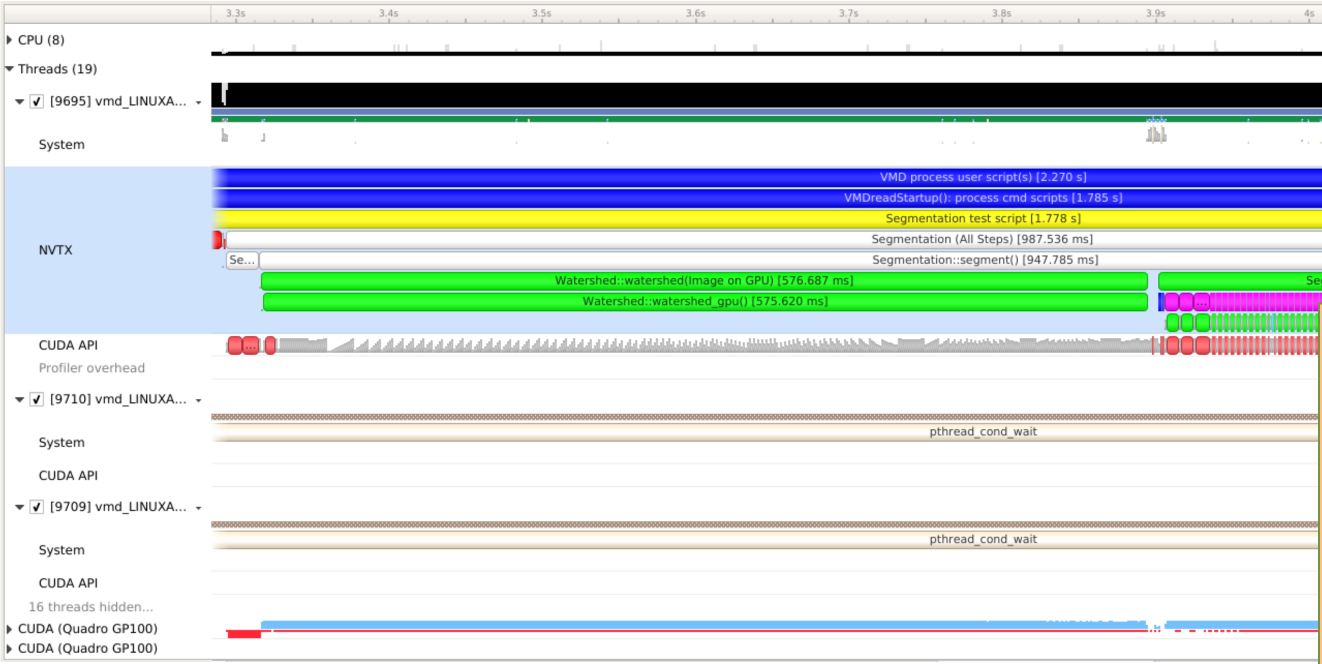
Scale-space segmentation variant does further blurring and group merging to reach a user-specified target segment count

Profiled VMD Segmentation w/ NVIDIA Nsight Systems



- See S8718 - Optimizing HPC Simulation and Visualization Codes using Nsight Systems
- Added NVTX tags clearly show algorithm phases in the Nsight System timeline.

VMD Optimized GPU Segmentation Pipeline



256^3 voxels:

Quadro GP100
Total time: 0.98s
Total speedup: 3.2x

Tesla V100
Total time: 0.67s
Total speedup: 4.1x

- **VMD GPU Segmentation now over 12x faster than competing tools**

Volta-Specific Segmentation Optimization Opportunities

- Optimized precision for 3-D density maps:
  - Improved memory bandwidth, lower arithmetic cost
  - FP16: half-precision EM density map representation
  - INT8: byte density map representation **for EM tomograms**
- Explore Tensor Core for iterative scale-space segmentation merge/blur convolutions, and initial noise filtering steps:
  - Difficult to prevent TC from becoming mem bandwidth-bound
  - Challenge: CUDA 9.x APIs for TC limit the range of data movement patterns that perform well
  - Some dimensionalities and matrix-based problem decompositions perform much better than others – this is an area of ongoing exploration

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!**

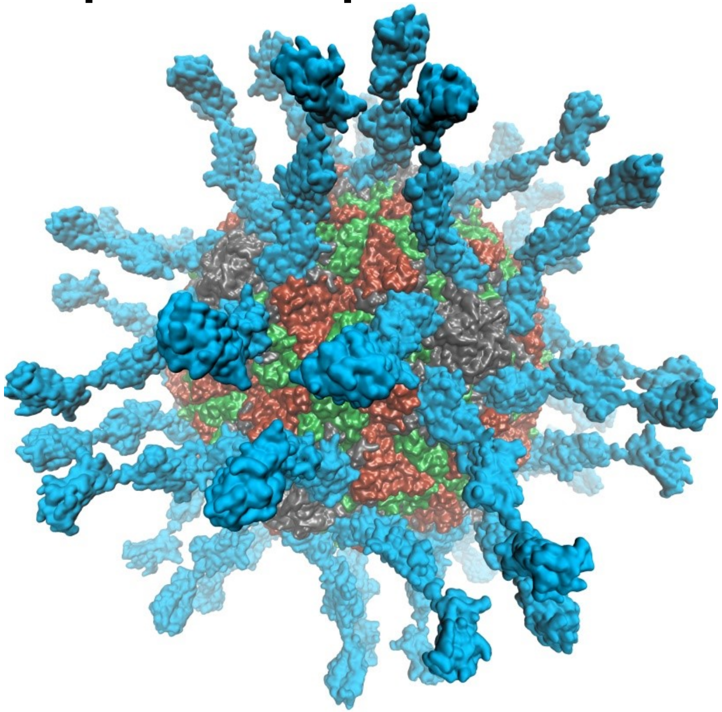
Parallel VMD currently available on:

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

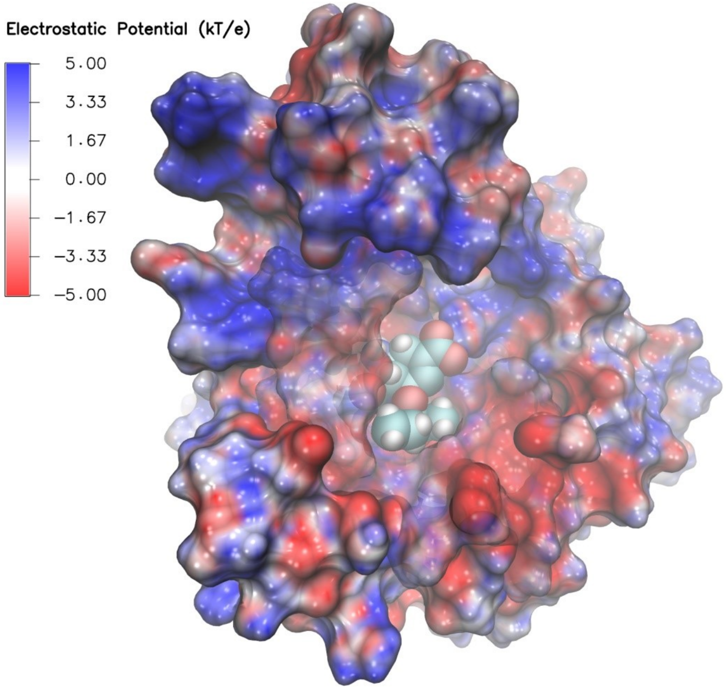
VMD supports EGL for in-situ and parallel rendering on clouds, clusters, and supercomputers

- **No windowing system dependency**
- Easily deploy parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features
- Support high-quality vendor-supported commercial OpenGL implementations in HPC systems that were previously limited to Mesa

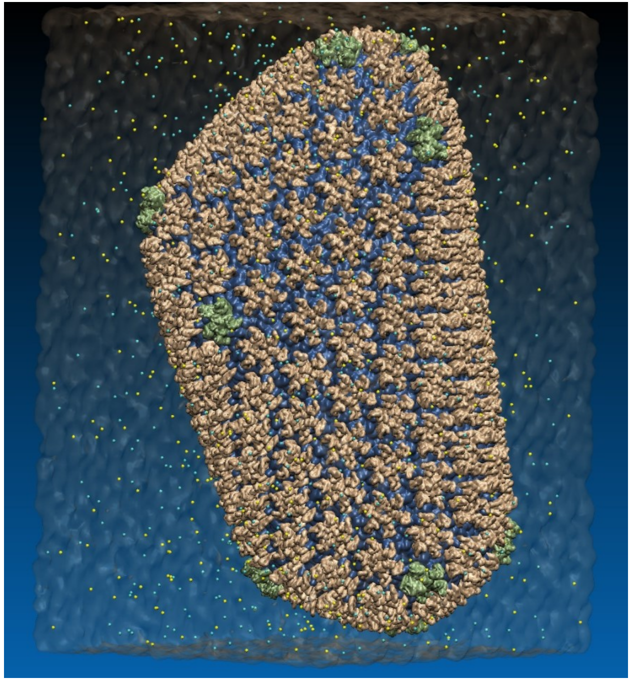


Poliovirus

VMD EGL Rendering: Supports full VMD GLSL shading features, multisample antialiasing, ray cast spheres, 3-D tex mapping, ...



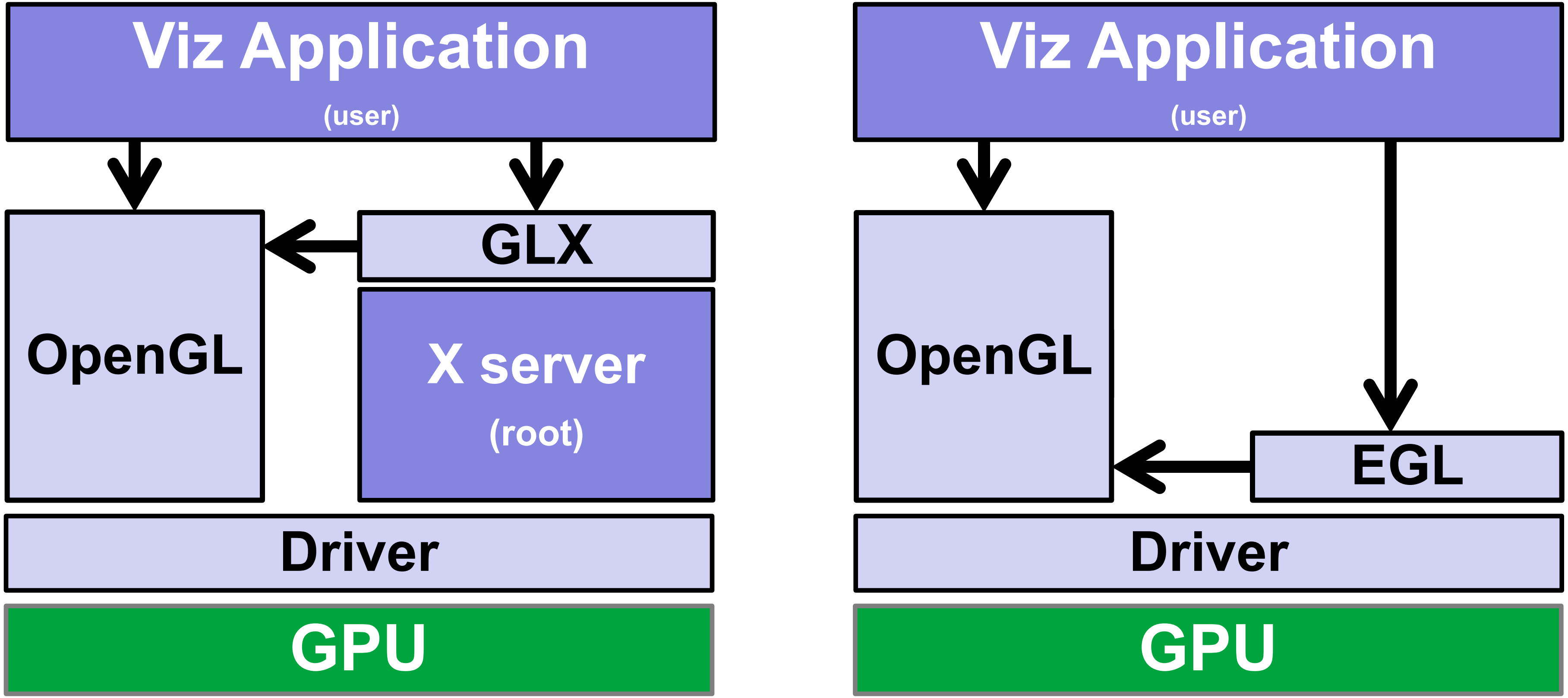
Swine Flu A/H1N1 neuraminidase bound to Tamiflu



64M atom HIV-1 capsid simulation

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 IPDPSW, pp. 1014-1023, 2016.

OpenGL: GLX vs. EGL



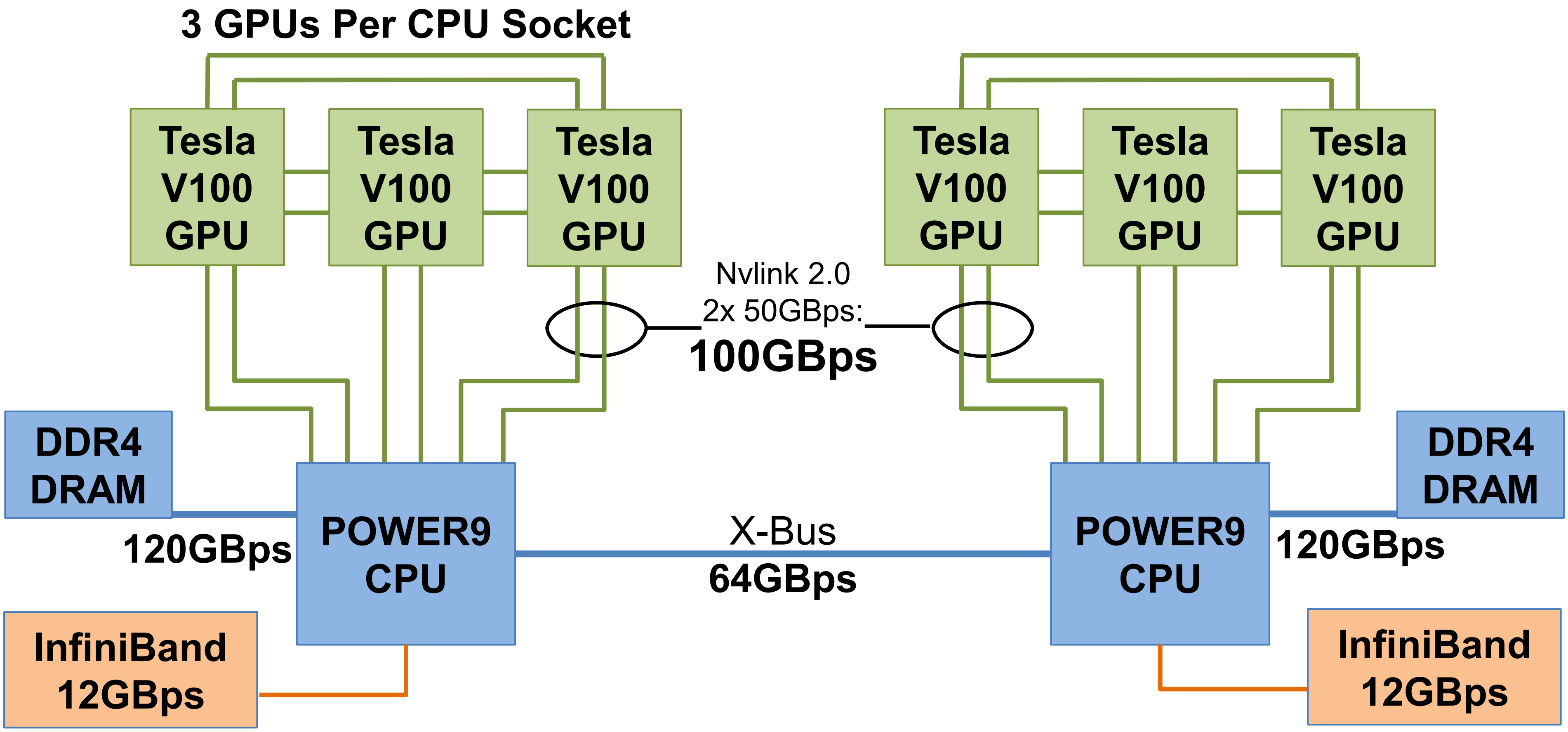
VMD Off-Screen Rendering w/ EGL

- Containers+Cloud+Workstations with recent NVIDIA drivers
- VMD on HPC systems w/ latest GPUs:
  - Cray XC50, CSCS Piz Daint
  - **ORNL Summit in progress now**
  - IBM OpenPOWER, drivers 375.66 and later support both GLX and EGL

Benefits of EGL Platform Interfaces

- **EGL interfaces make it EASY to bind a GPU** to a thread with optimal CPU affinity **with respect to NUMA topology, NVLink GPU topology**
  - High-perf. multi-GPU image compositing, video streaming
  - EGL plays nicely with MPI, CUDA/OpenCL, OptiX, NVENC, etc
  - NVIDIA EGL supports multiple GPU indexing schemes, e.g. **PCIe ordering**
  - **Exploit NVLink interconnect topology on IBM OpenPOWER platforms, DOE/ORNL "Summit" system**

IBM AC922 Summit Node

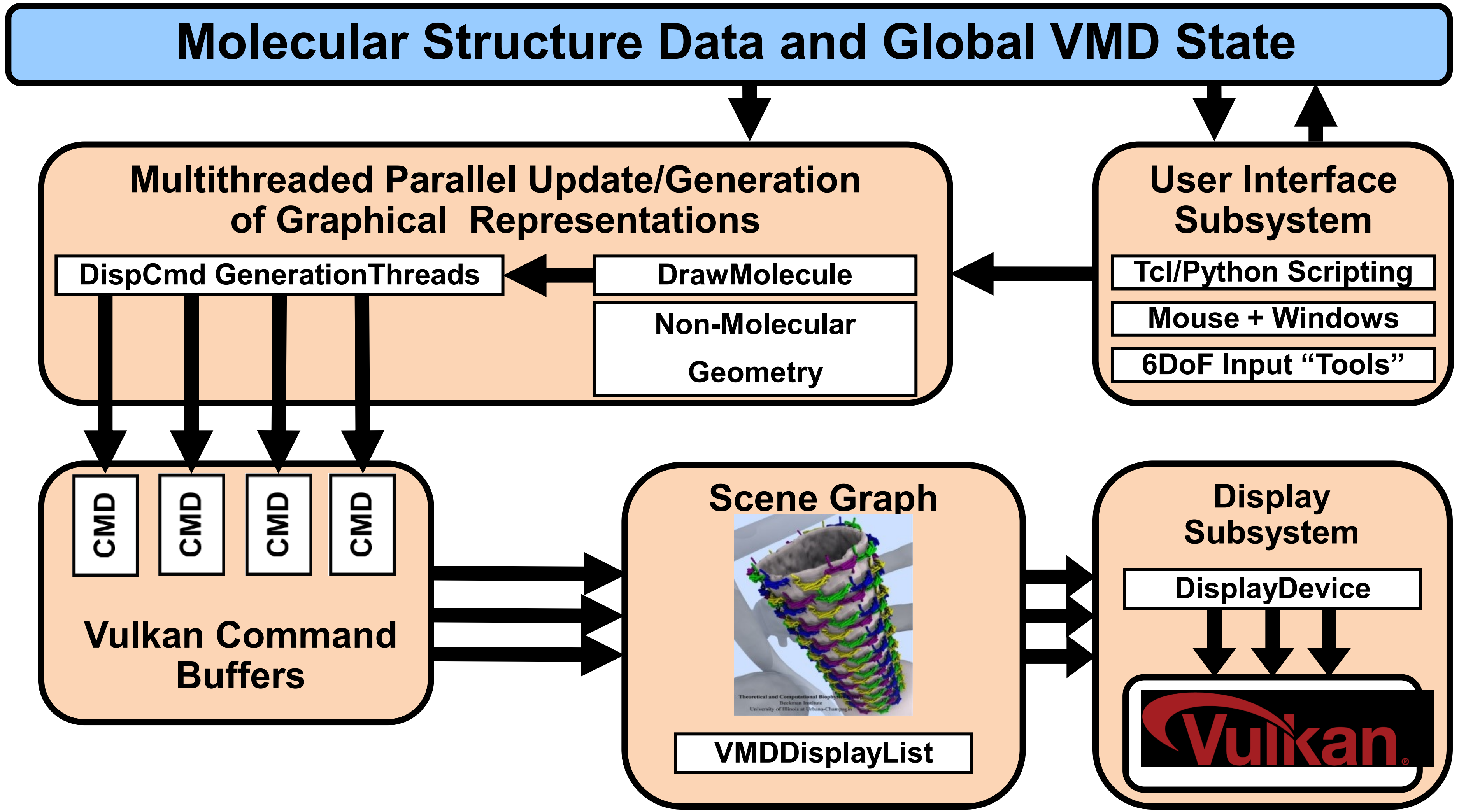


https://www.khronos.org/vulkan/

- **High performance, low-overhead, reduced abstraction, rasterization API:**
  - Modern API, benefits from past experiences with OpenGL, DX, etc
  - Core features essentially start w/ OpenGL 4.x function, and continue from there
  - Fewer extensions required for modern functionality
  - Significantly reduced API overheads relative to OpenGL, **some apps have seen up to ~3x performance gains vs. traditional OpenGL**
- Shaders (e.g. GLSL) compiled to SPIR-V intermediate code at **app compile time**
- **Compile-time validation** of shaders, rendering pipelines (lower runtime overhead)
- Core Vulkan doesn't deal with on-screen display, only rendering
  - Integration with windowing system is handled by Vulkan "WSI" extensions
- **Multi-GPU rendering included in the new Vulkan 1.1 spec!**

VMD on Vulkan®

- *In-progress:* **Vulkan-based rasterization path for VMD**
- **Vulkan opportunities for VMD:**
  - **Vulkan ideally suited** as the API for **high-end GPUs**
  - Maintain existing OpenGL renderer to support integrated/legacy GPUs
  - **Parallel Vulkan command buffer generation** will allow deep multithreading of time-varying VMD graphical representation updates
  - VMD Vulkan rendering path will be able to go all-in on techniques that are only viable on high-end GPUs
  - **Headless operation supported**, akin to EGL and GLX Pbuffer APIs


Molecular Structure Data and Global VMD State
Multithreaded Parallel Update/Generation of Graphical Representations
DispCmd GenerationThreads
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
6DoF Input "Tools"
CMD
CMD
CMD
CMD
Vulkan Command Buffers
Scene Graph
VMDDisplayList
Display Subsystem
DisplayDevice
Vulkan

Vulkan® on Cloud/HPC Systems

- Straightforward use within Amazon EC2 AMIs
- Containers: requires just a few additional steps beyond those for OpenGL, placement of **Vulkan-specific JSON files**, etc.
- **Early tests have demonstrated viability of off-screen Vulkan rendering on Cray XC50 supercomputers:**
  - **Headless Vulkan works on CSCS Piz Daint test and development system**
- Vulkan SDK open source, eases debug/testing/deployment on new or specialized systems such as HPC platforms:
  - Compilation of Vulkan SDK on IBM POWER9 pretty close to “out-of-box”
  - A few small missing pieces (assembly language in Vulkan loader) for POWER9 might be relatively easy to address
  - **Support OpenPOWER, ORNL Summit, with SDK updates, future drivers?**
  - **I will find out. Watch this space! ☺**

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/

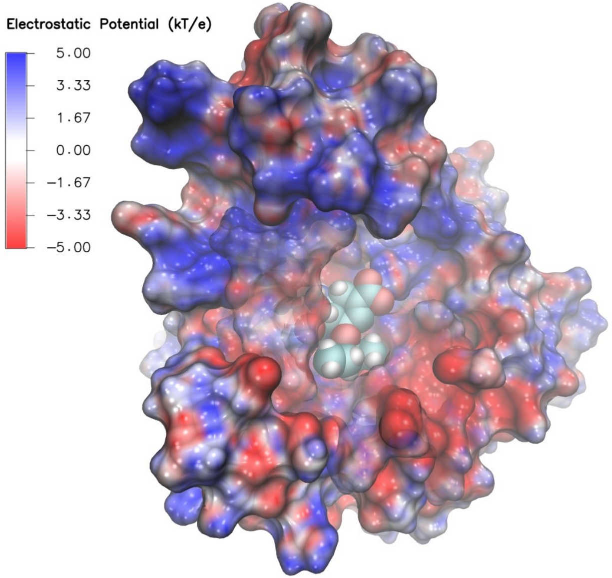
Clusters, Supercomputers

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.

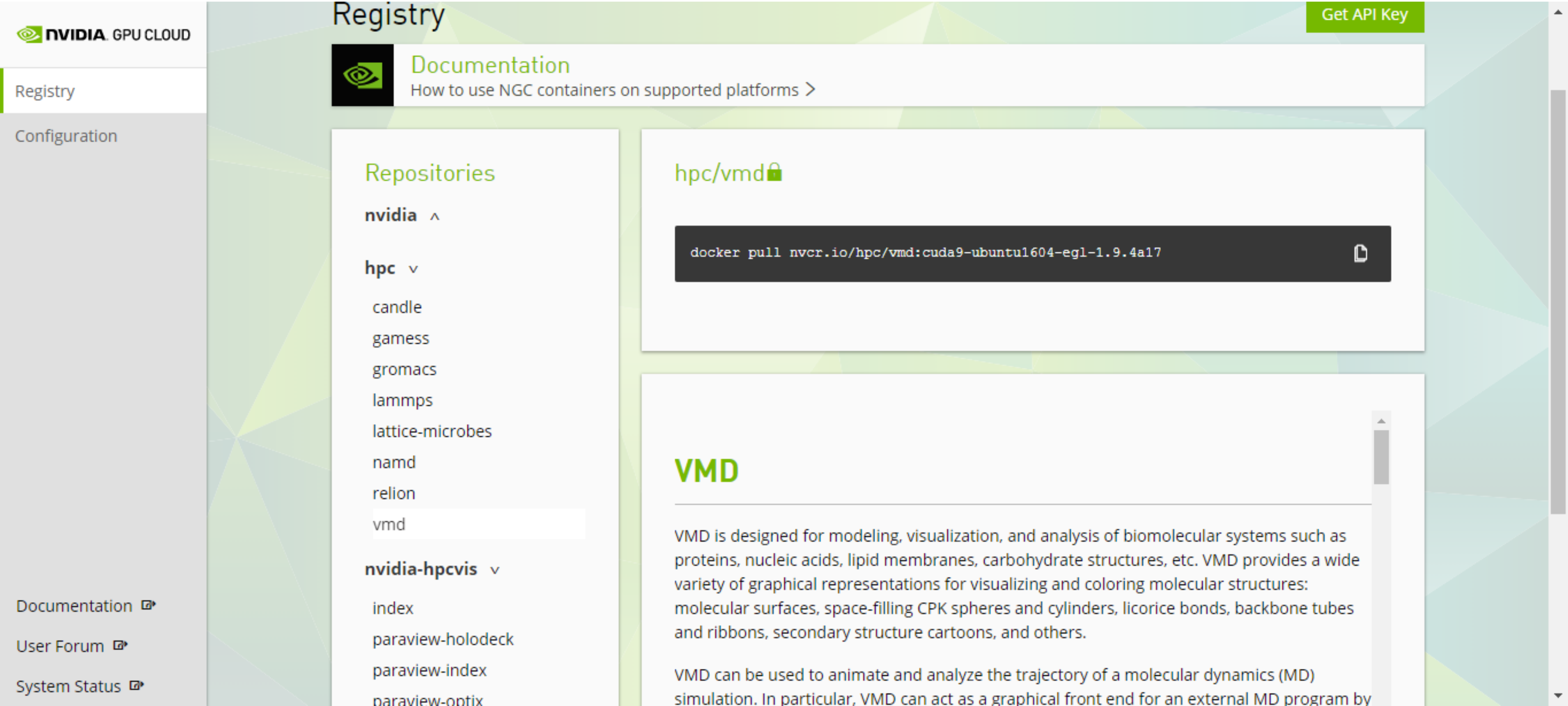
VMD OptiX/EGL NGC Container

- **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**



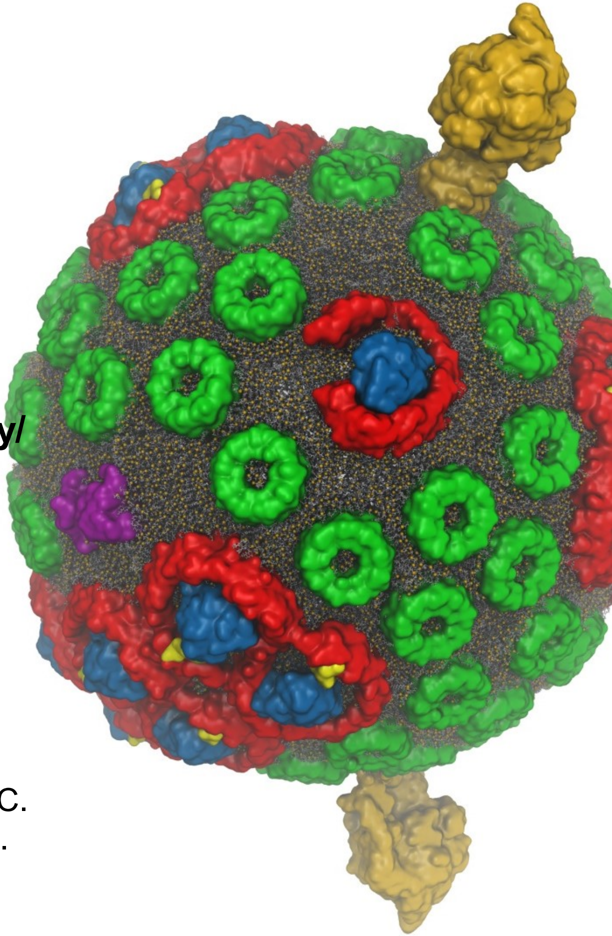
High performance molecular visualization: In-situ and parallel rendering with EGL. J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014-1023, 2016.

VMD / NAMD / LM, NGC Containers



VMD w/ OptiX 5

- 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 GP100, Tesla P100**
- **VMD+OptiX 5, NVIDIA NGC container: https://ngc.nvidia.com/registry/**
- **In-progress:**
  - **OptiX denoising support: fast turnaround w/ AO, DoF, etc**
  - **Denoising to enable practical use of path tracing in VMD**



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.

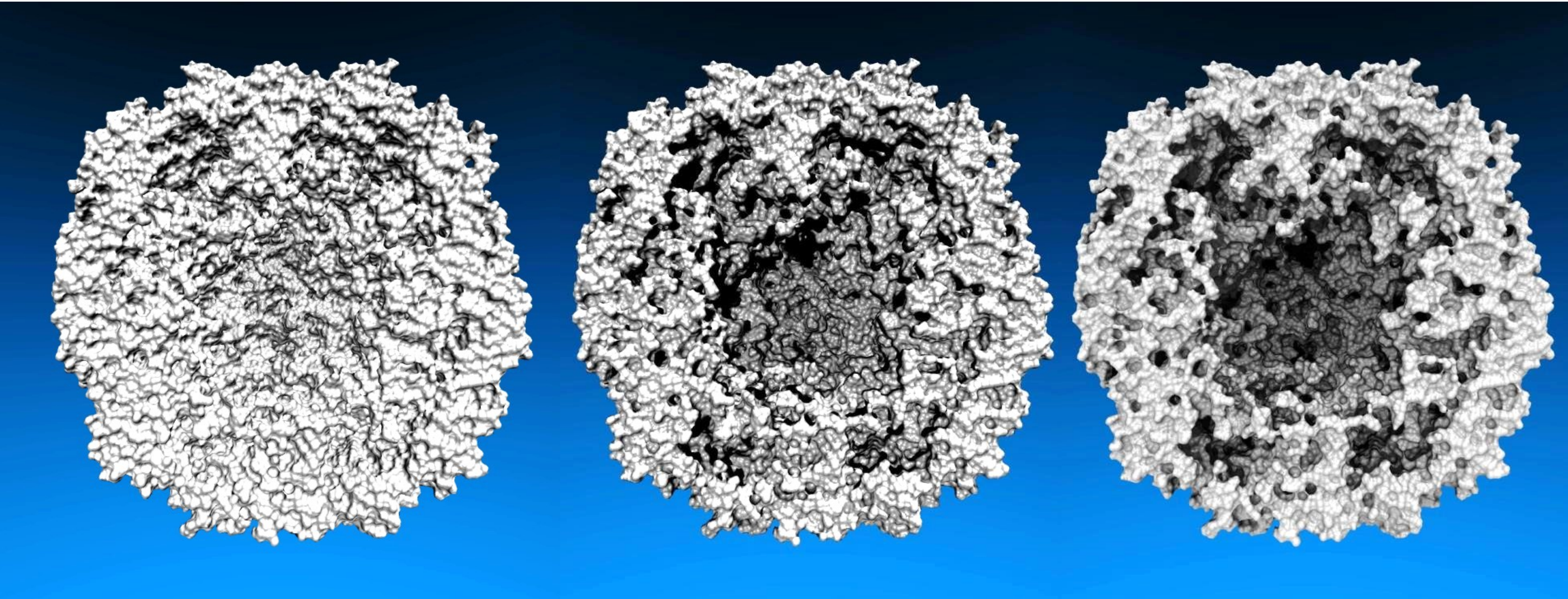
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering J. E. Stone, W. R. Sherman, and K. HPDAV, IPDPSW, pp. 1048-1057, 2016.

Lighting Comparison, STMV Capsid

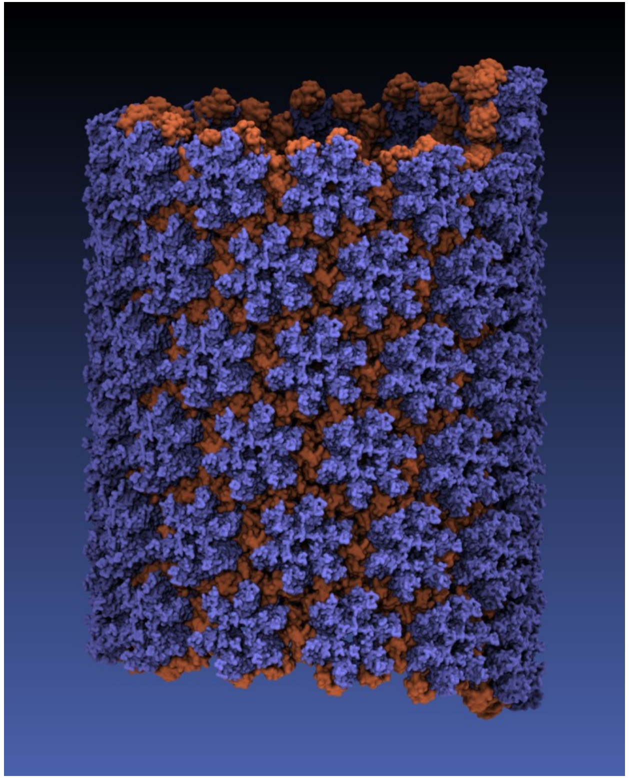
Two lights, no shadows

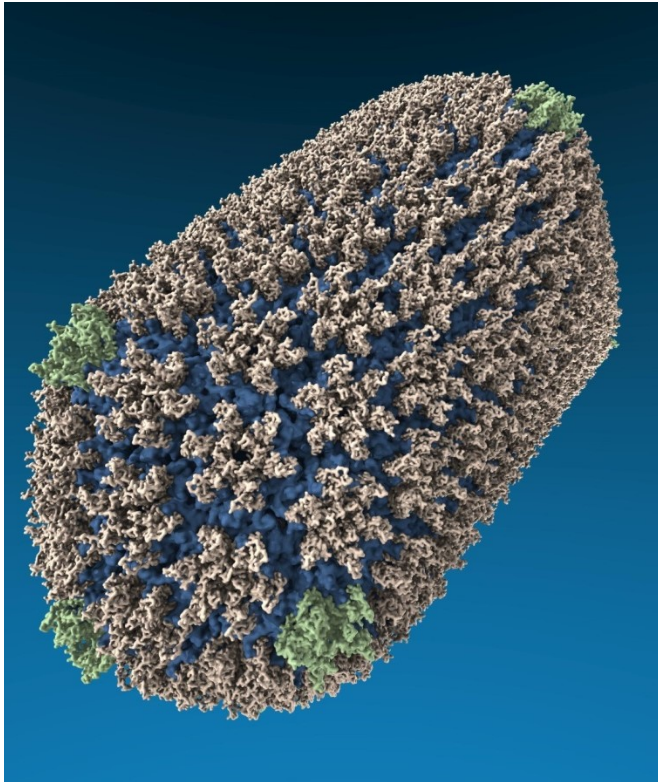
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit



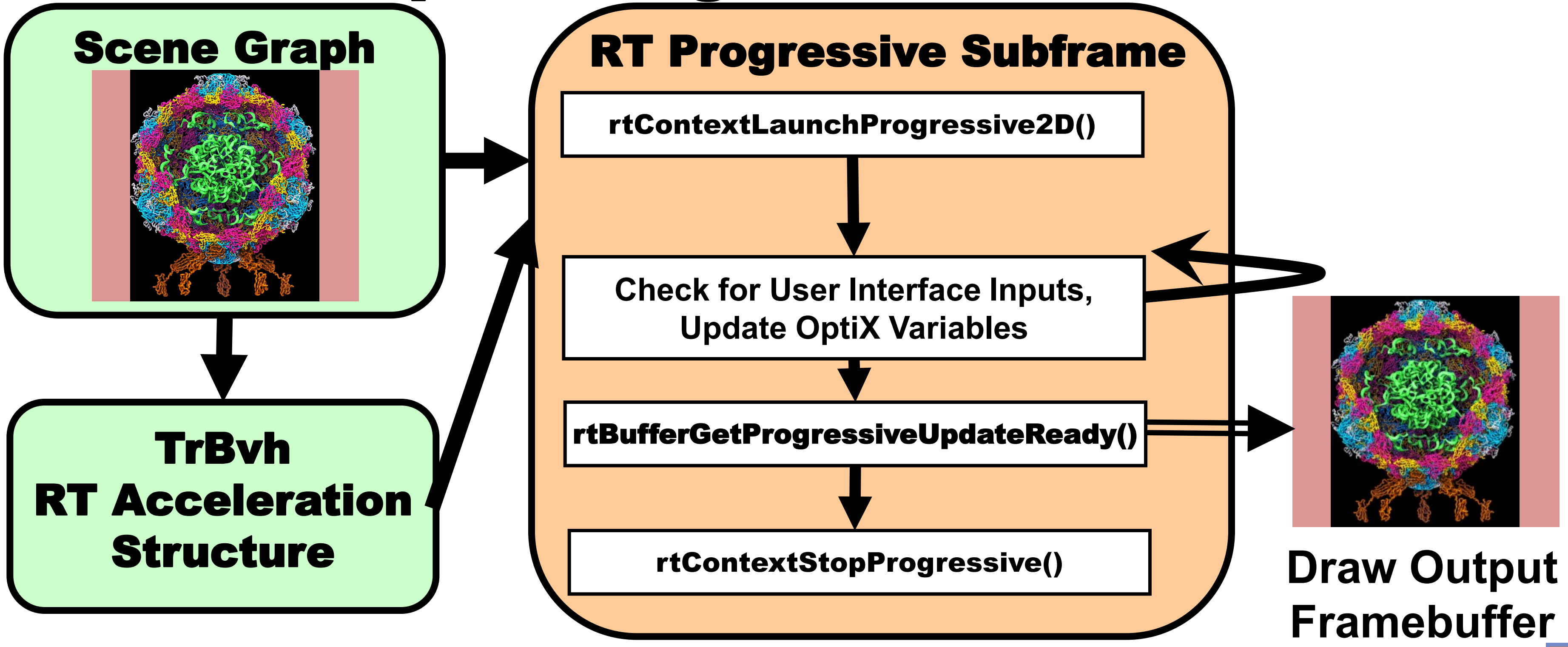
VMD “QuickSurf” Representation, Ray Tracing





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

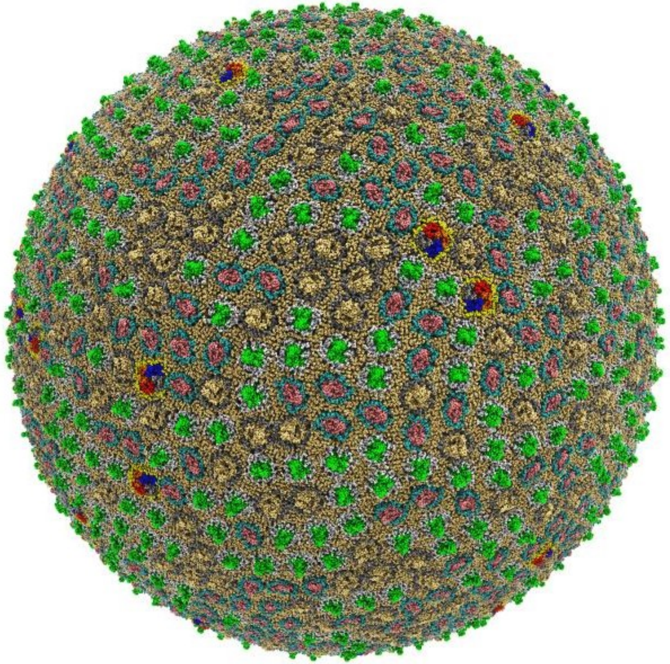
VMD TachyonL-OptiX Interactive RT w/ OptiX Progressive RT API



Preparation, Visualization, Analysis of All-Atom Cell-Scale Simulations

- Interactive rasterization w/ OpenGL/EGL now, **Vulkan** in future releases of VMD
- **Interactive ray tracing on CPUs and GPUs**
- Support for large host memory (TB), up to **2 billion atoms per “molecule” now**
- Parallel analysis, visualization w/ MPI

- 200 nm spherical envelope
- Membrane with ~50% occupancy by proteins
- 63M atoms in envelope model

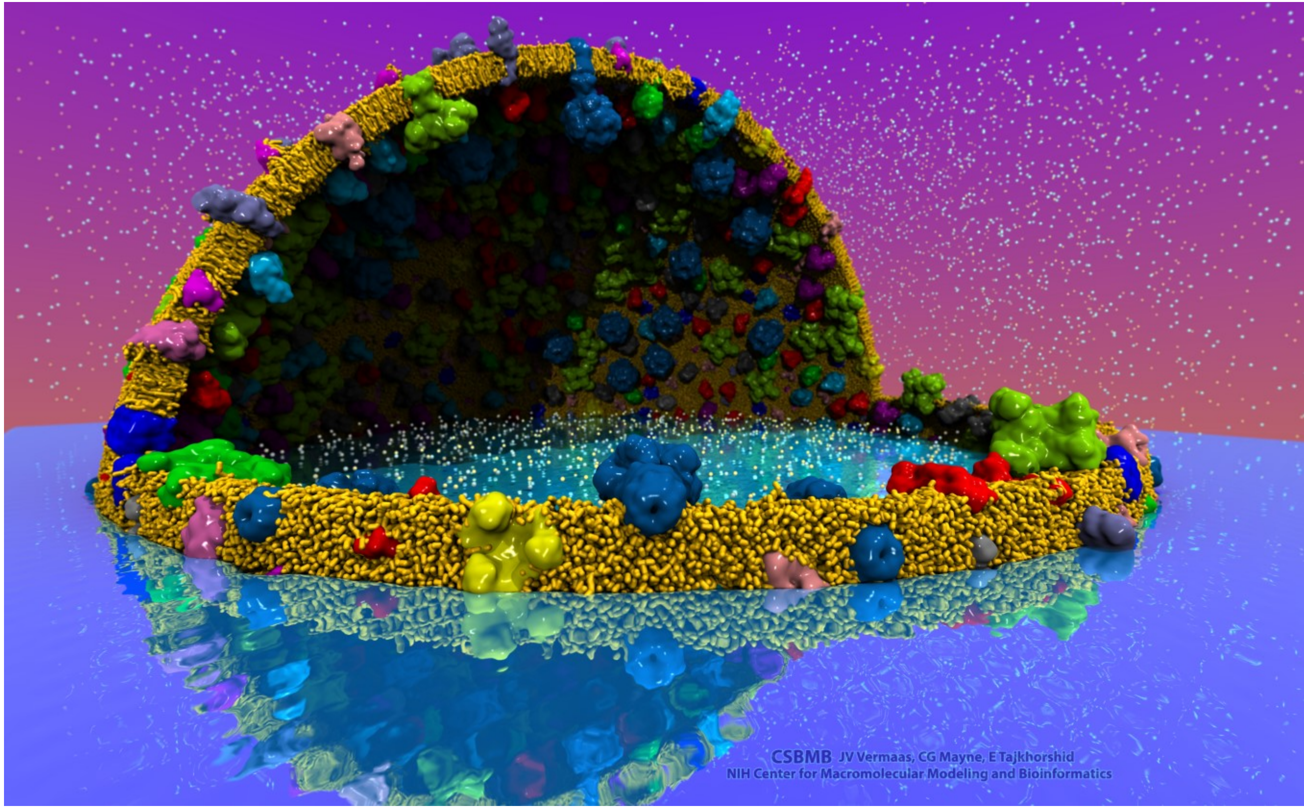


Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J.E. Stone, …, K. Schulten, J. Parallel Computing, 55:17-27, 2016.

High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL. J.E. Stone, ..., K. Schulten. IEEE High Performance Data Analysis and Visualization, IPDPSW, pp. 1014-1023, 2016.

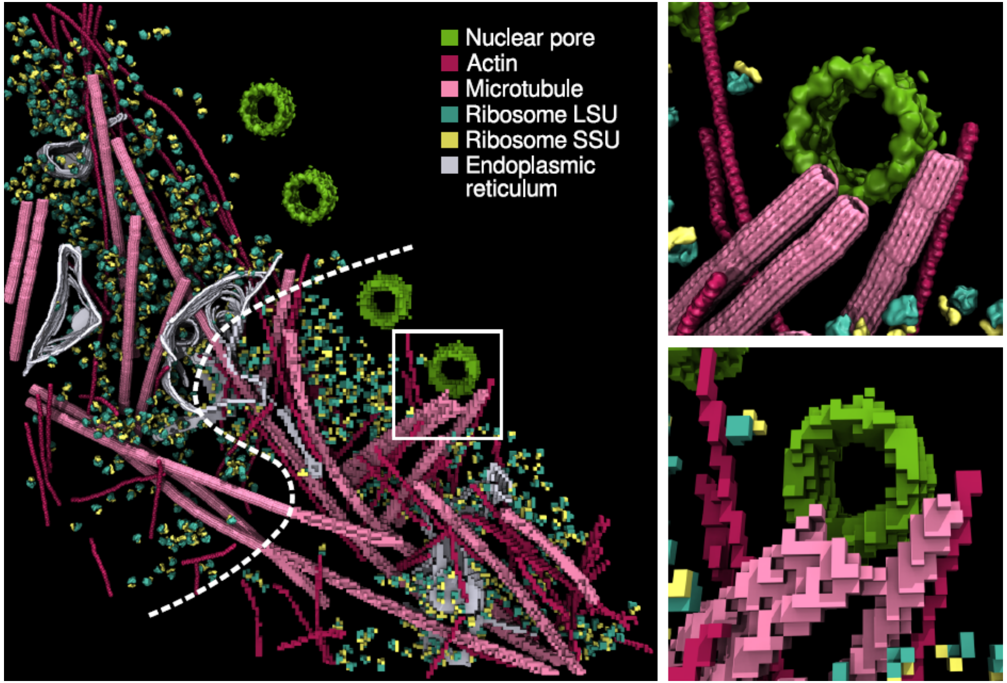
Proto-Cell Rendered with VMD+OptiX

- 113M particles
- 1,397 copies of 14 different membrane proteins
- Preparing for simulations on pre-exascale computers



Interactive Ray Tracing of Cells

- High resolution cellular tomograms, **billions of voxels**
- Even isosurface or lattice site graphical representations involve ~100M geometric primitives
- 24GB Quadro M6000s used for interactive RT of cellular tomograms of this size
- **Quadro GP100 / GV100 GPUs benefit from OptiX support for NVLink and distribution of scene data across multiple GPUs**



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

VMD Atomic Detail Visualization of Cellular Architecture with Instancing

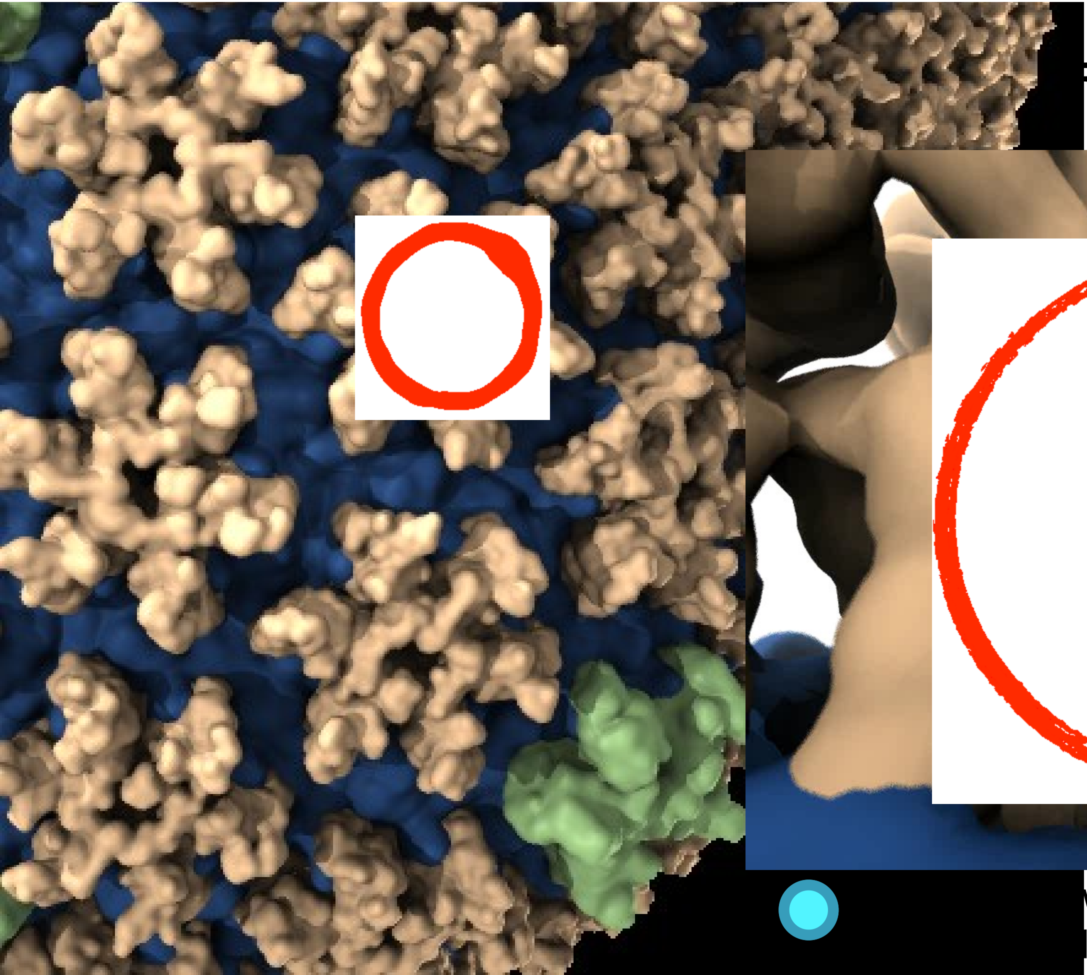
- VMD 1.9.4 supports instancing of graphical representations associated with molecules
- Exploit **VBO caching** in OpenGL to eliminate host-GPU geometry transfers
- **OptiX instancing** of geometry buffers to minimize GPU memory footprint for cell-scale scenes w/ atomic structures

Immersive Viz. w/ VMD

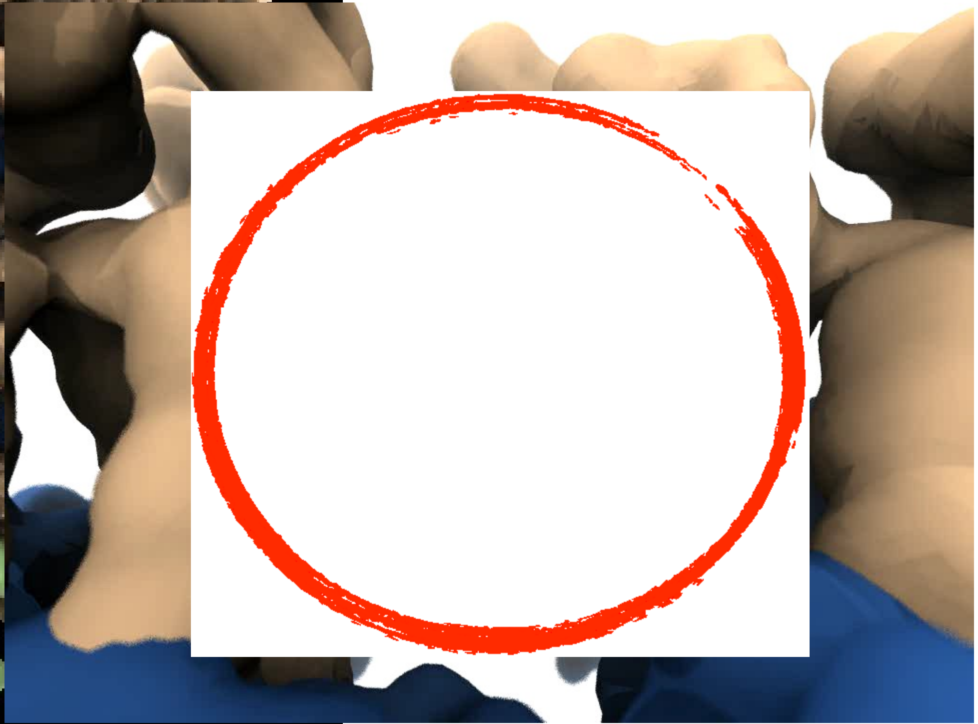
- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability, convenience
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support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

VMD running in a CAVE w/ VR Juggler

Goal: Intuitive interactive viz. in crowded molecular complexes



Results from 64 M atom, 1 μs sim!



v of chloride ions permeating

capsid hexameric centers

In-Progress VMD VR Development, Demos

VMD VR ray tracing:
- Google Cardboard [1]
- Demo w/ Indiana U., SC'15 [2]

Prototype of VR user interaction with VMD models in **room-scale VR** with NVIDIA @ SC'16

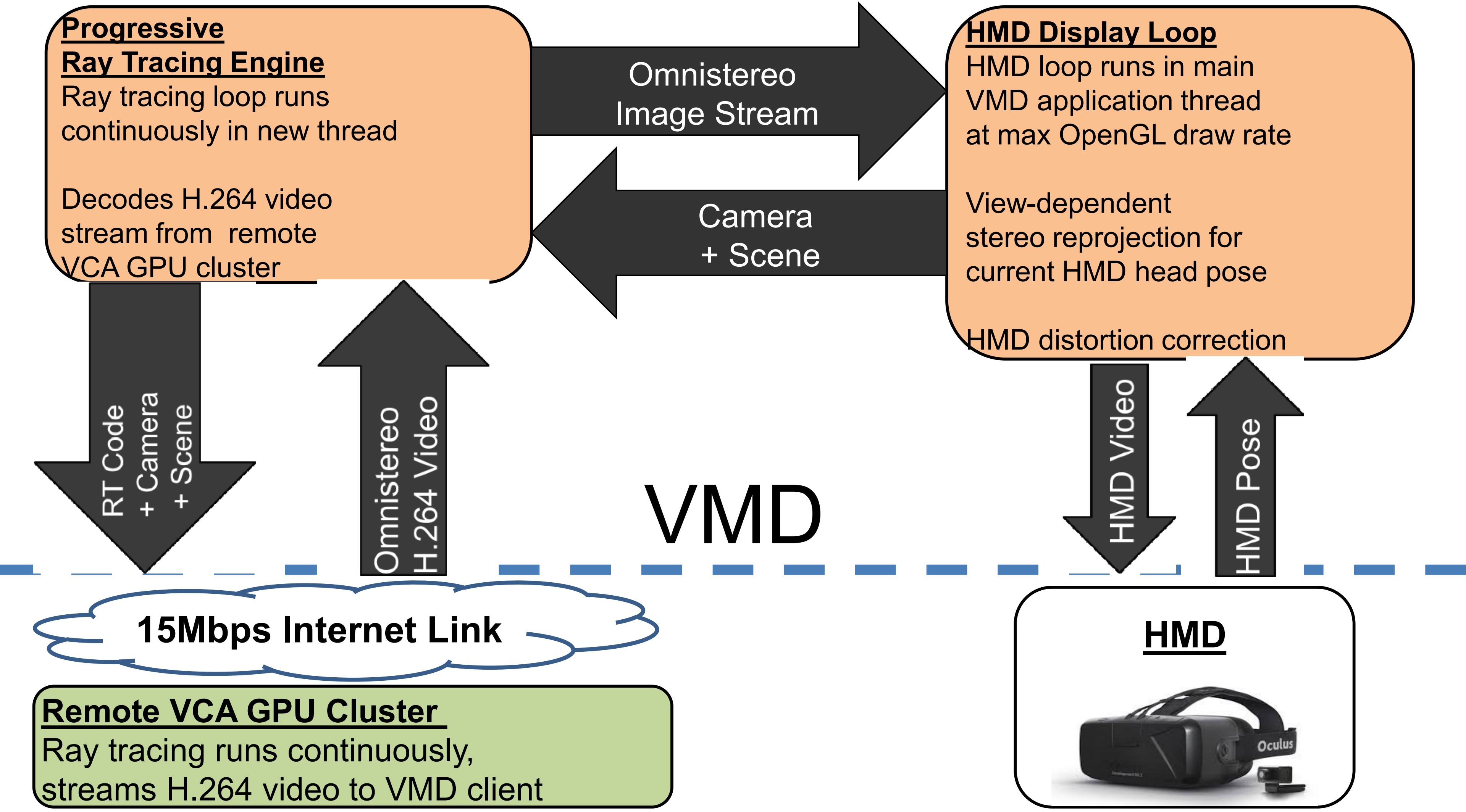
VMD Chromatophore Demo, NVIDIA VR Room at SC'16

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

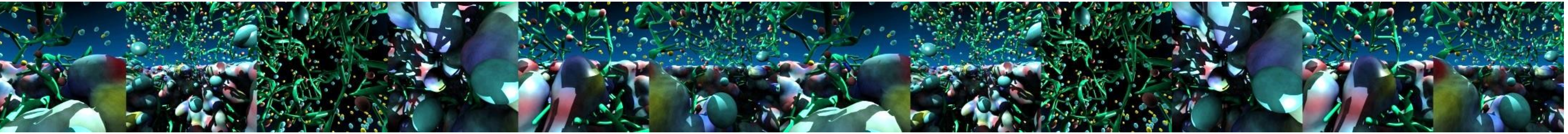
[2] Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J.E. Stone, W.R. Sherman, K. Schulten. IEEE HPDAV (IPDPSW), pp. 1048-1057, 2016.

HMD Ray Tracing Challenges

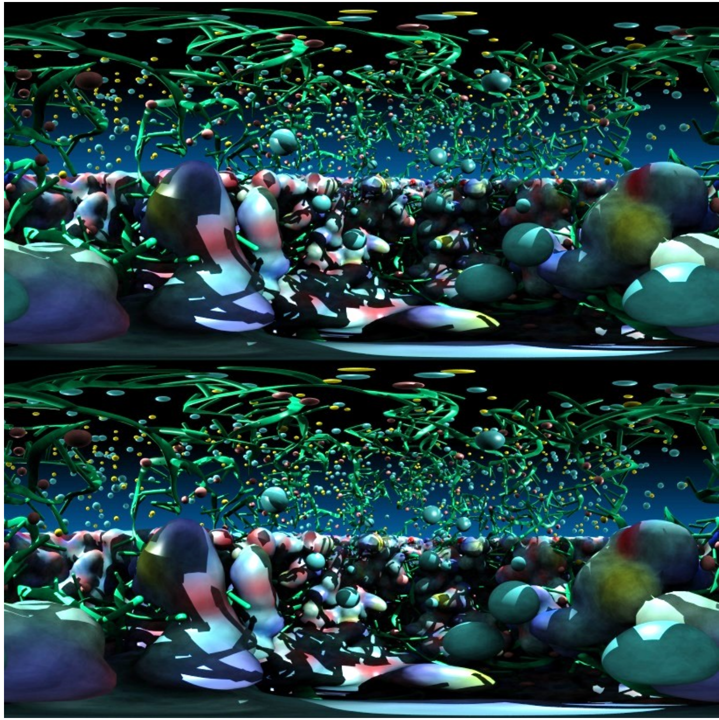
- HMDs require high frame rates **(90Hz or more)** and minimum latency between IMU sensor reads and presentation on the display
- Multi-GPU workstations fast enough to direct-drive HMDs at required frame rates for simple scenes with direct lighting, hard shadows
- Advanced RT effects such as AO lighting,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

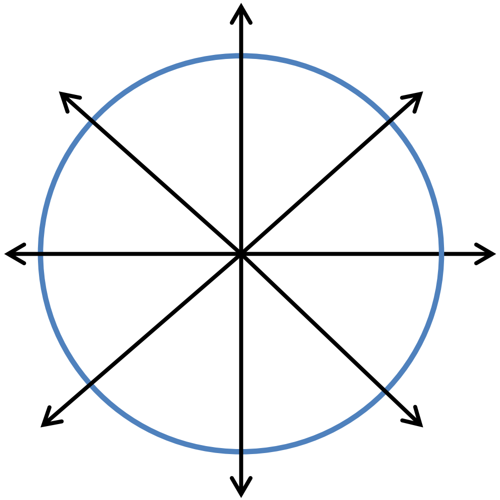

Progressive
Ray Tracing Engine
Ray tracing loop runs
continuously in new thread
Decodes H.264 video
stream from remote
VCA GPU cluster
Omnistereo
Image Stream
Camera
+ Scene
HMD Display Loop
HMD loop runs in main
VMD application thread
at max OpenGL draw rate
View-dependent
stereo reprojection for
current 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

Stereoscopic Panorama Ray Tracing w/ OptiX

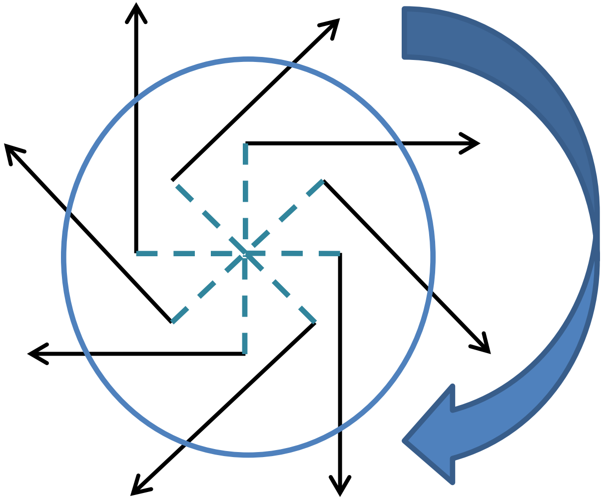


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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

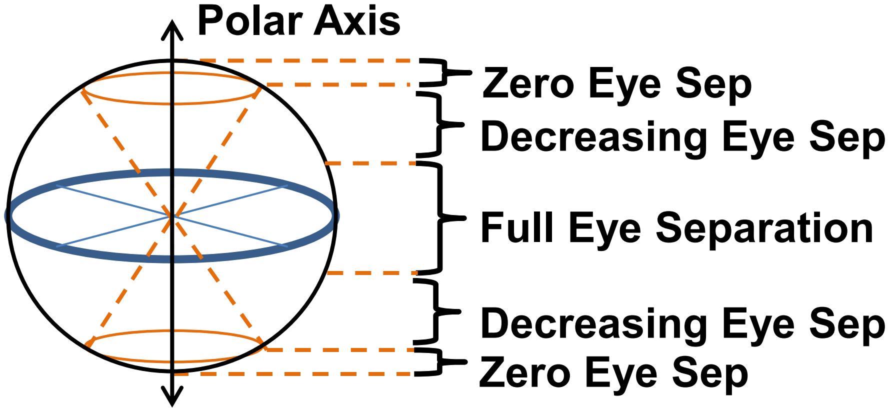




A) Monoscopic circular projection.
Eye at center of projection (COP).

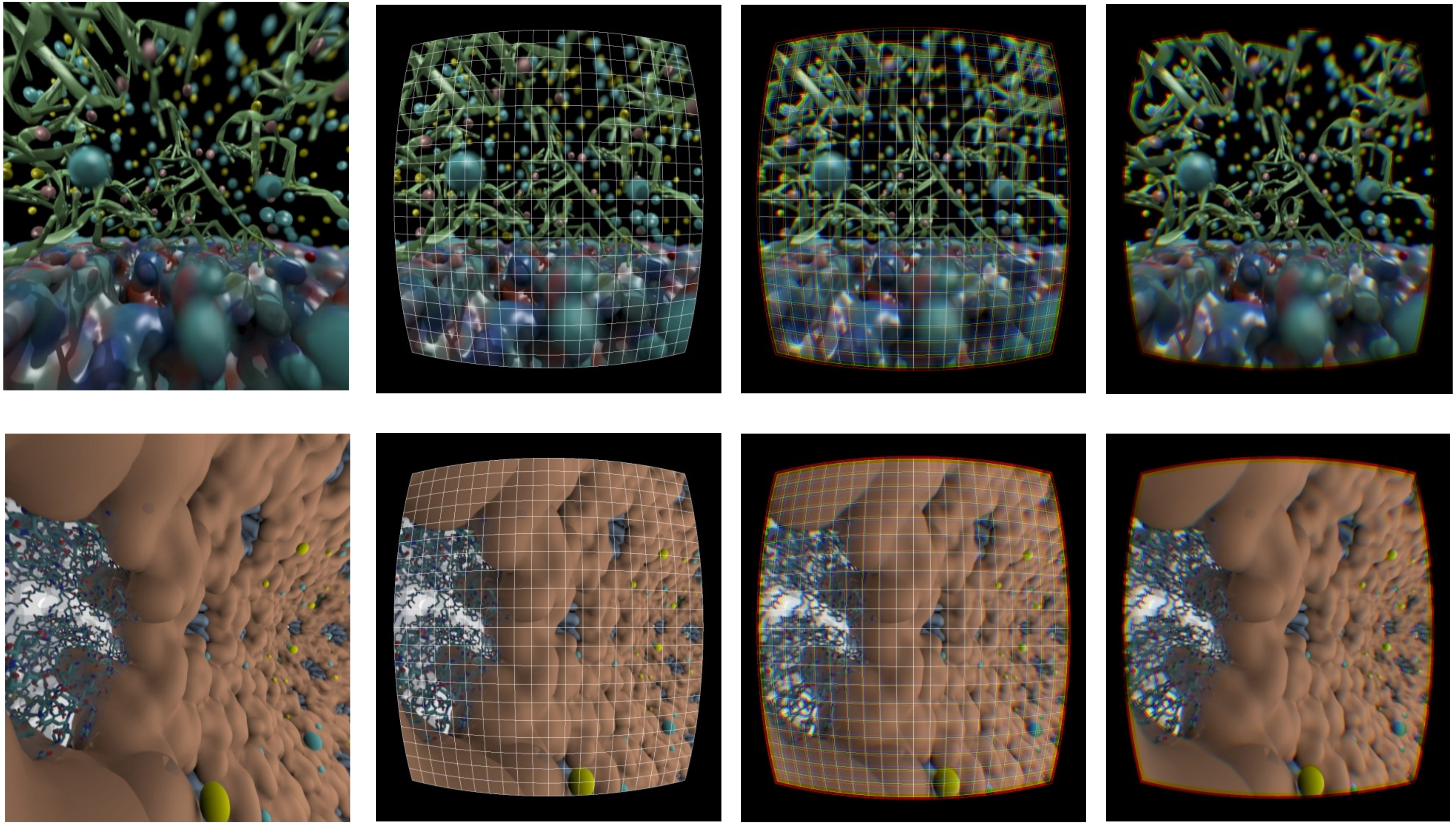


B) Left eye stereo circular projection.
Eye offset from COP by half of interocular distance.



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.

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.



Ongoing VR Work

- OpenXR – cross platform muti-vendor HMD support
- 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, …

Please See These Other Talks:

- S8727 - Improving NAMD Performance on Volta GPUs
- S8718 - Optimizing HPC Simulation and Visualization Codes using Nsight Systems
- S8747 - ORNL Summit: Petascale Molecular Dynamics Simulations on the Summit POWER9/Volta Supercomputer
- SE150572 - OpenACC User Group Meeting
- S8665: VMD: Biomolecular Visualization from Atoms to Cells Using Ray Tracing, Rasterization, and VR

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  - NSF Blue Waters:
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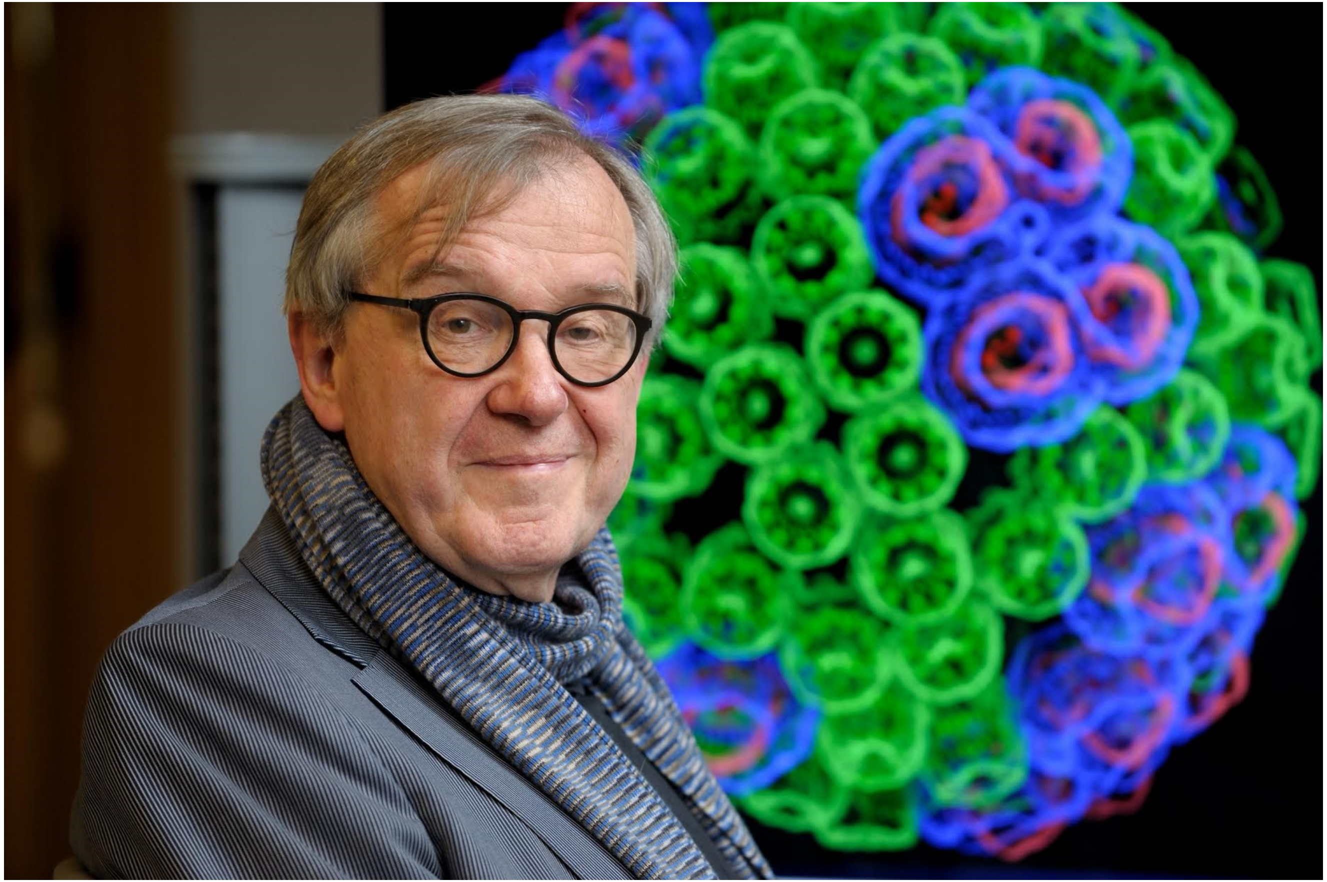
    ACI-1238993, ACI-1440026



“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**)
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