S7391—Turbocharging VMD Molecular Visualizations with State-of-the-Art Rendering and VR Technologies

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

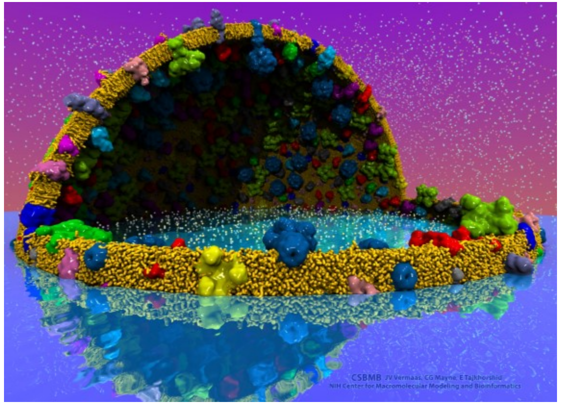
S7391, GPU Technology Conference

14:00-14:50, Room 212B, San Jose Convention Center,

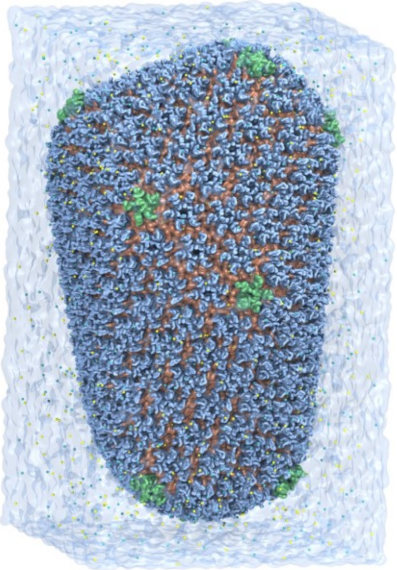
San Jose, CA, Tuesday May 9th, 2017

VMD – "Visual Molecular Dynamics"

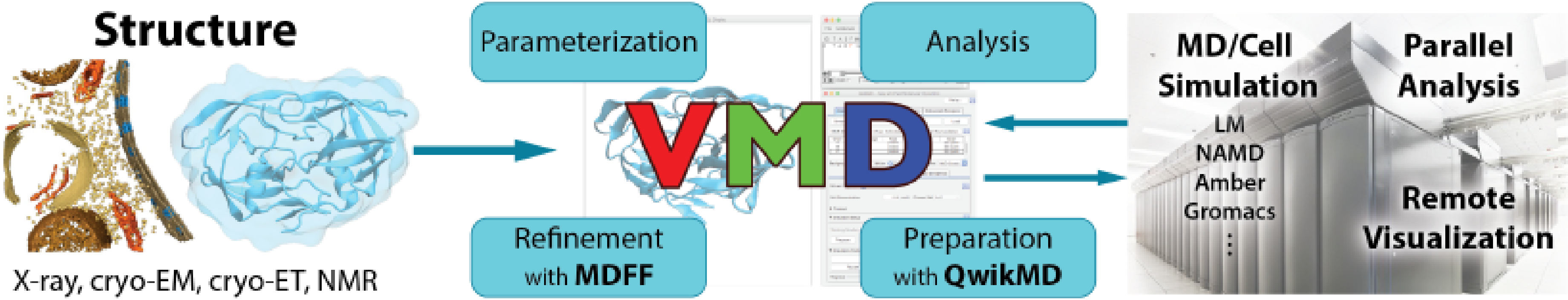
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
  - Sequence information
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



MD Simulation



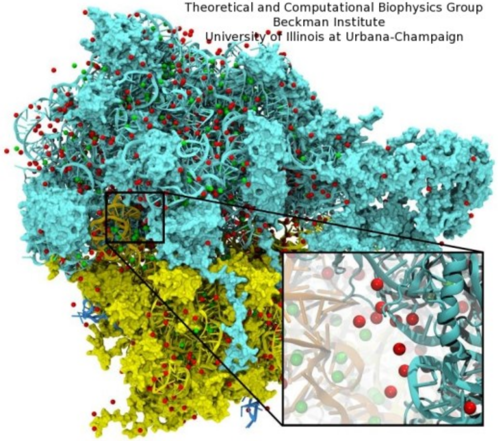
10 Years of GPU Computing in VMD

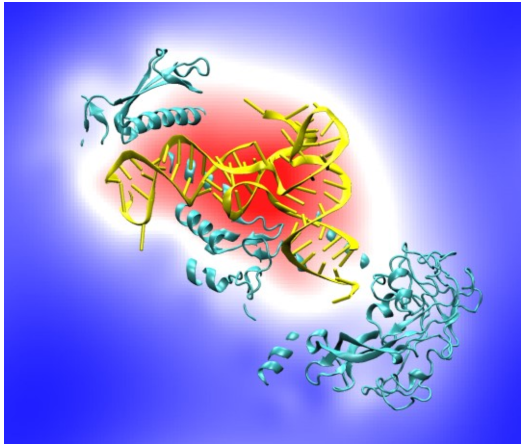
- Has stood the test of time
- Modeling, Visualization, Rendering, and Analysis

Blast from the past:

CUDA starting with version 0.7 !!!

Quad core Intel QX6700, three NVIDIA GeForce 8800GTX GPUs, RHEL4 Linux



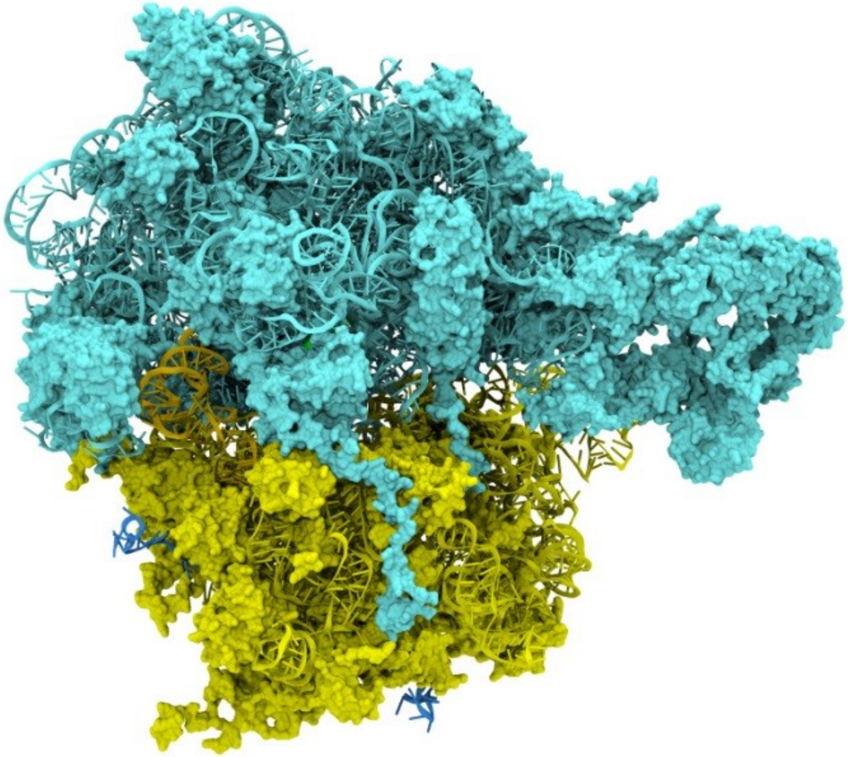


Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.

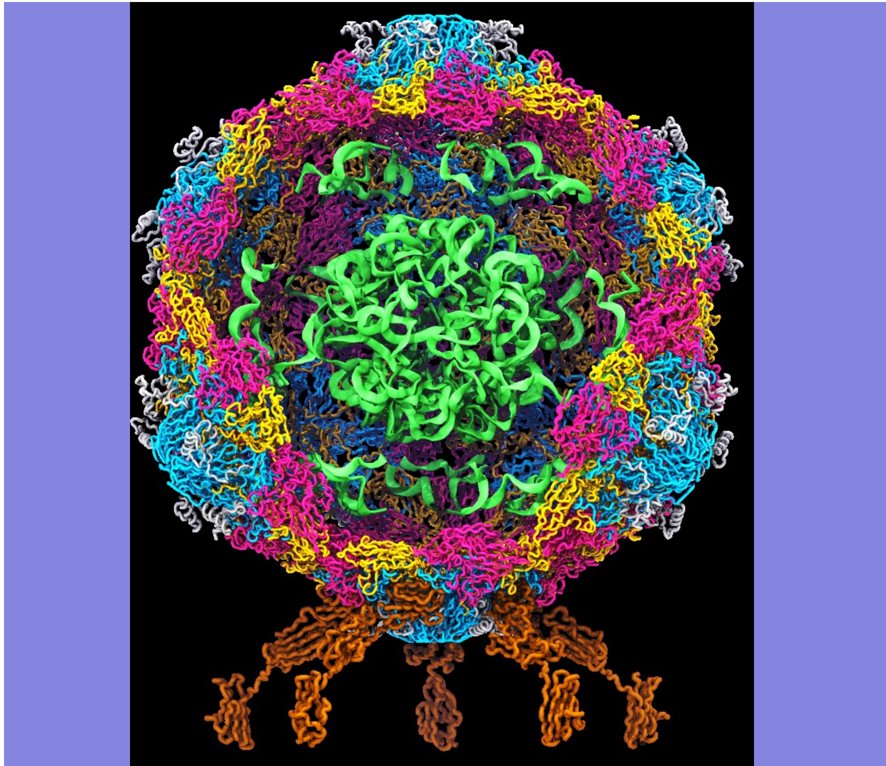
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus



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!**

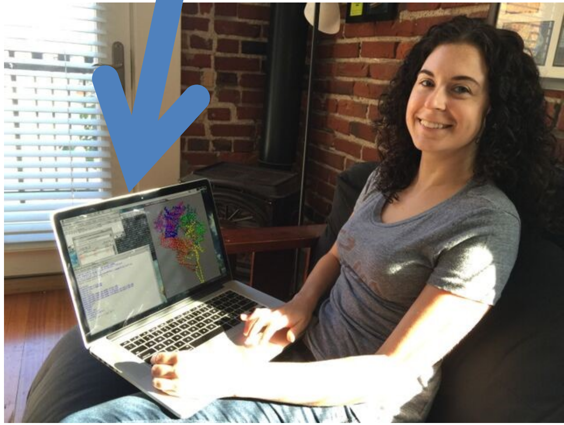
Parallel VMD currently available on:

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

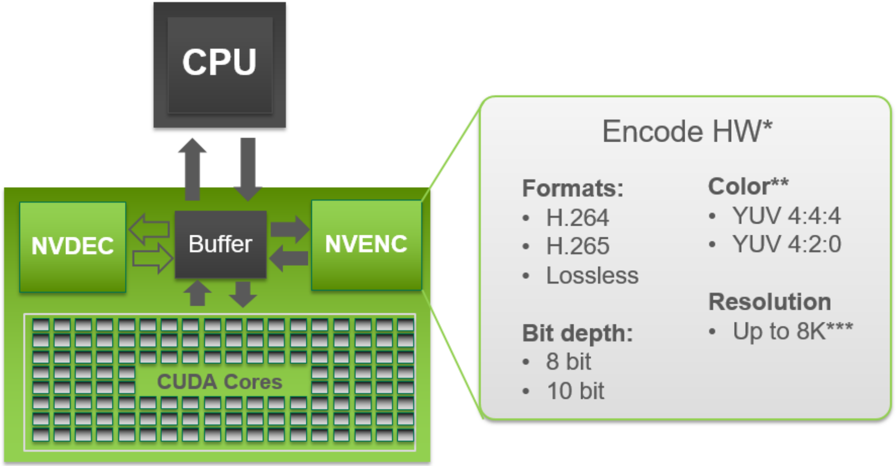
Interactive Remote Visualization and Analysis

- Enabled by hardware H.264/H.265 video encode/decode
- Enable visualization and analyses not possible with conventional workstations
- Access data located anywhere in the world
  - Same VMD session available to any device
- Linux prototype in-development using NVIDIA Video Codec SDK, easy-to-use ***NvPipe*** wrapper library



NVIDIA Video CODEC SDK and NvPipe

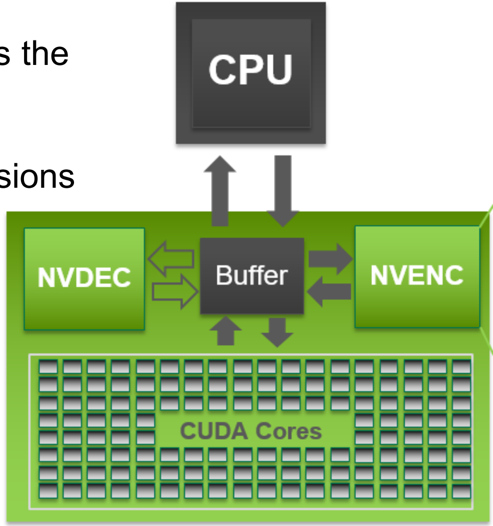
- GPUs (Kepler-on) include NVENC and NVDEC video codec acceleration hardware
- Independent of GPU compute hardware
- Hardware-accelerated codecs can ***overlap*** with interactive **rendering**, and **computation**
- ***NvPipe*** provides an easy to use API for interactive video streaming, abstracting many low level codec details, ideal for basic remote visualization implementations: **https://github.com/NVIDIA/NvPipe**



NvPipe

https://github.com/NVIDIA/NvPipe

- Simplified API for producing a basic encoder/decoder system.
- **Roughly 100 lines of code for basic encode/decode "Hello World" loops with minimal error handling logic**
- Encode/decode ends up being **simpler than your networking code** ☺
- Encode loop structure:
  - User selects encoder type***, e.g. NVPIPE_H264_NV***, and target encoder bitrate parameter
  - User provides uncompressed **RGB** or **RGBA** image buffer, image dimensions, and size of the output memory buffer
  - NvPipe compresses the frame using the NVENC hardware encoder, and returns the number of bytes of output written to the output buffer
- Symmetric decode loop structure:
  - Provide decoder with compressed buffer, buffer size in bytes, and image dimensions as input
  - Decoder produces uncompressed output image
- Optionally supports FFMPEG back-ends (but I haven't tried those yet)

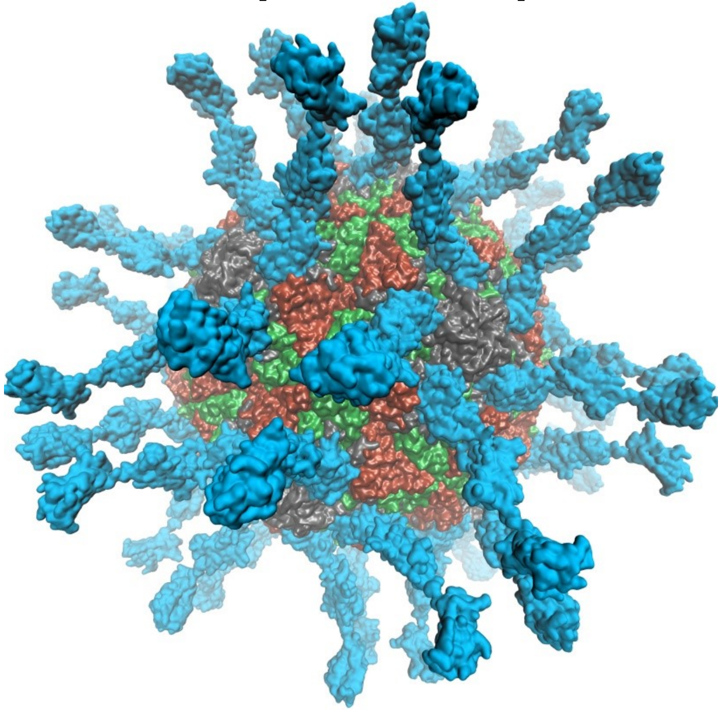


https://www.khronos.org/vulkan/

- ***In-progress:* Vulkan-based rasterization path for VMD**
  - Modern API, reduced dependence on extensions for modern functionality
  - Significantly reduced API overheads relative to OpenGL, **some other apps have seen ~2x performance gains vs. OpenGL**
  - Shaders (e.g. GLSL) compiled to SPIR-V intermediate code
  - Compile-time rather than runtime verification of rendering pipelines
  - Integration with windowing system is handled by Vulkan extensions
  - Multi-GPU rendering wasn’t part of Vulkan 1.0 spec, but is in development

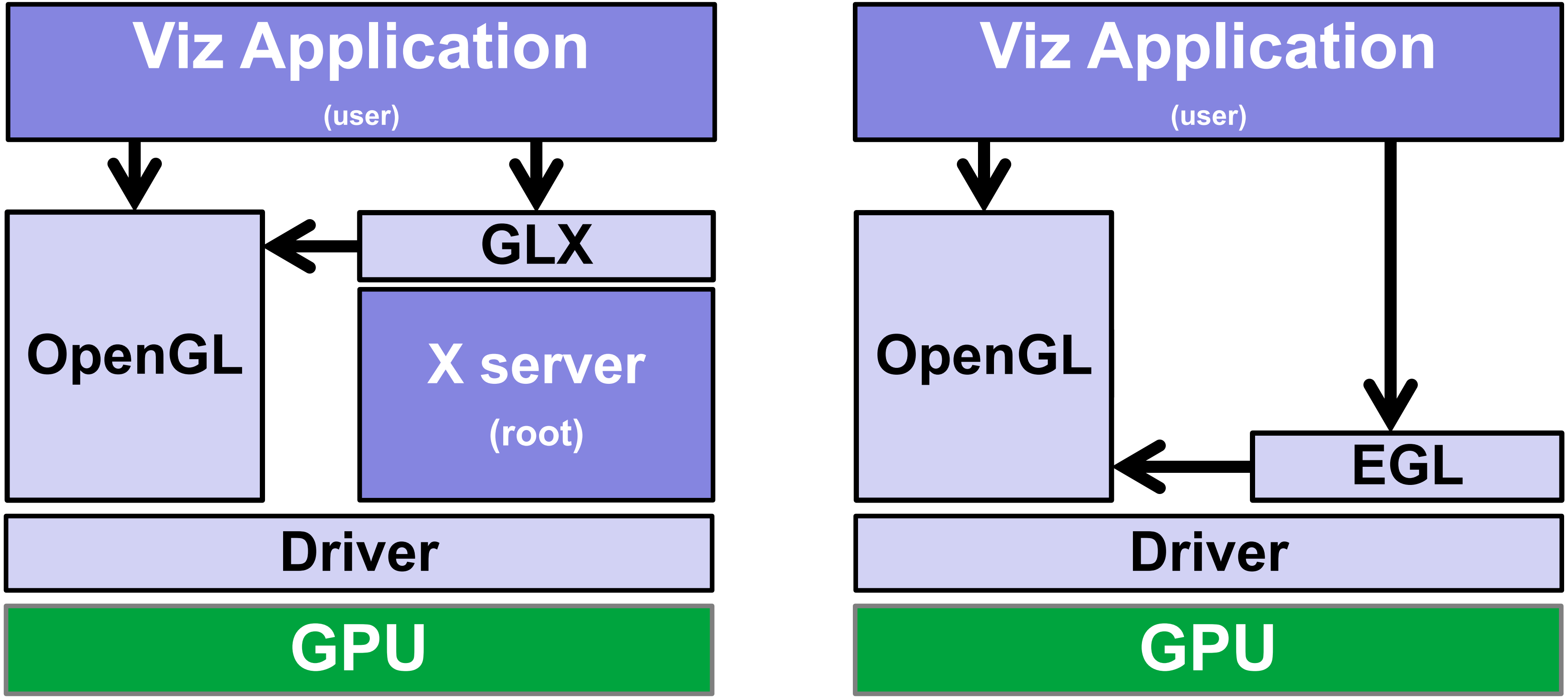
VMD 1.9.3 supports EGL for in-situ and parallel rendering on clouds, clusters, and supercomputers

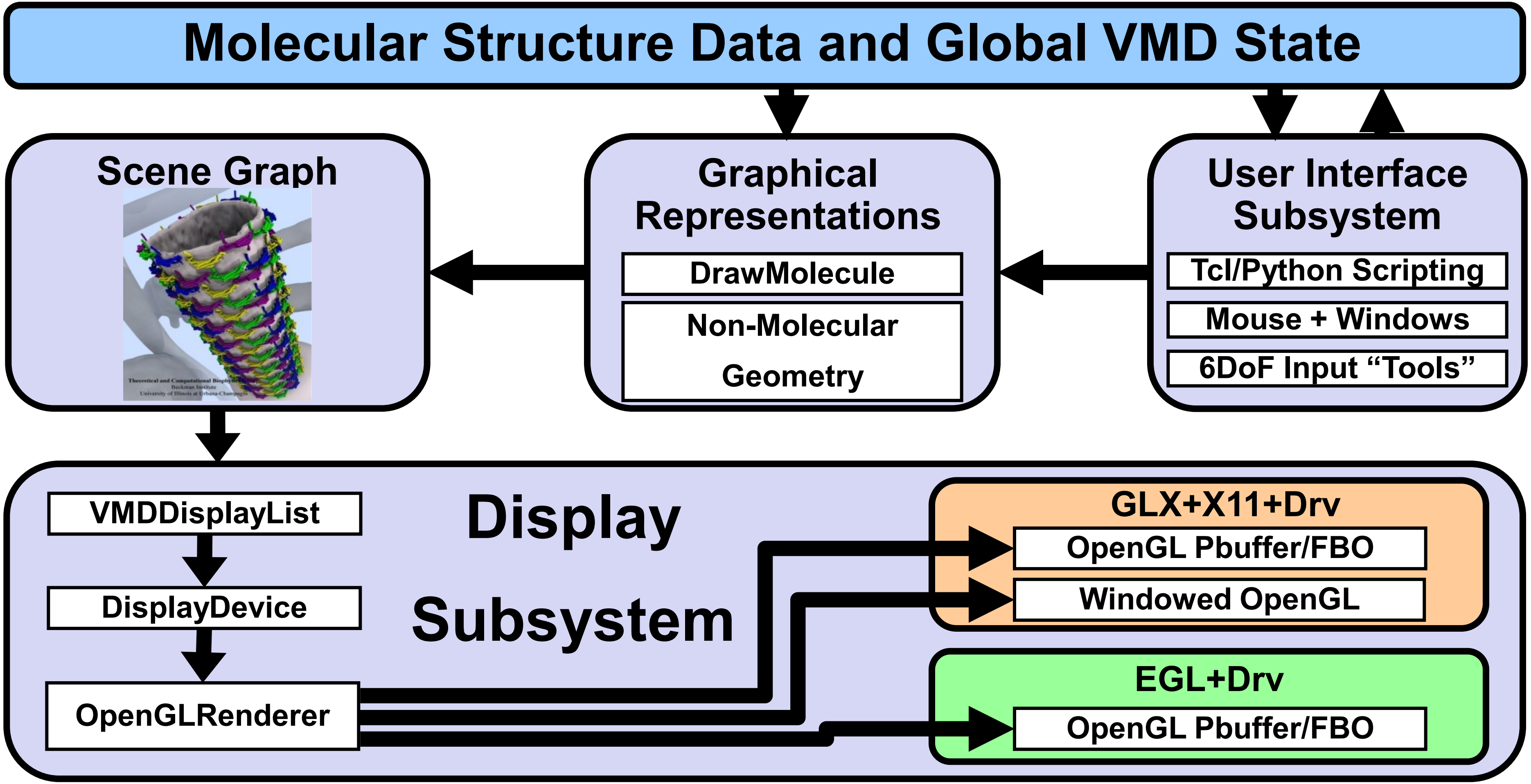
- Eliminate dependency on windowing systems
- Simplified deployment of parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features
- Support high-quality vendor-supported commercial OpenGL implementations in HPC systems that were previously limited to Mesa

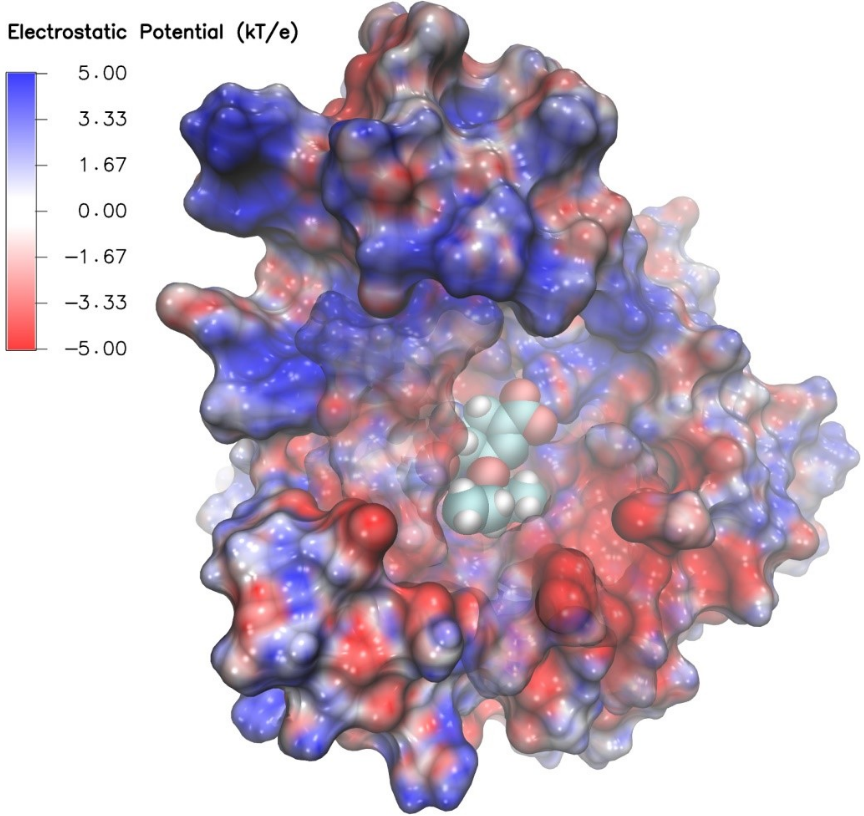


Poliovirus

OpenGL: GLX vs. EGL




Molecular Structure Data and Global VMD State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
6DoF Input "Tools"
VMDDisplayList
DisplayDevice
OpenGLRenderer
Display Subsystem
GLX+X11+Drv
OpenGL Pbuffer/FBO
Windowed OpenGL
EGL+Drv
OpenGL Pbuffer/FBO

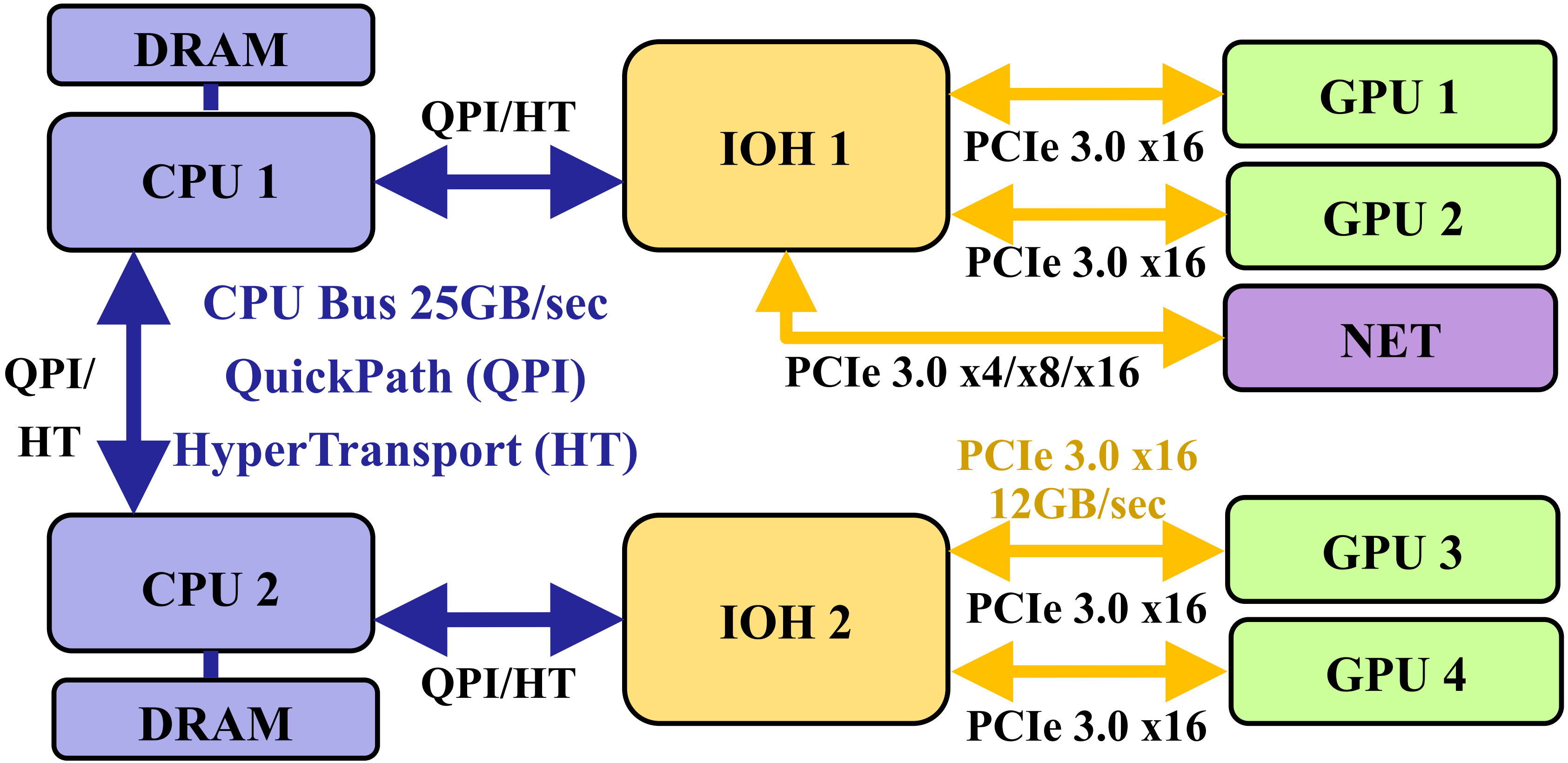


Swine Flu A/H1N1 neuraminidase bound to Tamiflu: VMD EGL rendering demonstrating full support for all VMD shaders and OpenGL features, multisample antialiasing, ray cast spheres, 3-D texture mapping, ...

Benefits of EGL Platform Interfaces

- Enumerate and select among available platforms, potentially supporting multiple vendors in the same host/node
  - Allows specific target implementation to be bound, e.g. GPU, CPU-integrated GPU, software rasterizer
- **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, e.g. "Minsky", upcoming DOE/ORNL "Summit" system**

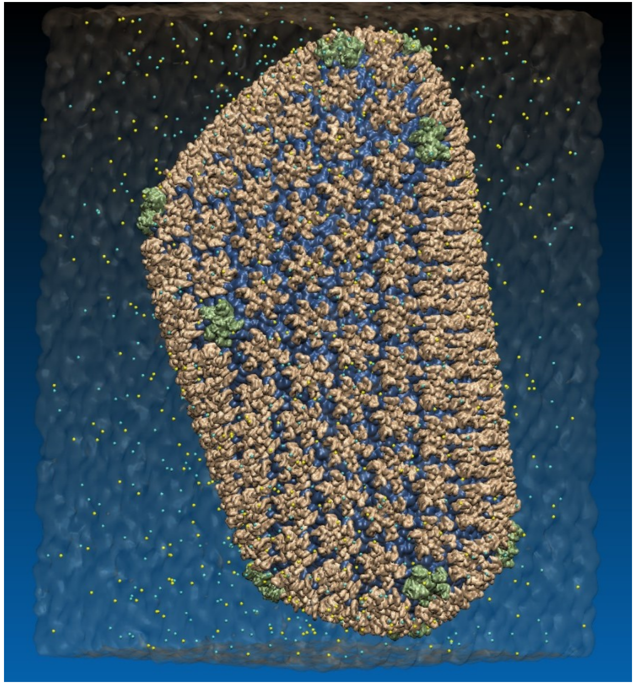
Example Node NUMA Topology



VMD EGL Performance on Amazon EC2 Cloud

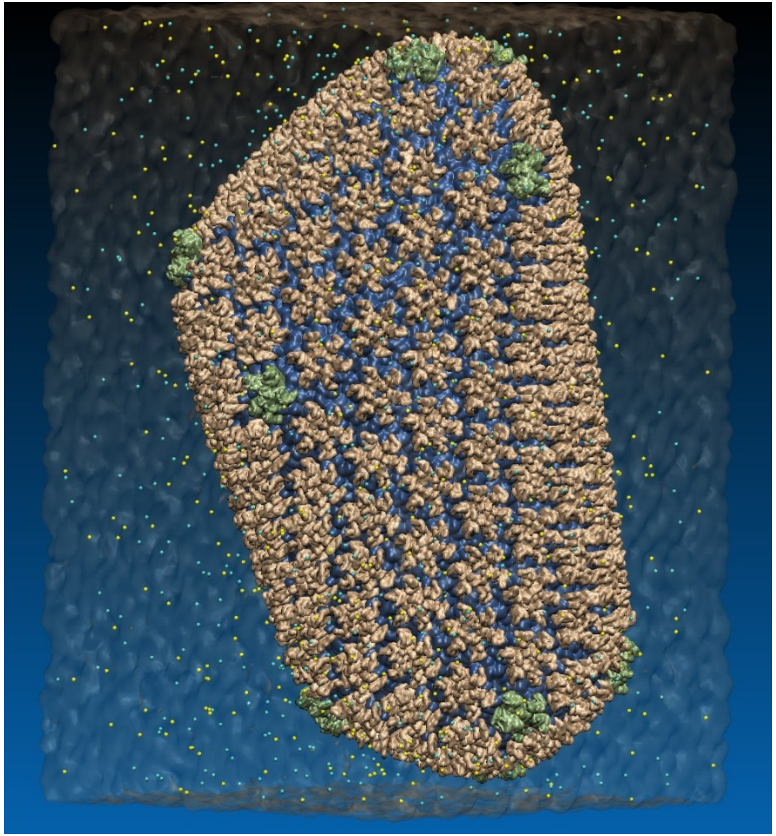
MPI Ranks	EC2 "G2.8xlarge" GPU Instances	HIV-1 movie rendering time (sec), (I/O %) 3840x2160 resolution
1	1	626s (10% I/O)
2	1	347s (19% I/O)
4	1	221s (31% I/O)
8	2	141s (46% I/O)
16	4	107s (64% I/O)
32	8	90s (76% I/O)

Performance at 32 nodes reaches ~48 frames per second



64M atom HIV-1 capsid simulation rendered via EGL

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.



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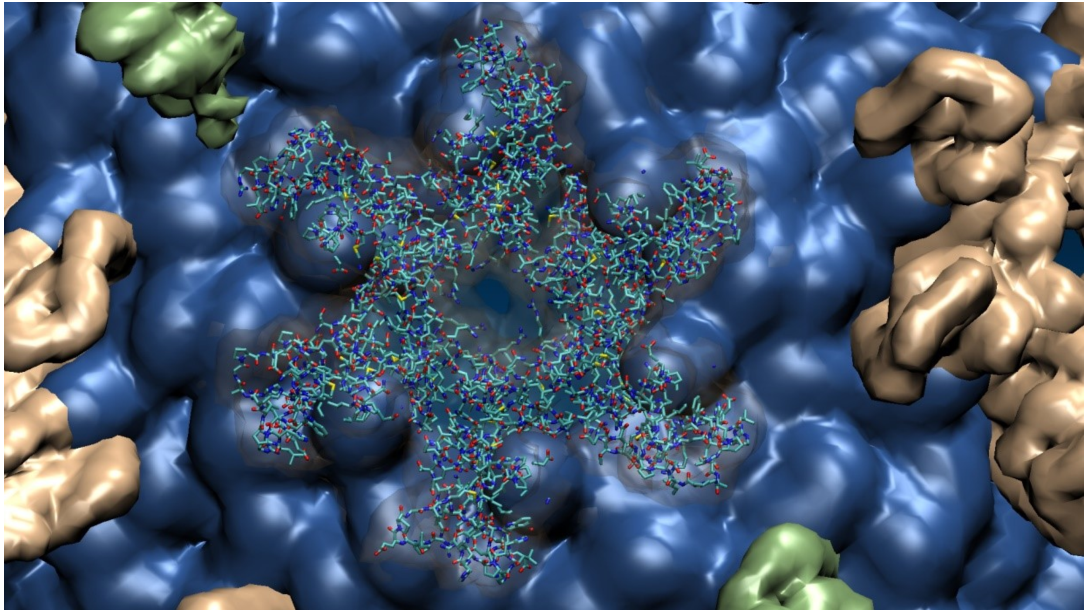


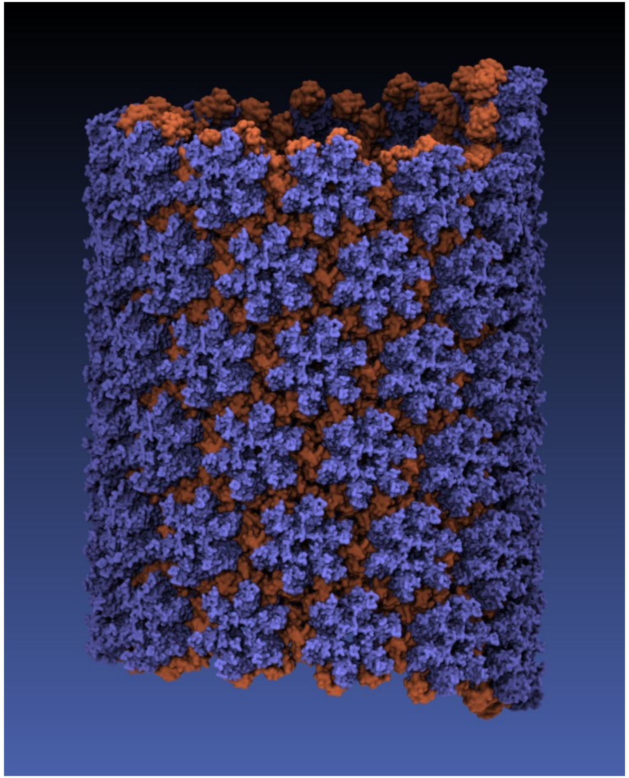
Close-up view of HIV-1 hexamer rendered via EGL

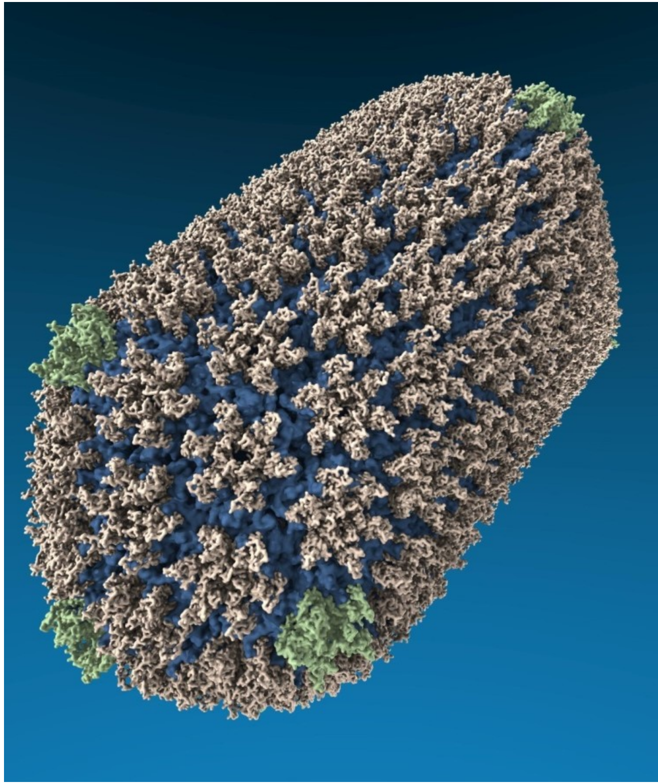
EGL Is Supported Now!

- Cloud+Workstations with most recent NVIDIA drivers
- VMD on HPC systems w/ latest Tesla P100 GPUs:
  - Cray XC50, CSCS Piz Daint, driver 375.39
  - IBM OpenPOWER, drivers 375.66 and later support both GLX and EGL

```
Info) VMD for OPENPOWER, version 1.9.3 (April 27, 2017)
Info) http://www.ks.uiuc.edu/Research/vmd/
[…]
Info) Multithreading available, 160 CPUs detected.
Info) Free system memory: 501GB (98%)
Info) Creating CUDA device pool and initializing hardware...
Info) Detected 4 available CUDA accelerators:
Info) [0] Tesla P100-SXM2-16GB 56 SM_6.0 @ 1.48 GHz, 16GB RAM, AE3, ZCP
[…]
Info) EGL: node[0] bound to display[0], 4 displays total
Info) EGL version 1.4
Info) OpenGL Pbuffer size: 4096x2400
Info) OpenGL renderer: Tesla P100-SXM2-16GB/PCIe
Info)   Features: STENCIL MSAA(4) MDE CVA MTX NPOT PP PS GLSL(OVFGS)
Info)   Full GLSL rendering mode is available.
Info)   Textures: 2-D (32768x32768), 3-D (16384x16384x16384), Multitexture (4)
Info) Created EGL OpenGL Pbuffer for off-screen rendering
```

VMD "QuickSurf" Representation, Ray Tracing

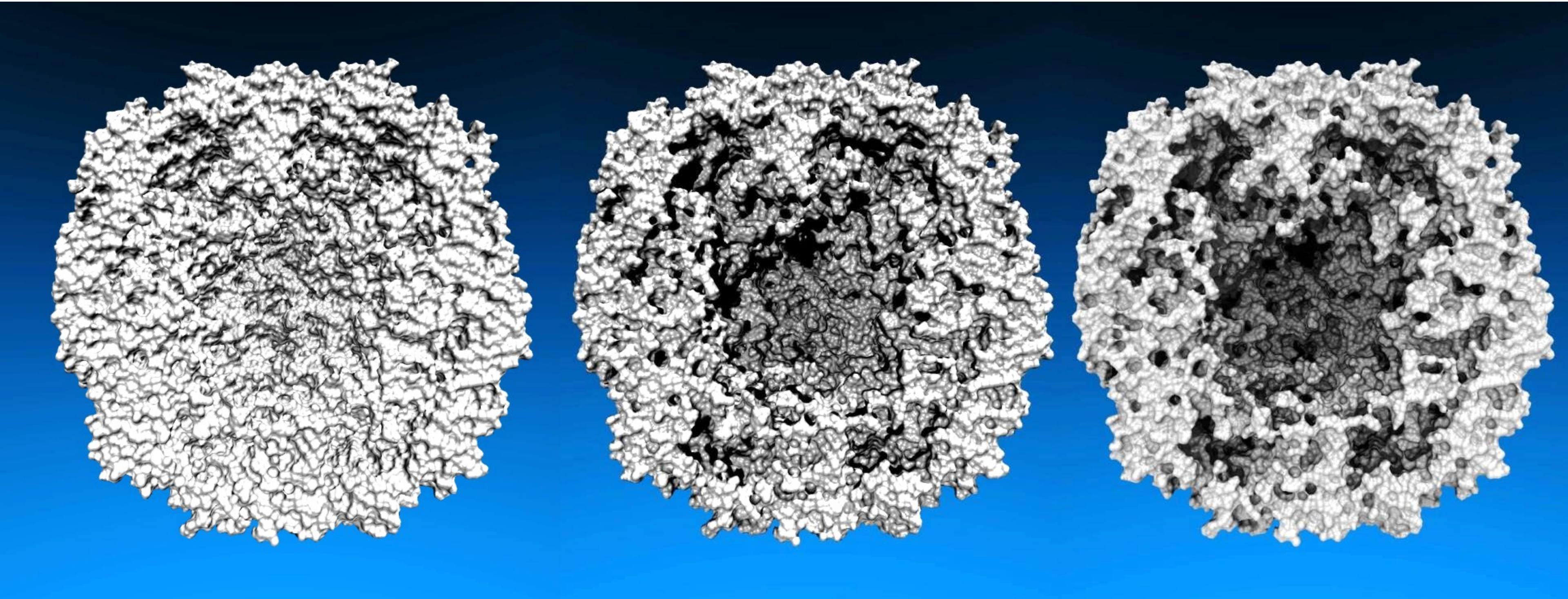




All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

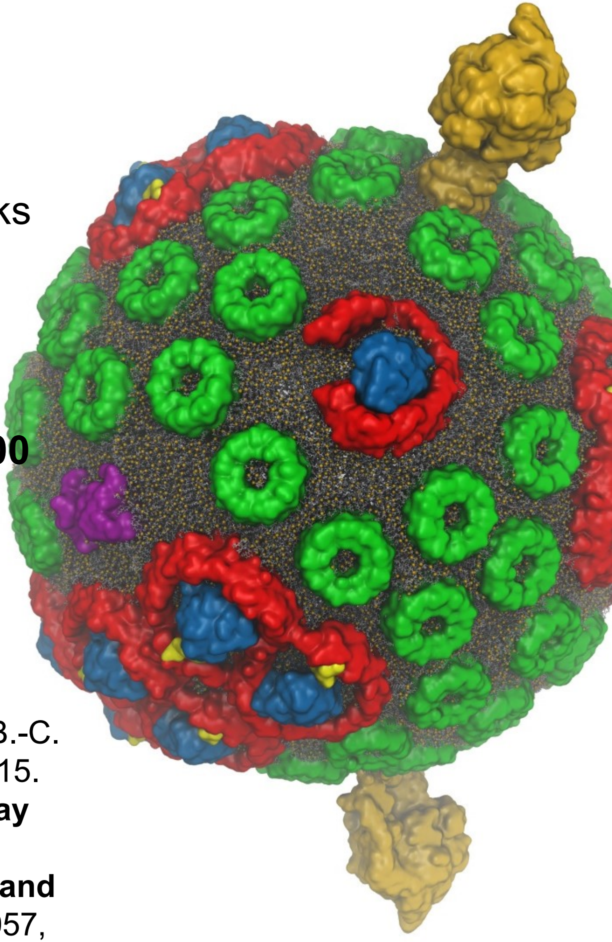
Lighting Comparison, STMV Capsid

Two lights, no shadows	Two lights, hard shadows, 1 shadow ray per light	Ambient occlusion + two lights, 144 AO rays/hit



VMD w/ OptiX 4.1

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization tasks
- Remote RT on NVIDIA VCA clusters
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- **Top-end Pascal Tesla GPUs roughly 2x faster than Kepler**
- **GPU memory sharing via NVLink on Quadro GP100, Tesla P100**



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.

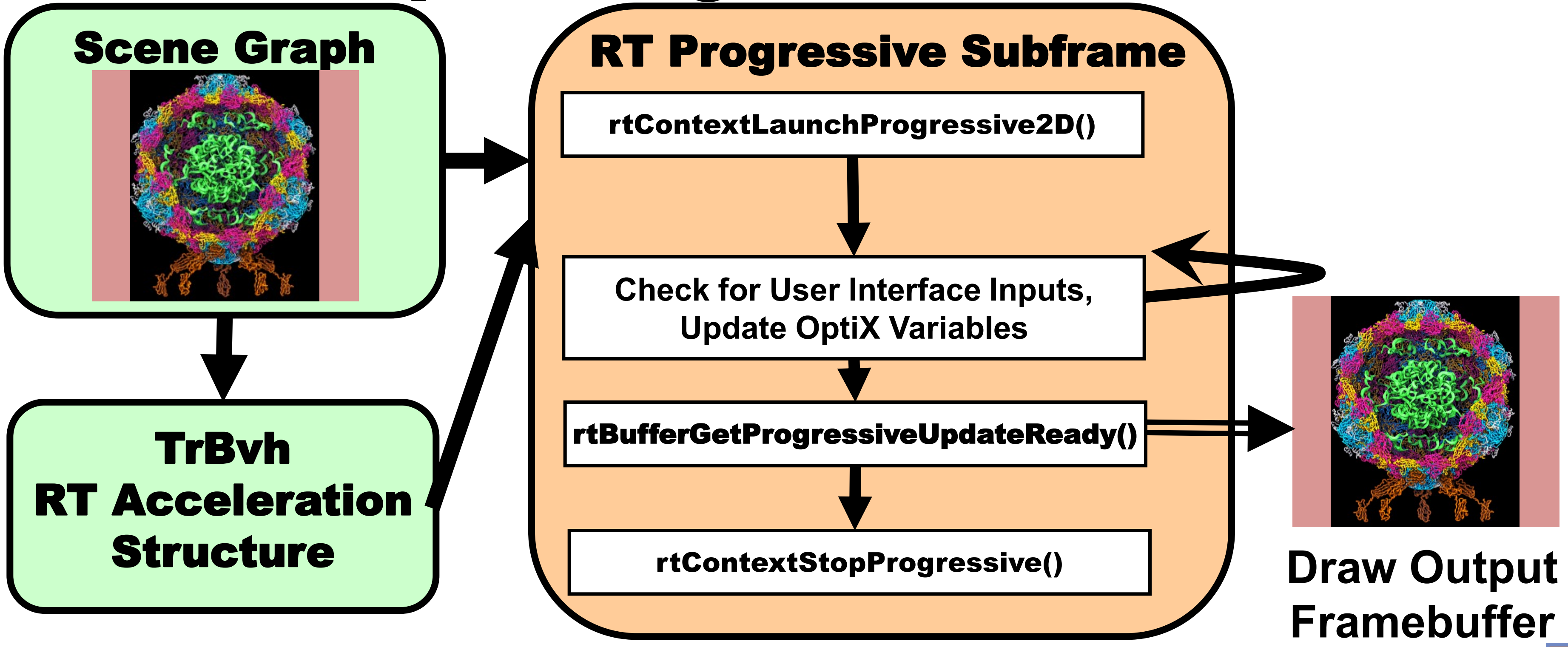
Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

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.

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

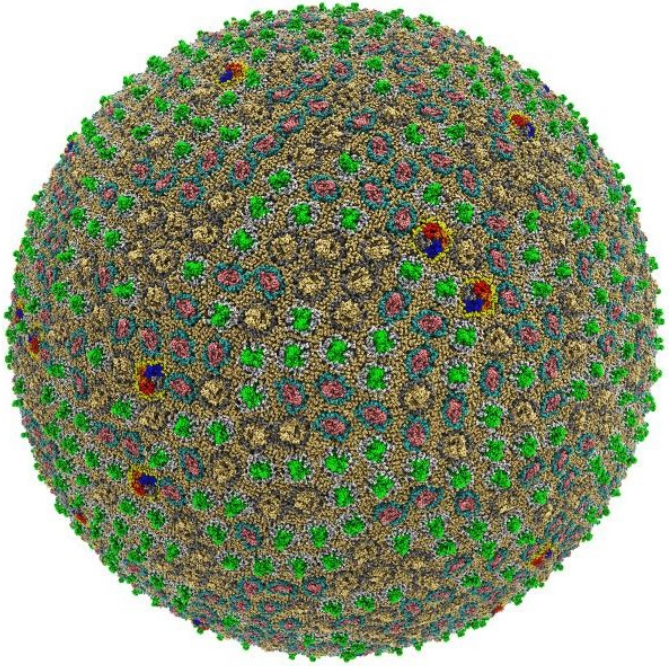
VMD TachyonL-OptiX Interactive RT w/ OptiX Progressive RT API



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

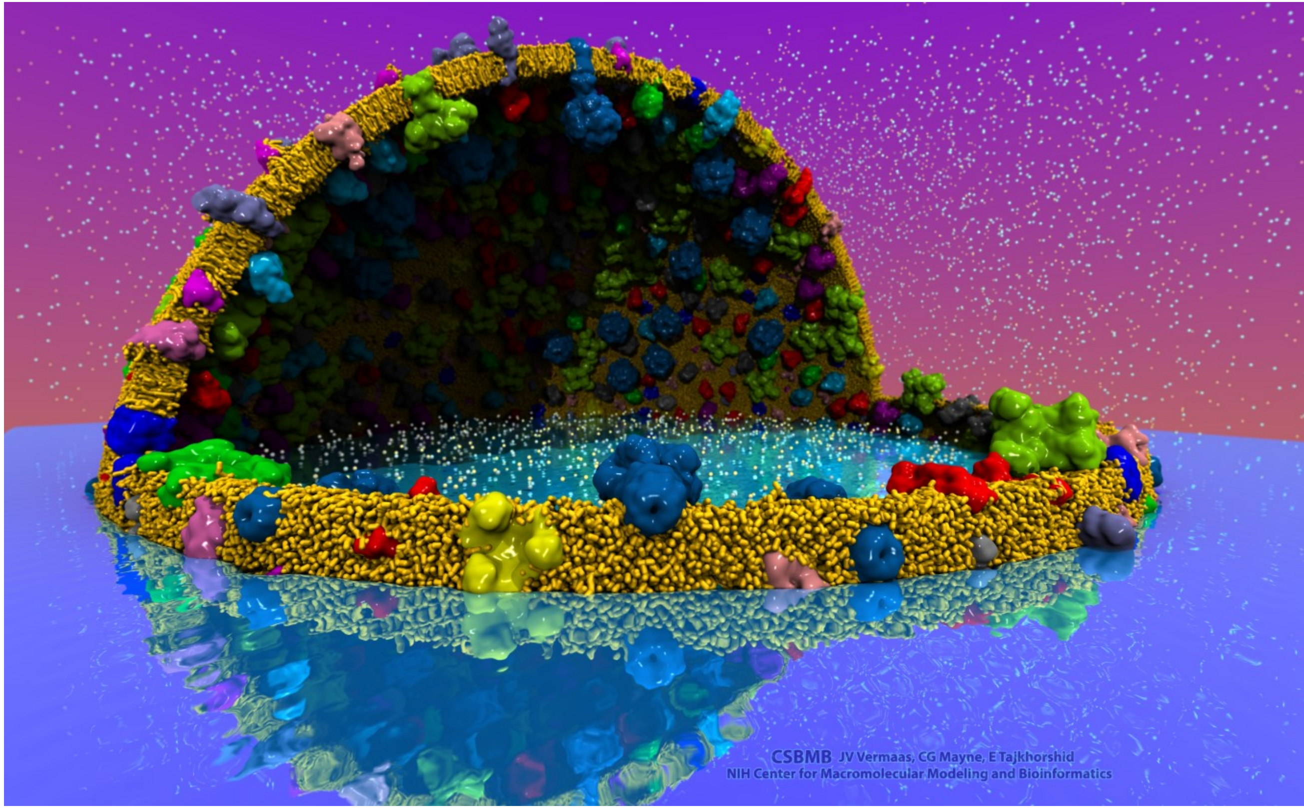


Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J.E. Stone, …, K. Schulten, J. Parallel Computing, 55:17-27, 2016.

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.

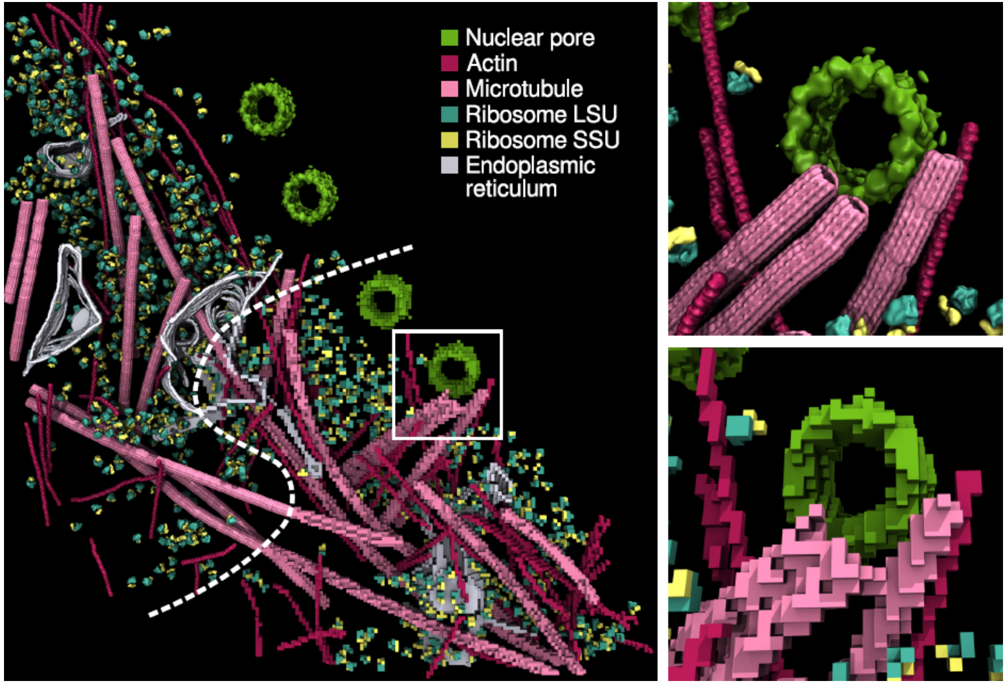
Proto-Cell Rendered with VMD+OptiX

- 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
- **Latest Quadro GP100 GPUs benefit from OptiX 4.1 support for NVLink and distribution of scene data across multiple GPUs**



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

VMD Molecule Instancing: In-Progress Development

- VMD 1.9.4 supports instancing of graphical representations associated with molecules
- Will exploit VBO caching in OpenGL to eliminate host-GPU geometry transfers
- OptiX instancing of geometry buffers to eliminate GPU memory consumption for instances

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

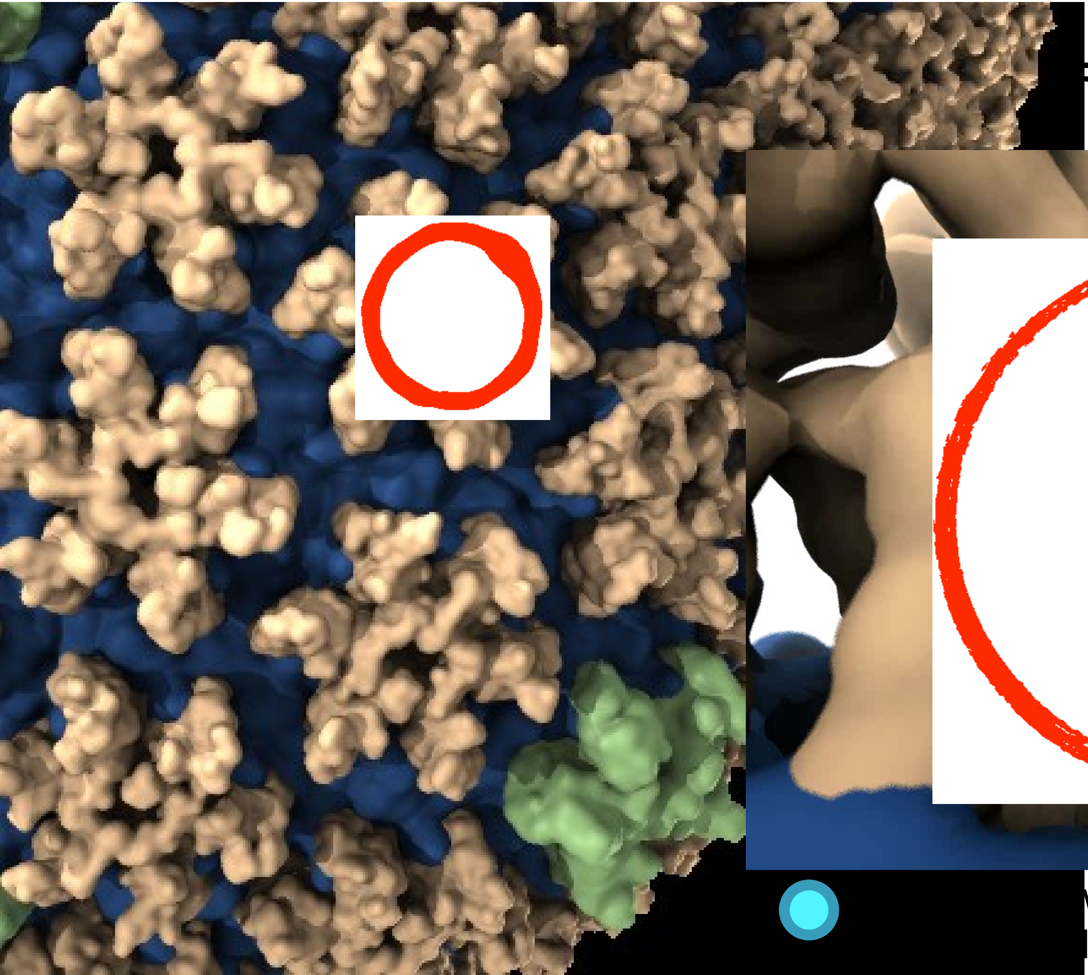
VMD Chromatophore Demo, NVIDIA VR Room at SC'16

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

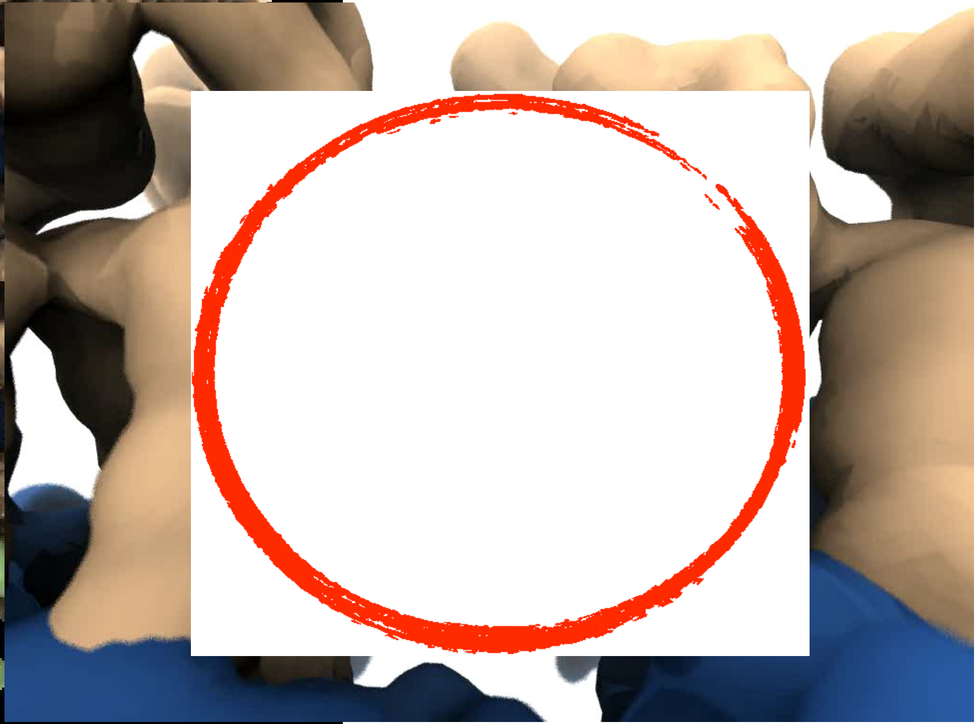
[2] Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J.E. Stone, W.R. Sherman, K. Schulten. IEEE HPDAV (IPDPSW), pp. 1048-1057, 2016.

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.

Goal: Intuitive interactive viz. in crowded molecular complexes



Results from 64 M atom, 1 μs sim!



v of chloride ions permeating
l capsid hexameric centers

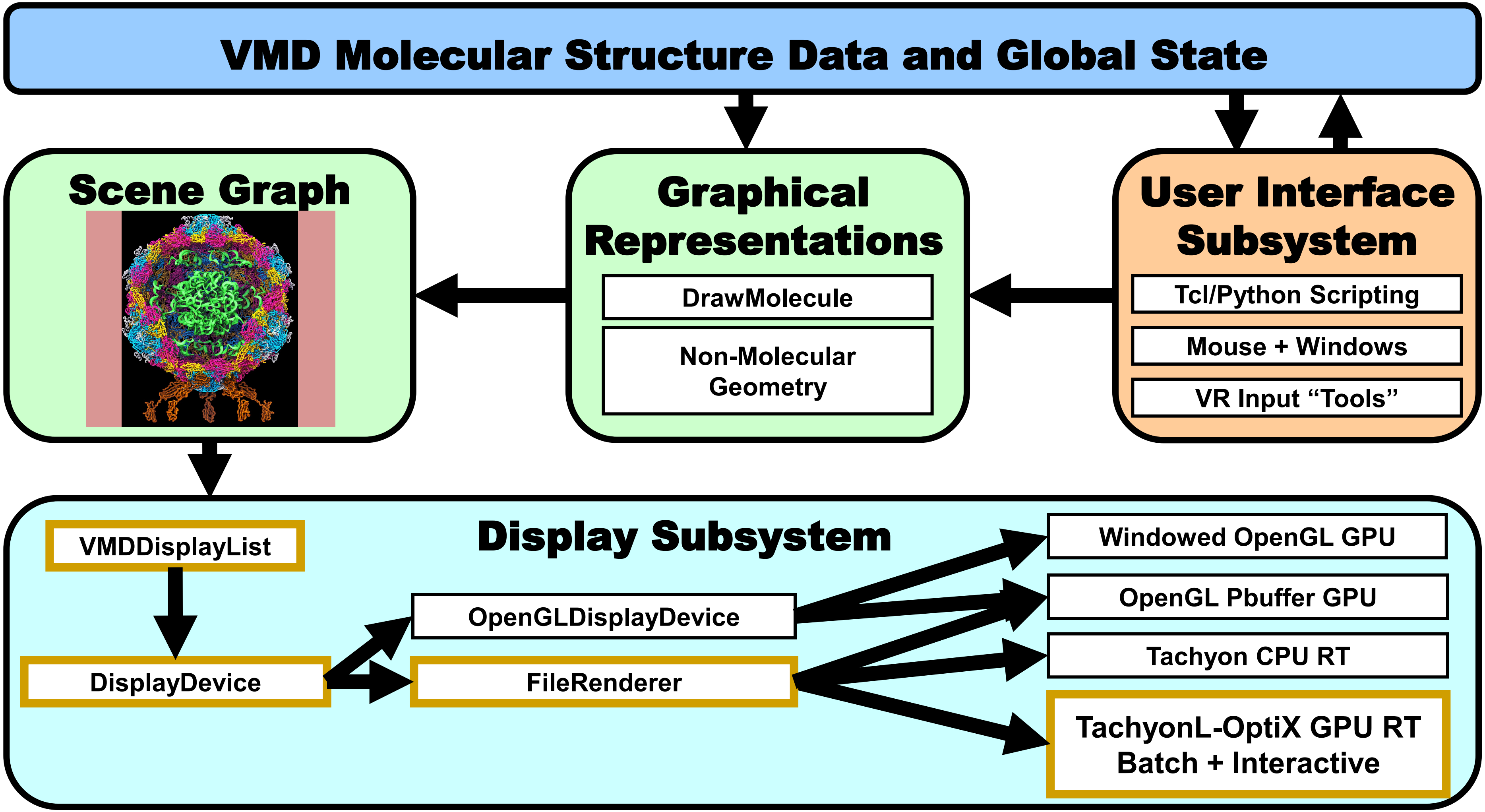
Immersive Viz. w/ VMD

- 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
  - Accomodating limitations idiosynchracies of commercial HMDs

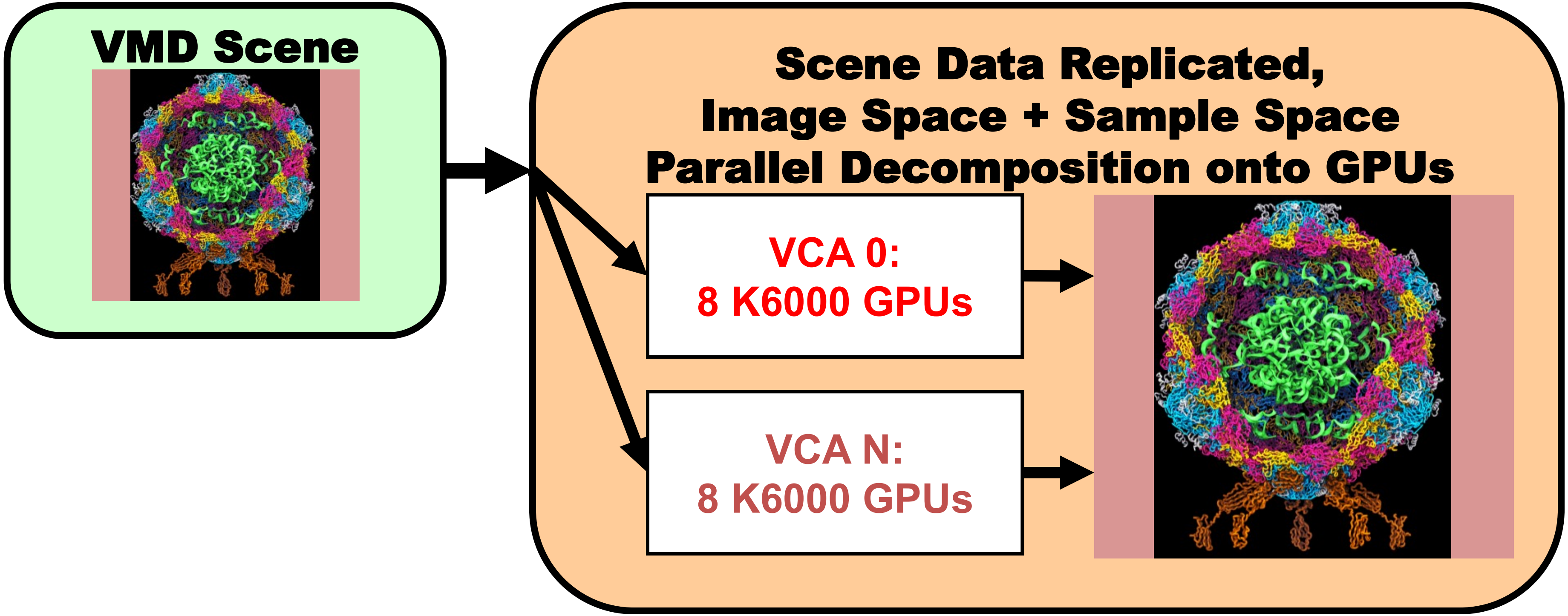
VMD running in a CAVE w/ VR Juggler

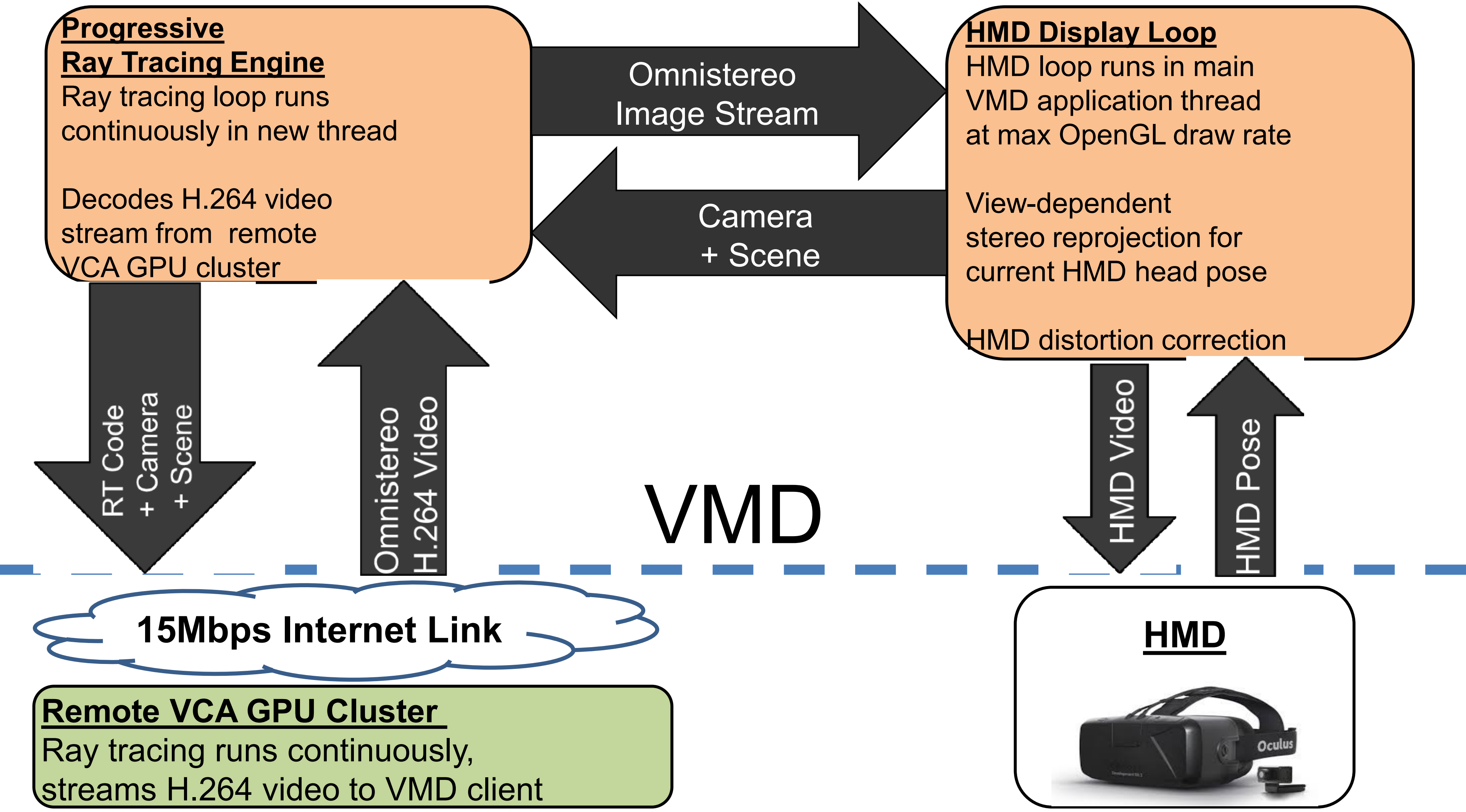
HMD Ray Tracing Challenges

- HMDs require high frame rates **(90Hz or more)** and minimum latency between IMU sensor reads and presentation on the display
- Multi-GPU workstations fast enough to direct-drive HMDs at required frame rates for simple scenes with direct lighting, hard shadows
- Advanced RT effects such as AO lighting, depth of field require much **larger sample counts**, impractical for direct-driving HMDs
- **Remote viz. required for** many HPC problems due to **large data**
- **Remote viz. latencies too high for direct-drive of HMD**
- **Our two-phase approach: moderate-FPS remote RT combined with local high-FPS view-dependent HMD reprojection w/ OpenGL**

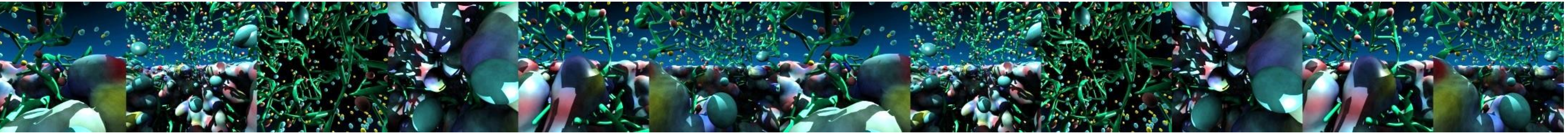

VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input "Tools"
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL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

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

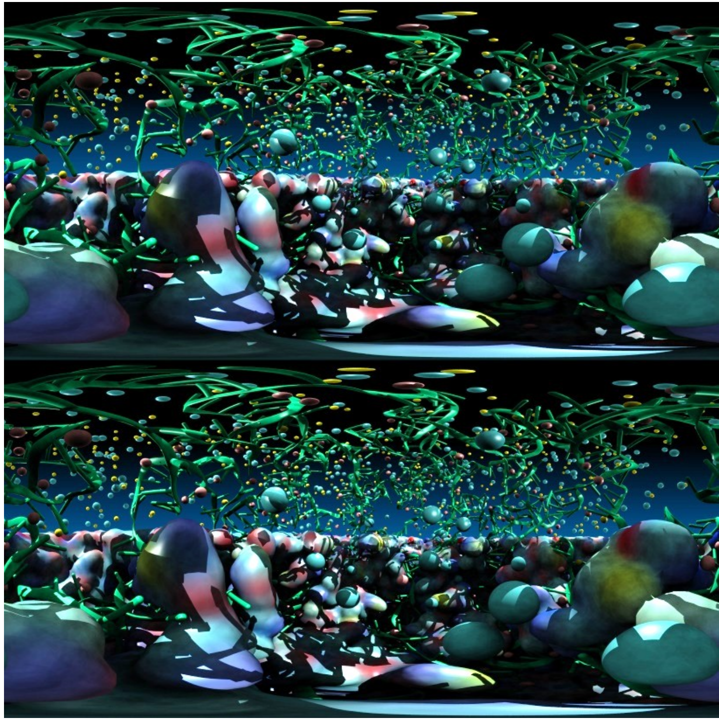


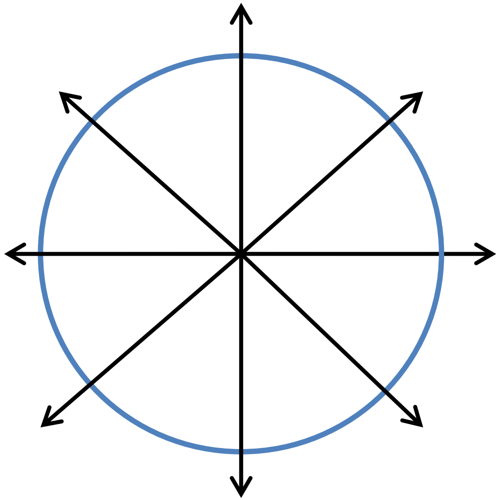

Progressive
Ray Tracing Engine
Ray tracing loop runs
continuously in new thread
Decodes H.264 video
stream from remote
VCA GPU cluster
Omnistereo
Image Stream
Camera
+ Scene
HMD Display Loop
HMD loop runs in main
VMD application thread
at max OpenGL draw rate
View-dependent
stereo reprojection for
current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

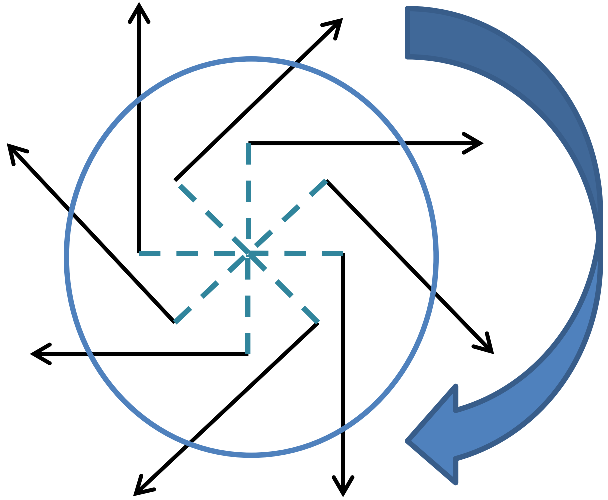


- **Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard**
- Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
- Stereo requires spherical camera projections **poorly suited to rasterization**
-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



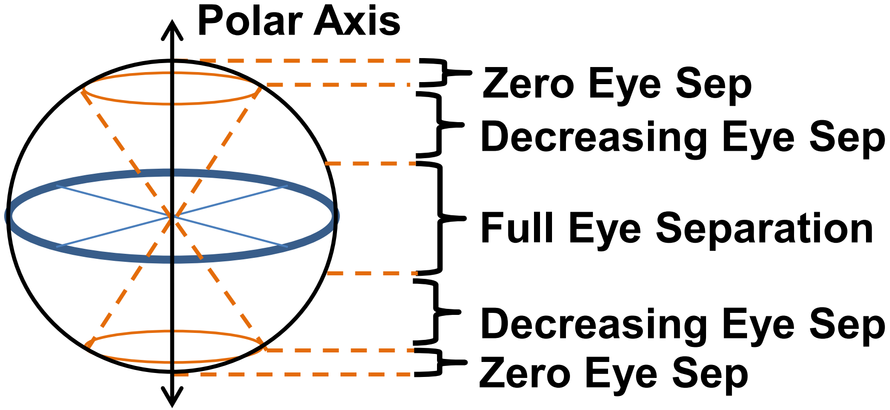


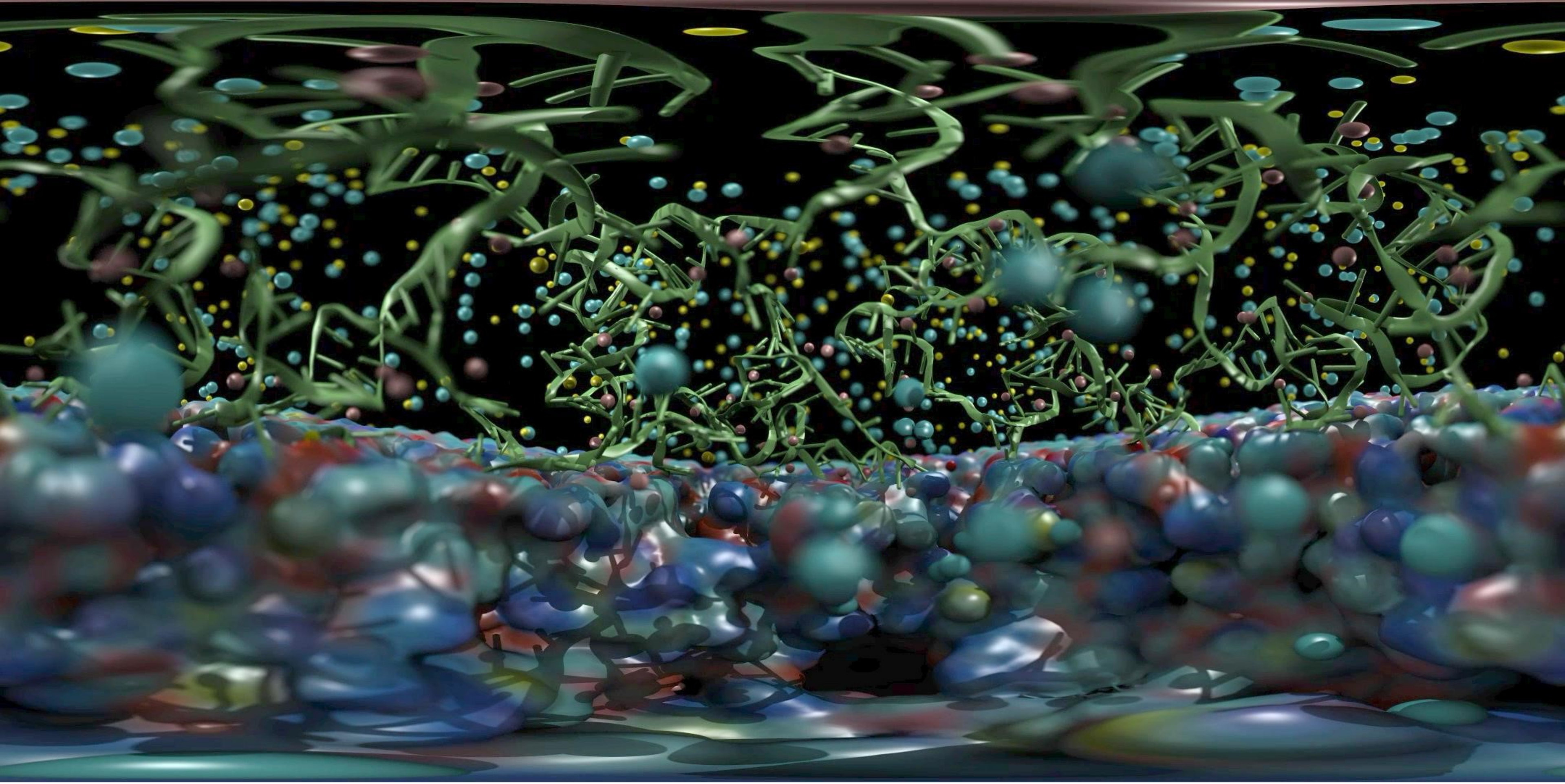
A) Monoscopic circular projection.
Eye at center of projection (COP).

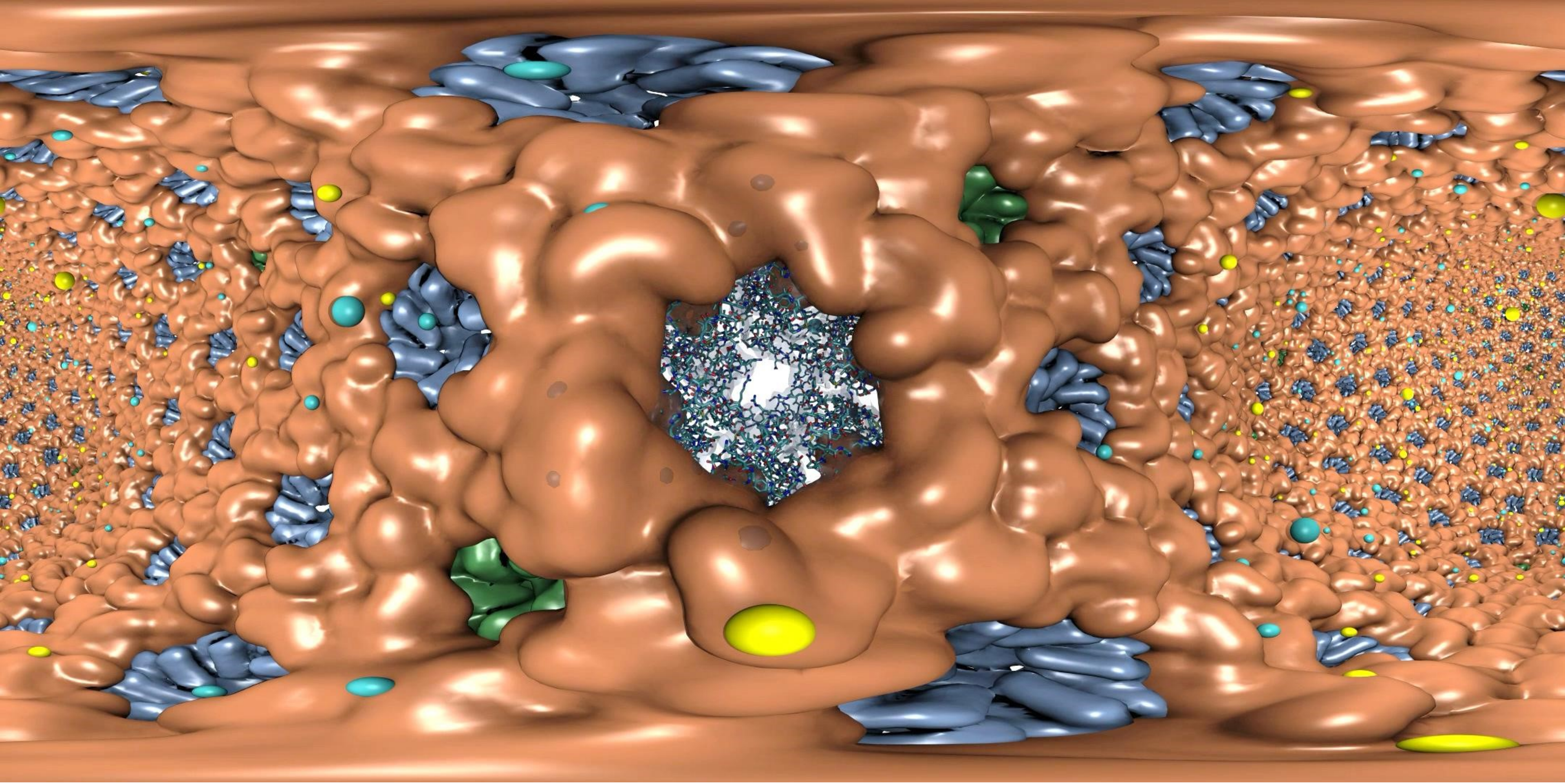


B) Left eye stereo circular projection.
Eye offset from COP by half of interocular distance.

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.







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+Do F	1:1 2:1 2:2	16.1 11.1 8.5
HIV-1 Shadows	1:0 2:0 4:0	20.1 18.1 10.2
HIV-1 Shadows+AO	1:1 1:2 1:4	17.4 12.2 8.1

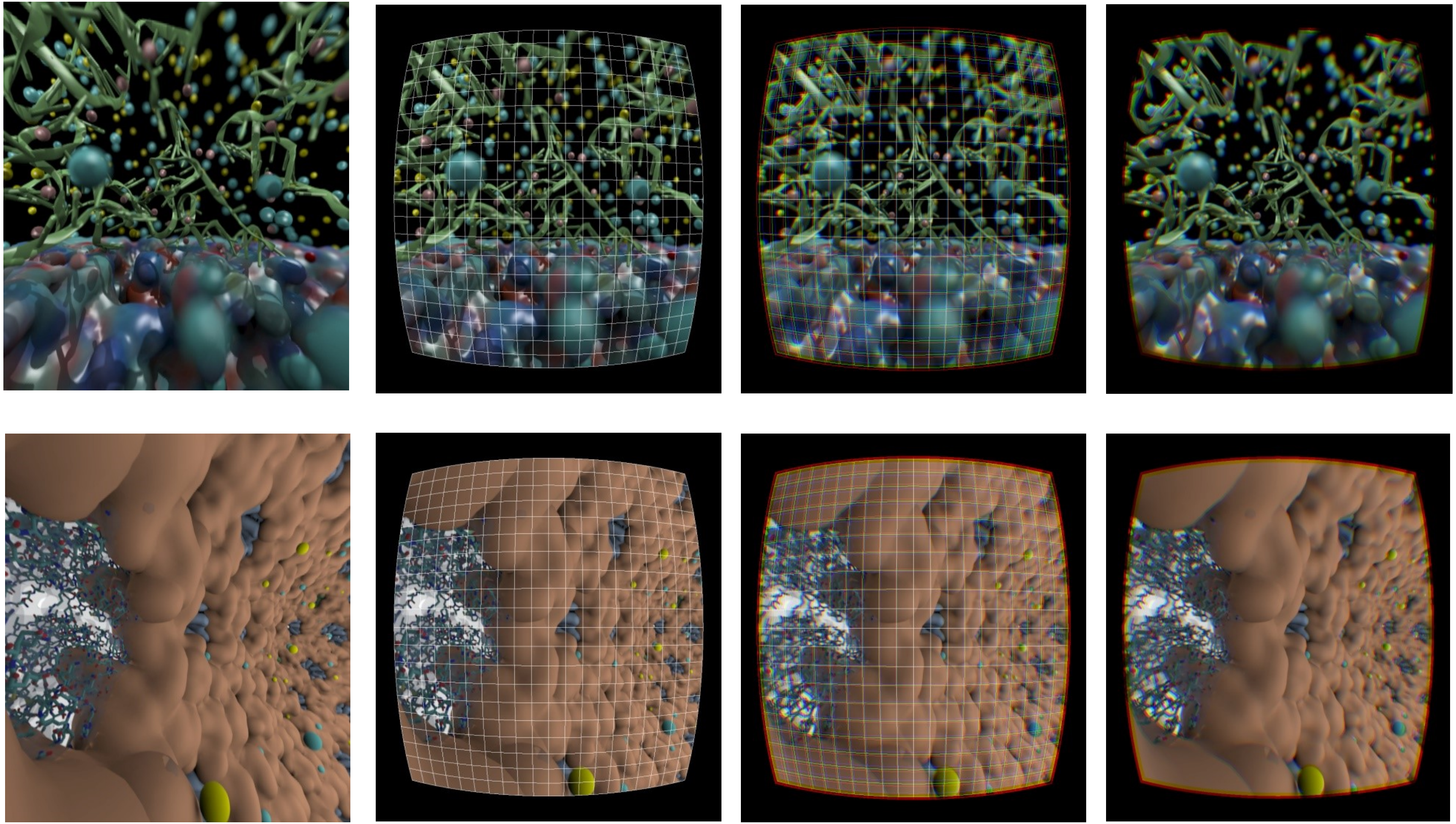
HMD View-Dependent Reprojection with OpenGL

- Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface (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)**

VMD can support a variety of HMD lens designs, e.g.

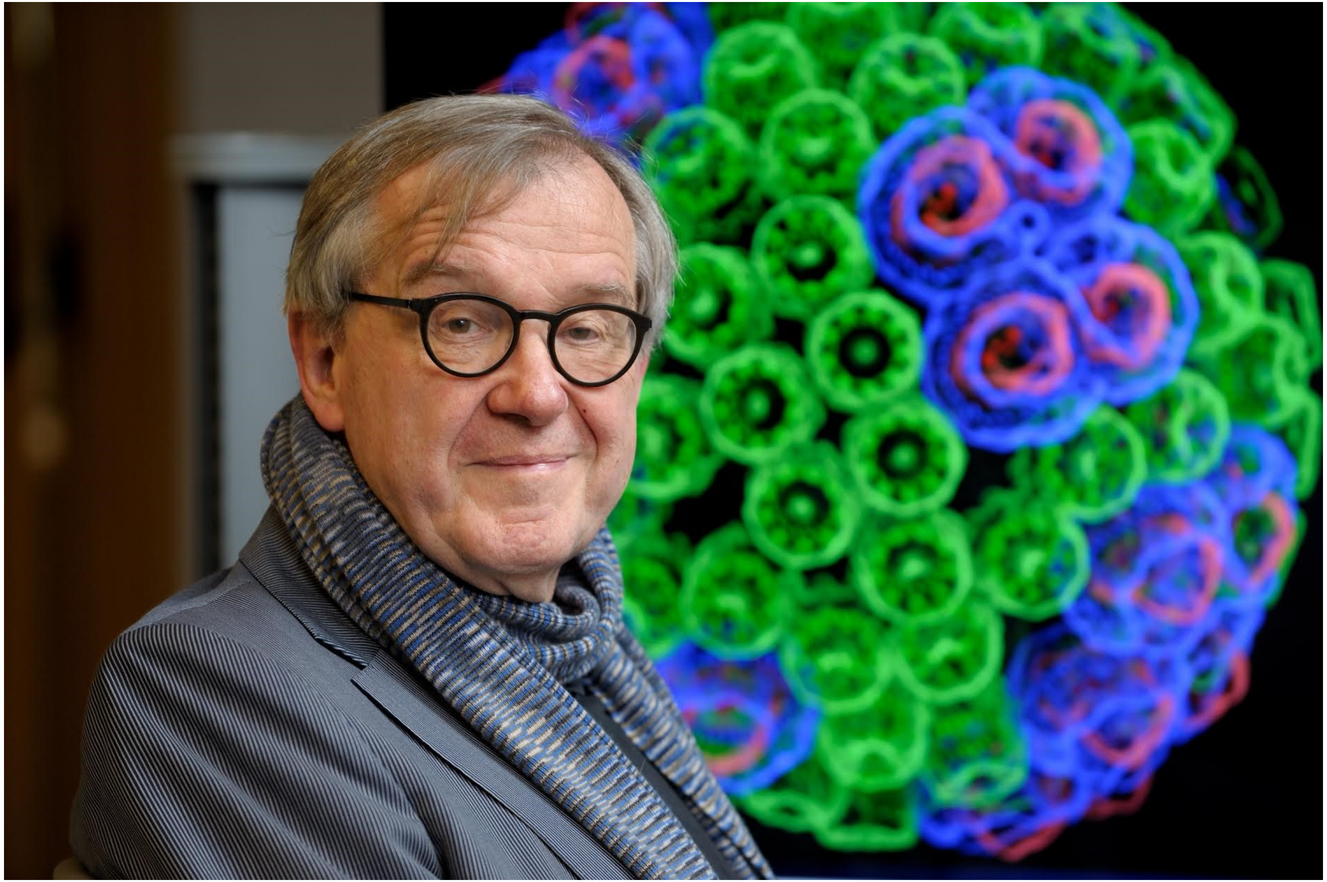
http://research.microsoft.com/en-us/um/redmond/projects/lensfactory/oculus/


A



Future Work

- Support for more commodity HMDs as they become generally available
- Support for OSes besides Linux
- Ray tracing engine and optimizations:
  – **Multi-node parallel RT and remote viz. on general clusters and supercomputers, e.g. NCSA Blue Waters, ORNL Titan**
  – Interactive RT stochastic sampling strategies to improve interactivity
  – Improved omnidirectional cubemap/spheremap sampling approaches
- Tons of work to do on VR user interfaces, multi-user collaborative visualization, …



“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

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