VMD: Immersive Molecular Visualization with High-Fidelity Ray Tracing

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

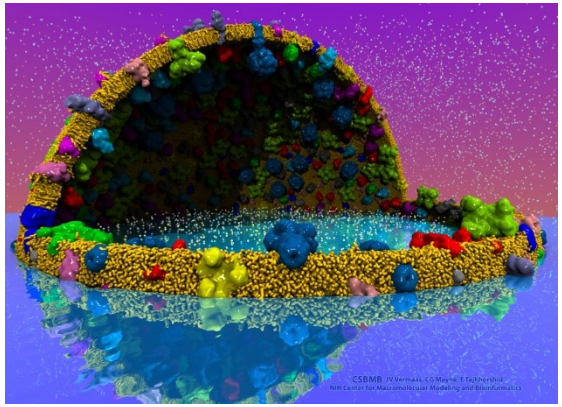
9:00am, Monday August 13, 2018

BOF: Immersive Visualization for Science and Research

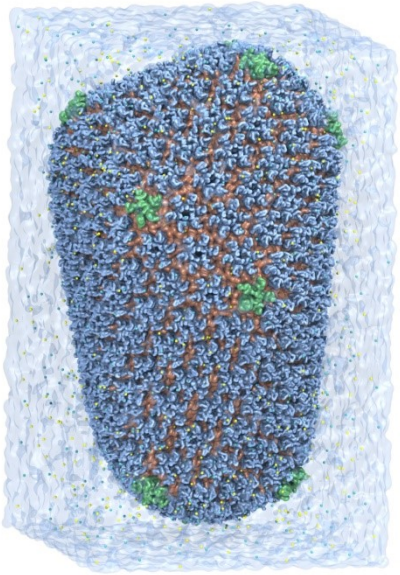
Siggraph 2018, Vancouver, BC, Canada

VMD – “Visual Molecular Dynamics”

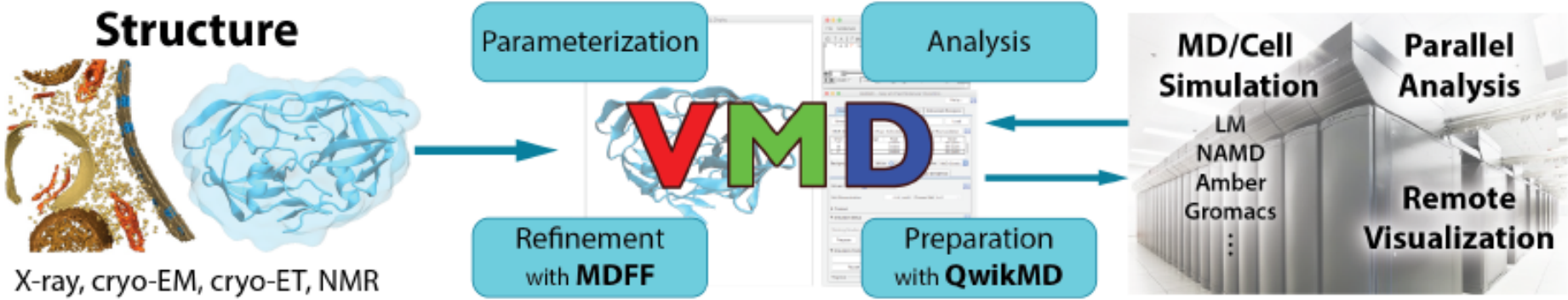
- 100,000 active users worldwide
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



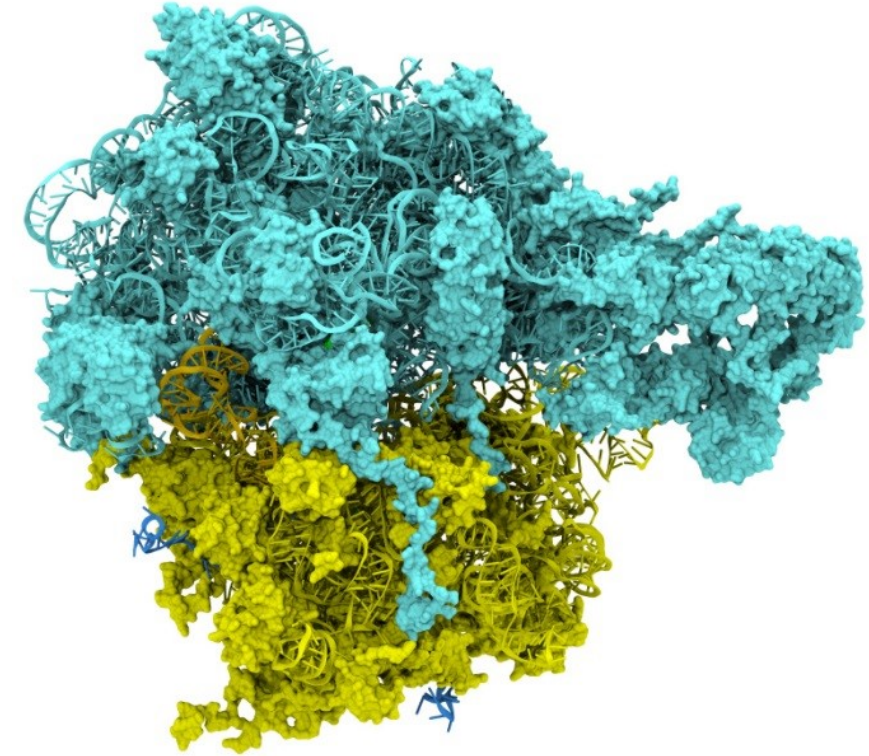
MD Simulation



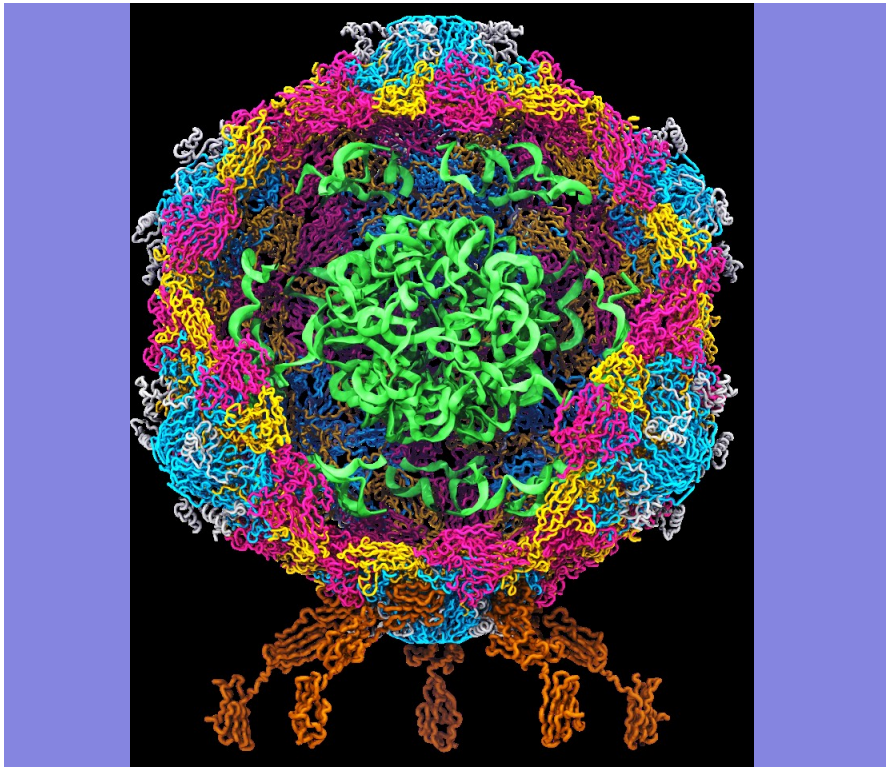
Goal: A Computational Microscope

Study the molecular machines in living cells

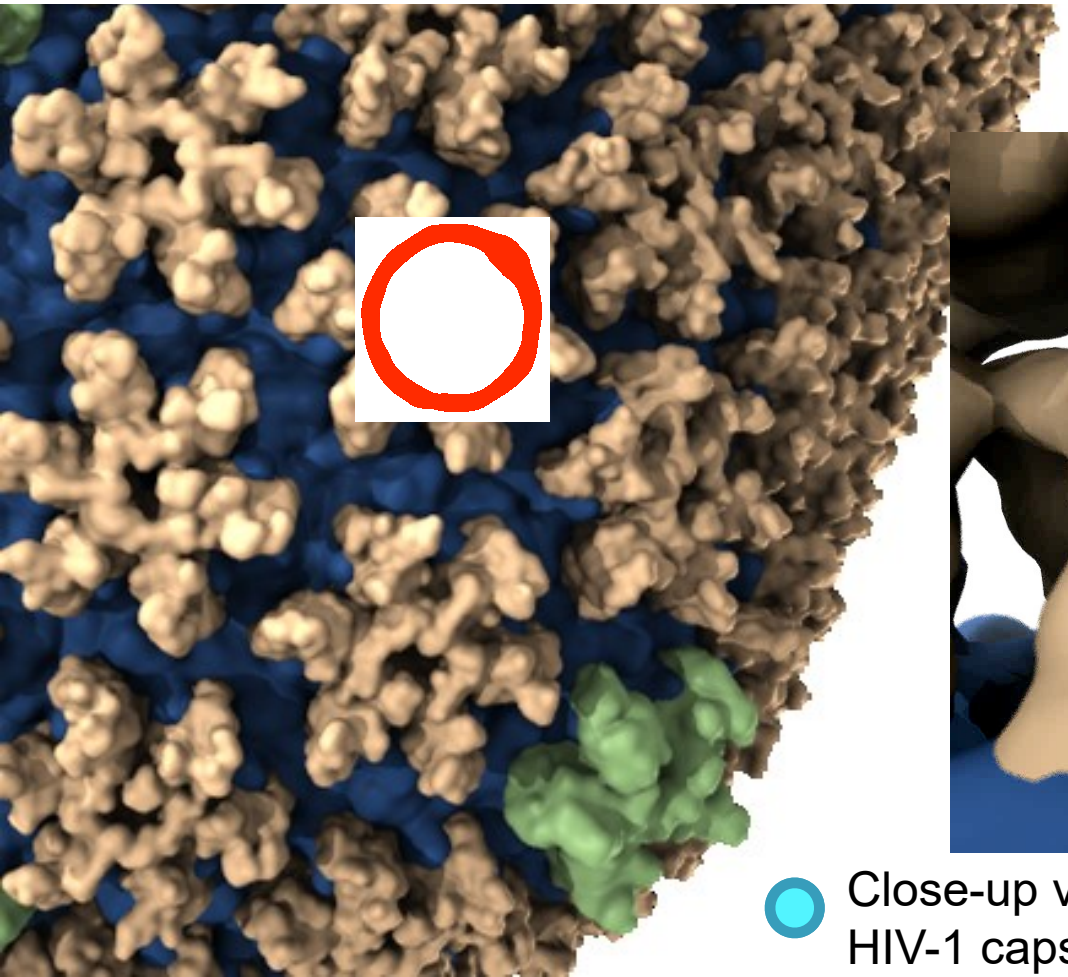
Ribosome: target for antibiotics



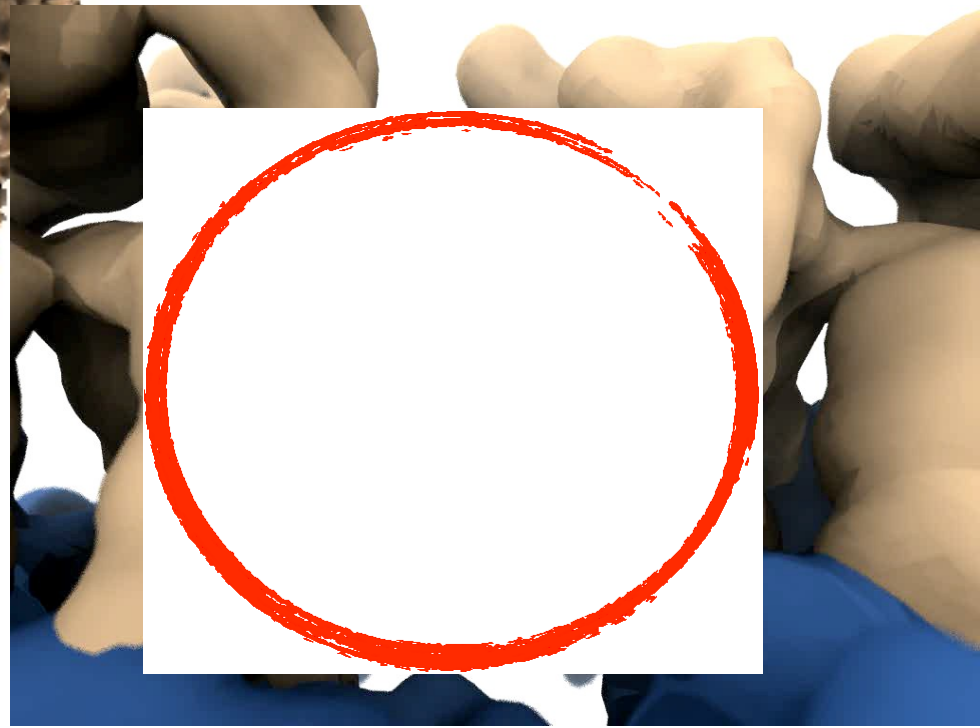
Poliovirus



Goal: Intuitive interactive viz. in crowded molecular complexes



Results from 64M atom, 1 μs sim!

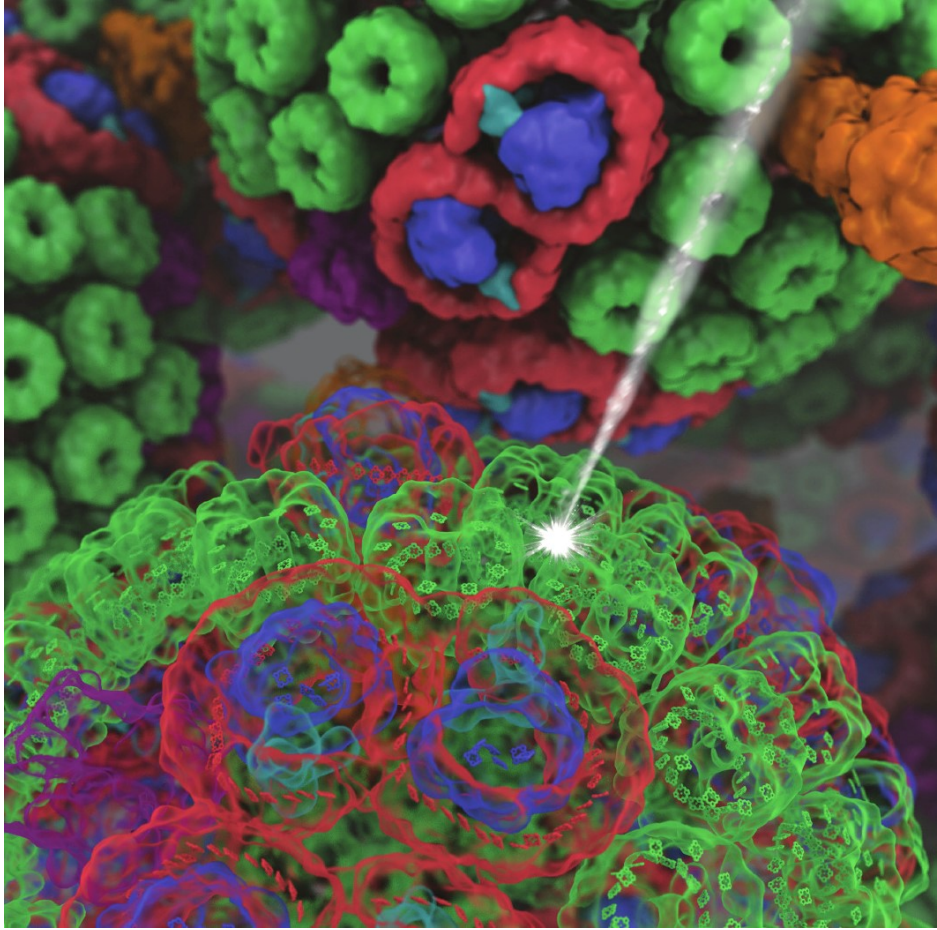


- Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers

High Fidelity Ray Tracing

- Ambient Occlusion, Depth of Field, high quality transparency, instancing, ….
- **Interactive RT** on laptop, desk, cloud
- Large-scale parallel rendering: in situ or post hoc visualization tasks
- **Stereoscopic panorama and full-dome projections**
- **Omnidirectional VR: YouTube, HMDs**

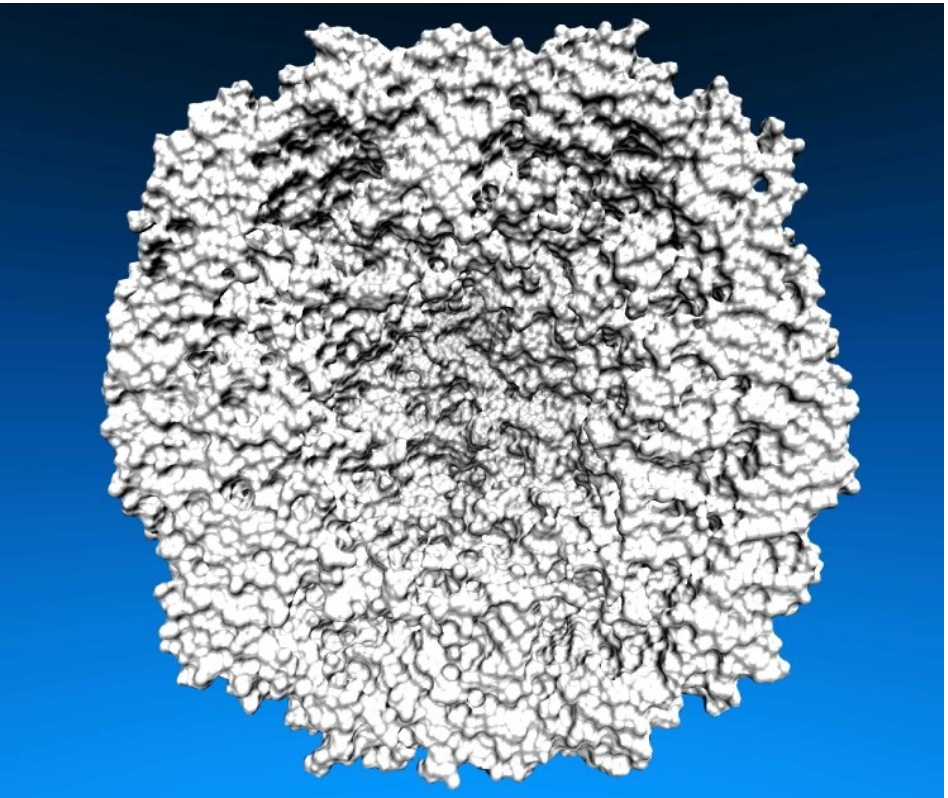
- Built-in ray tracing engines:
  - **Tachyon:** cross-platform RT
  - **NVIDIA OptiX:** GPU-accelerated and remote RT on VCA clusters
  - **Intel OSPRay:** CPU x86/Phi-optimized parallel rendering w/ MPI



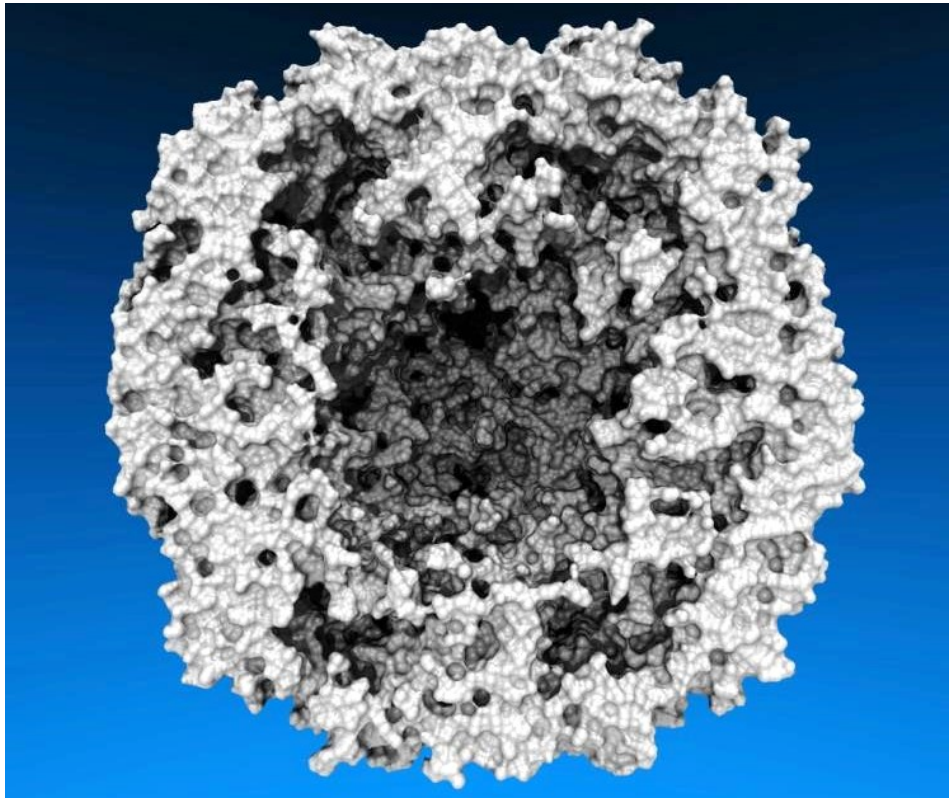
VMD/OptiX all-atom Chromatophore

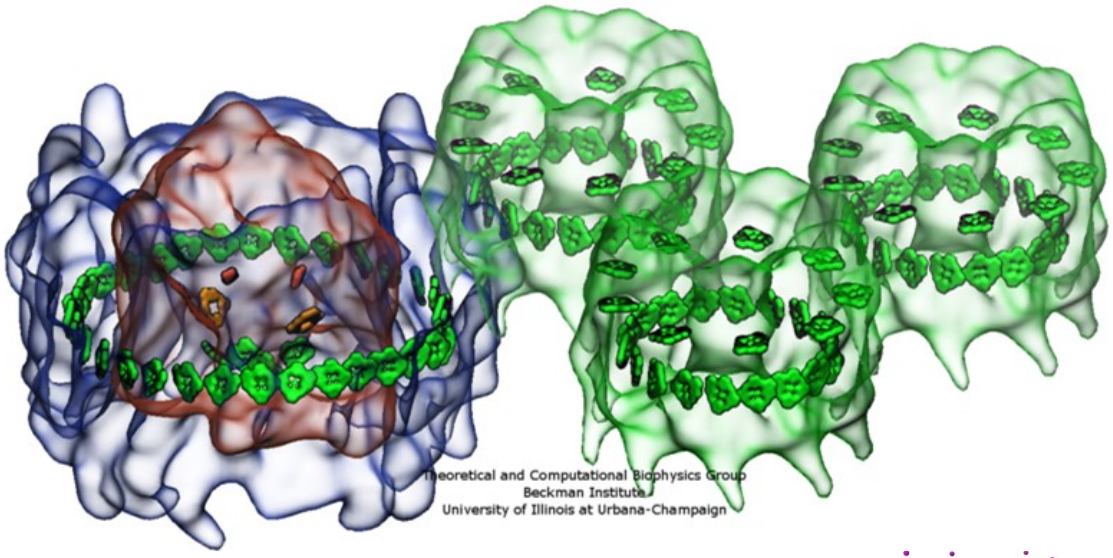
Lighting Comparison, STMV Capsid

Two lights, no shadows



Ambient occlusion + two lights, 144 AO rays/hit

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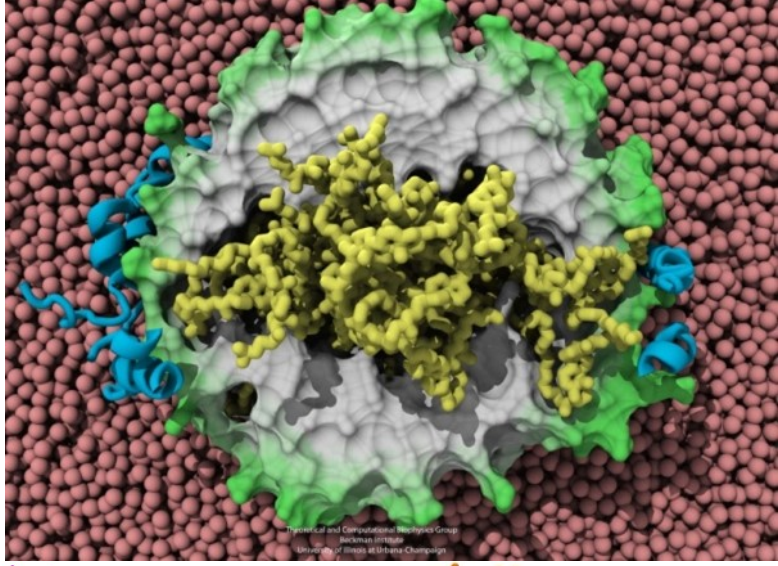
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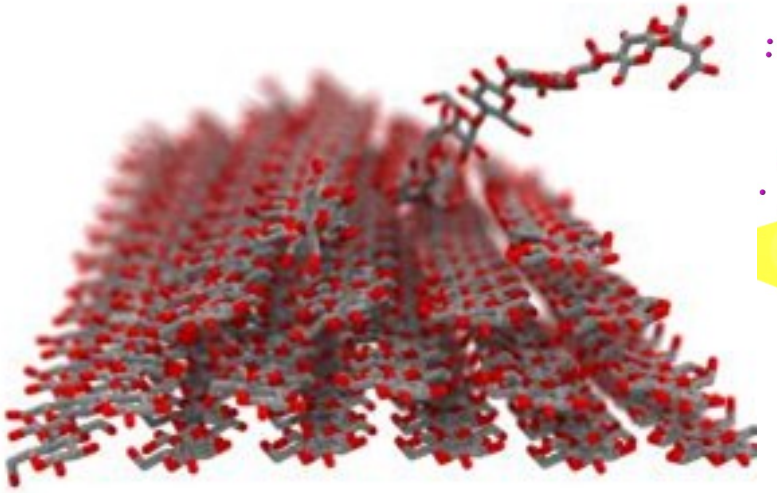
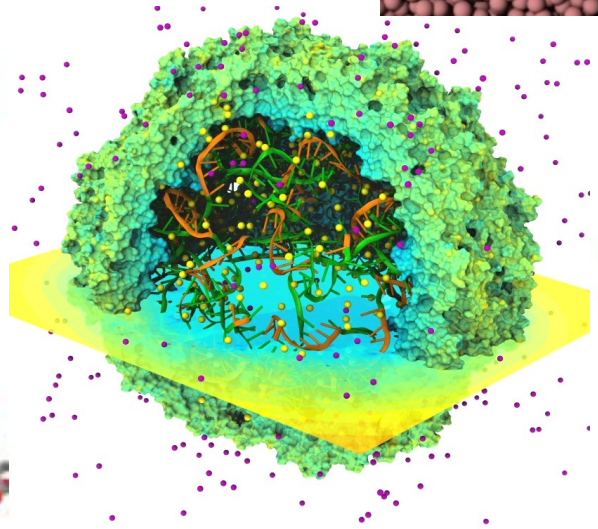
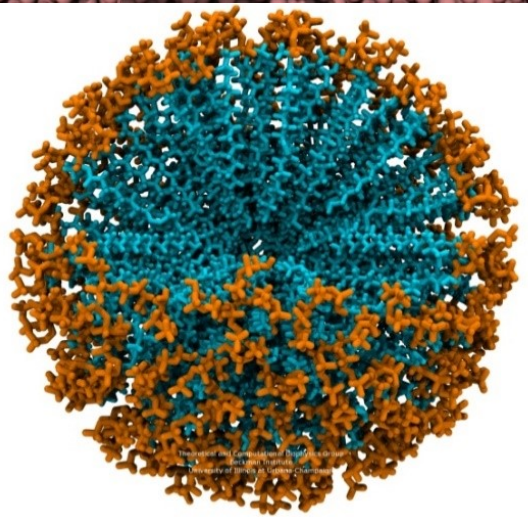
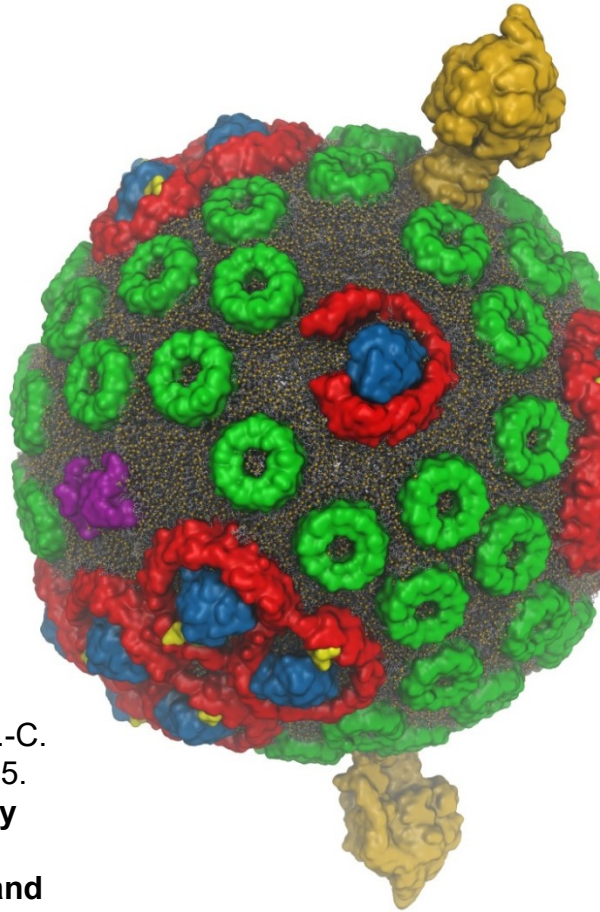






VMD w/ OptiX

- 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**
- **GPU memory sharing via NVLink**



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.

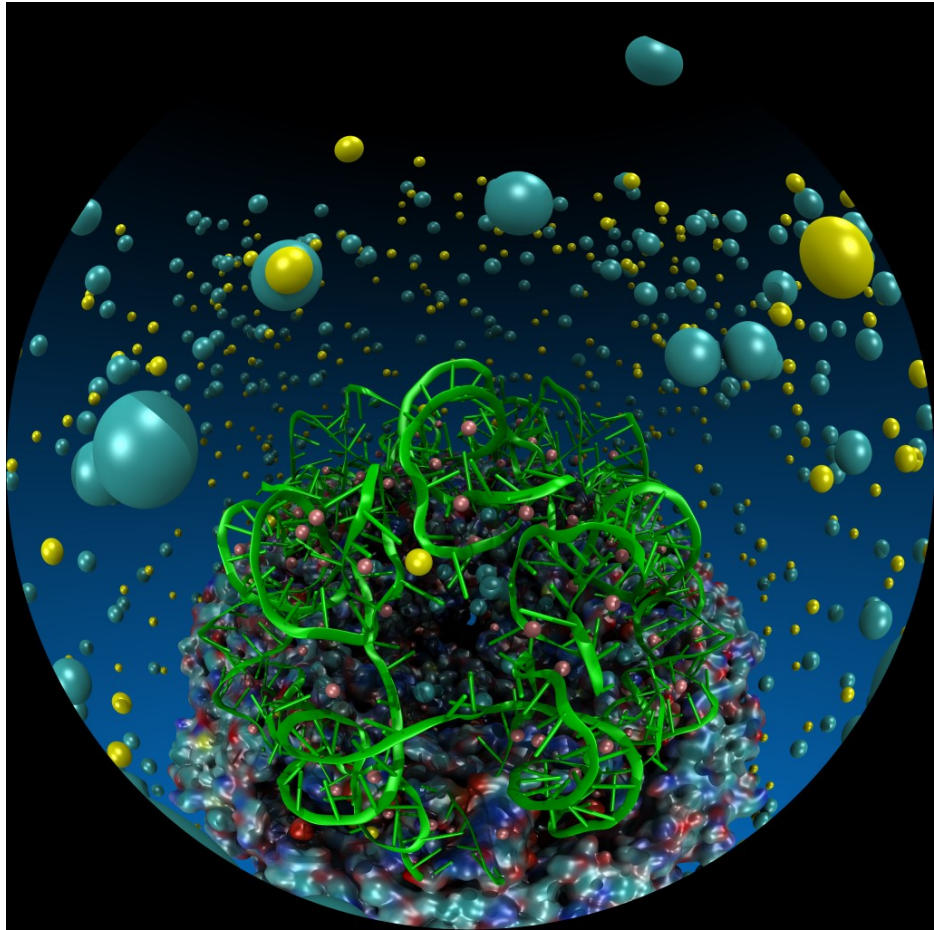
Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

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. Schulten. HPDAV, IPDPSW, pp. 1048-1057, 2016.

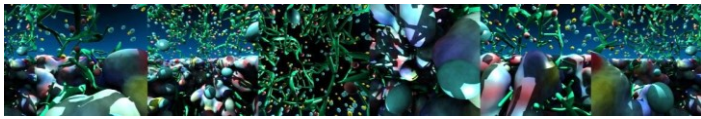
VMD Planetarium Dome Master Camera

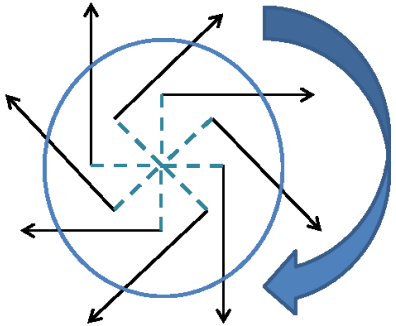
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required

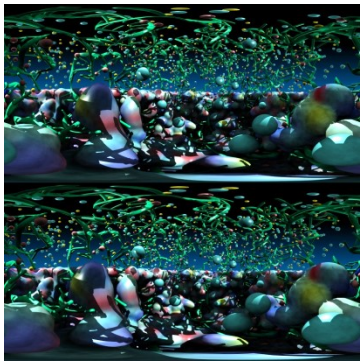


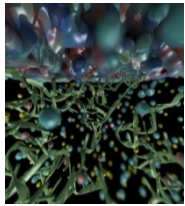
Omnidirectional Stereoscopic Ray Tracing

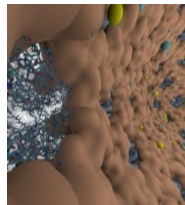
- **Ray trace 360° images and movies for Desk and VR HMDs: Oculus, Vive, Cardboard**
- Stereo spheremaps or cubemaps allow very high-frame-rate interactive OpenGL display
- **AO lighting, depth of field**, shadows, transparency, curved geometry, …











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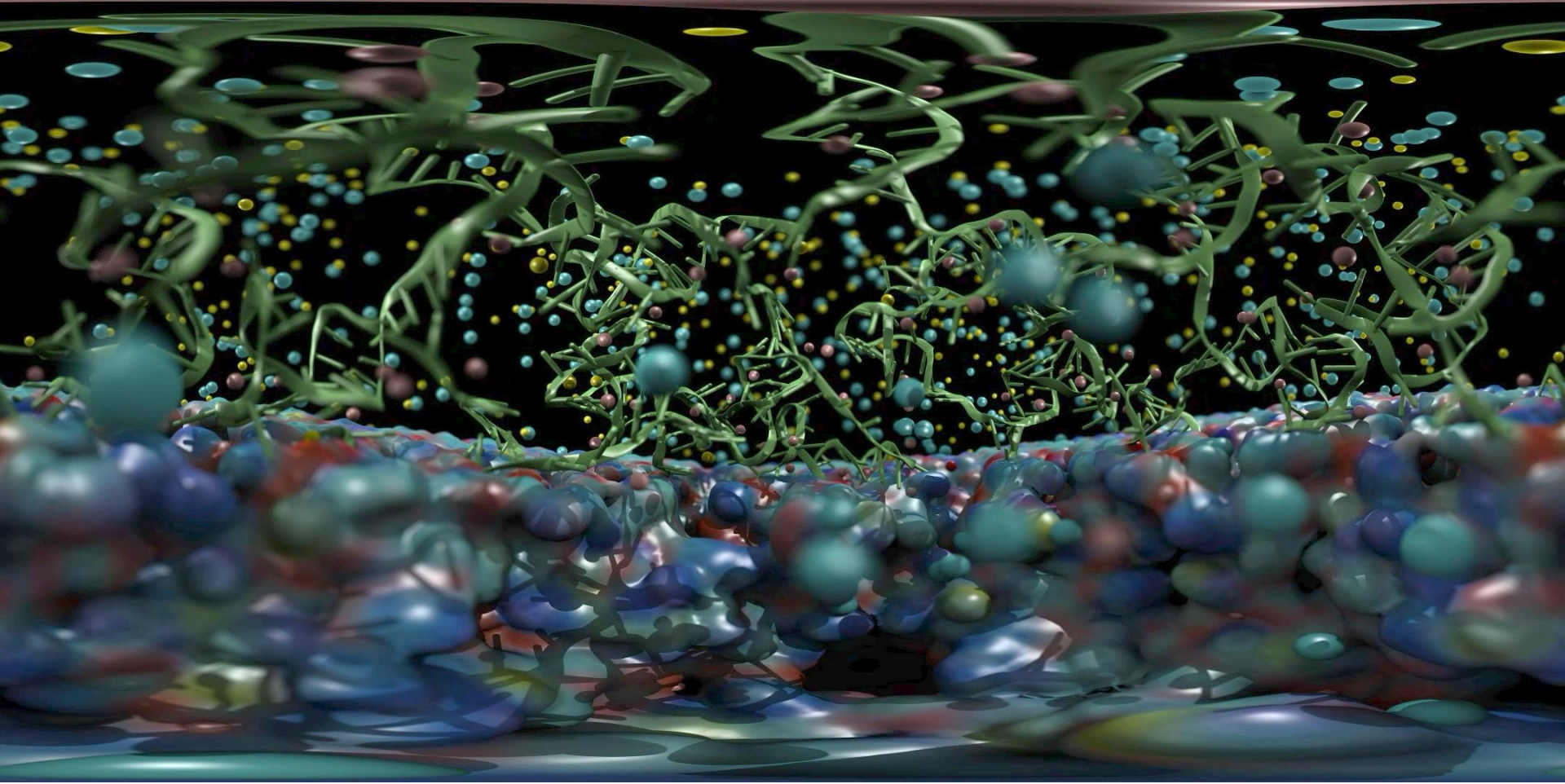
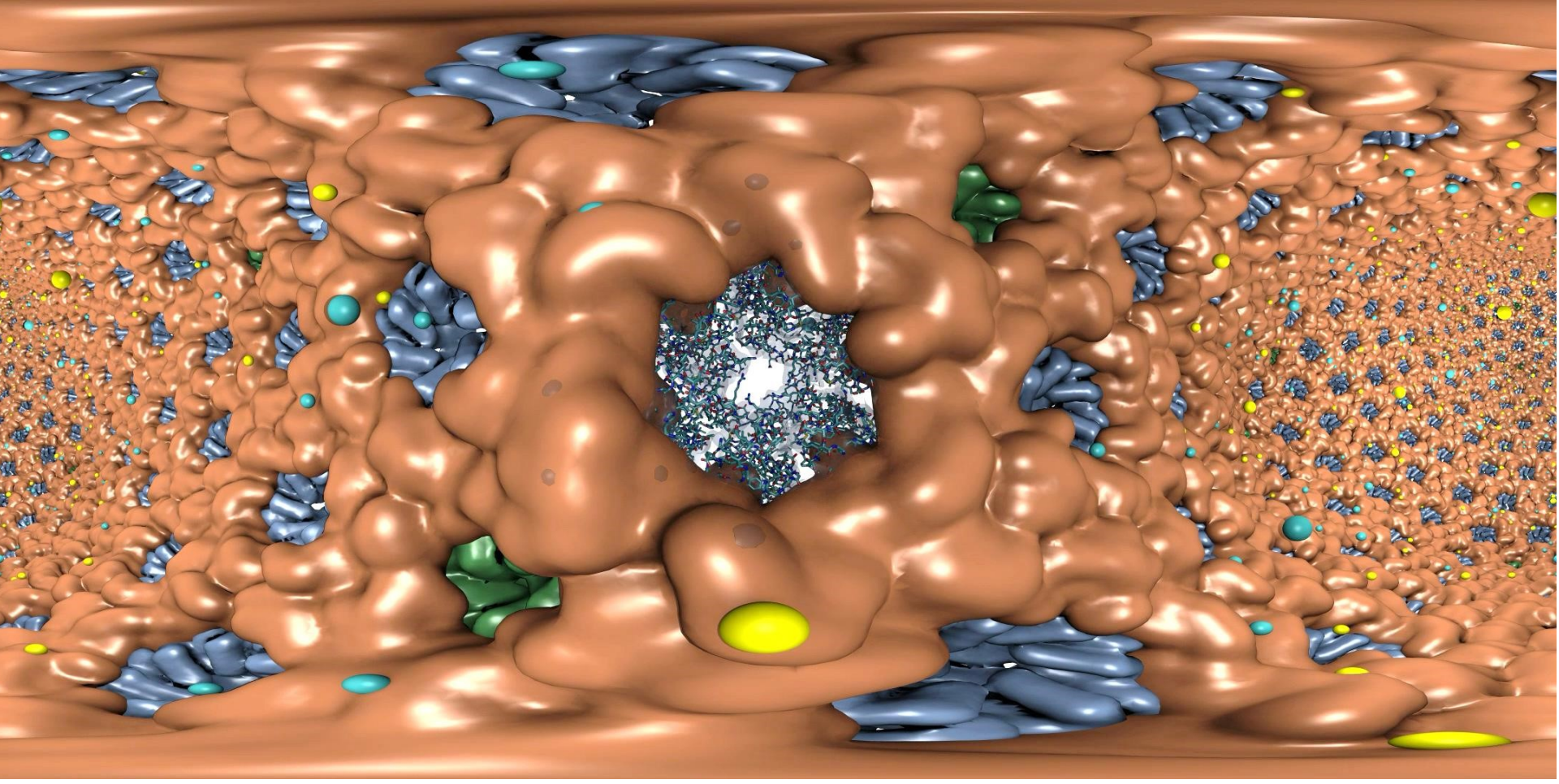
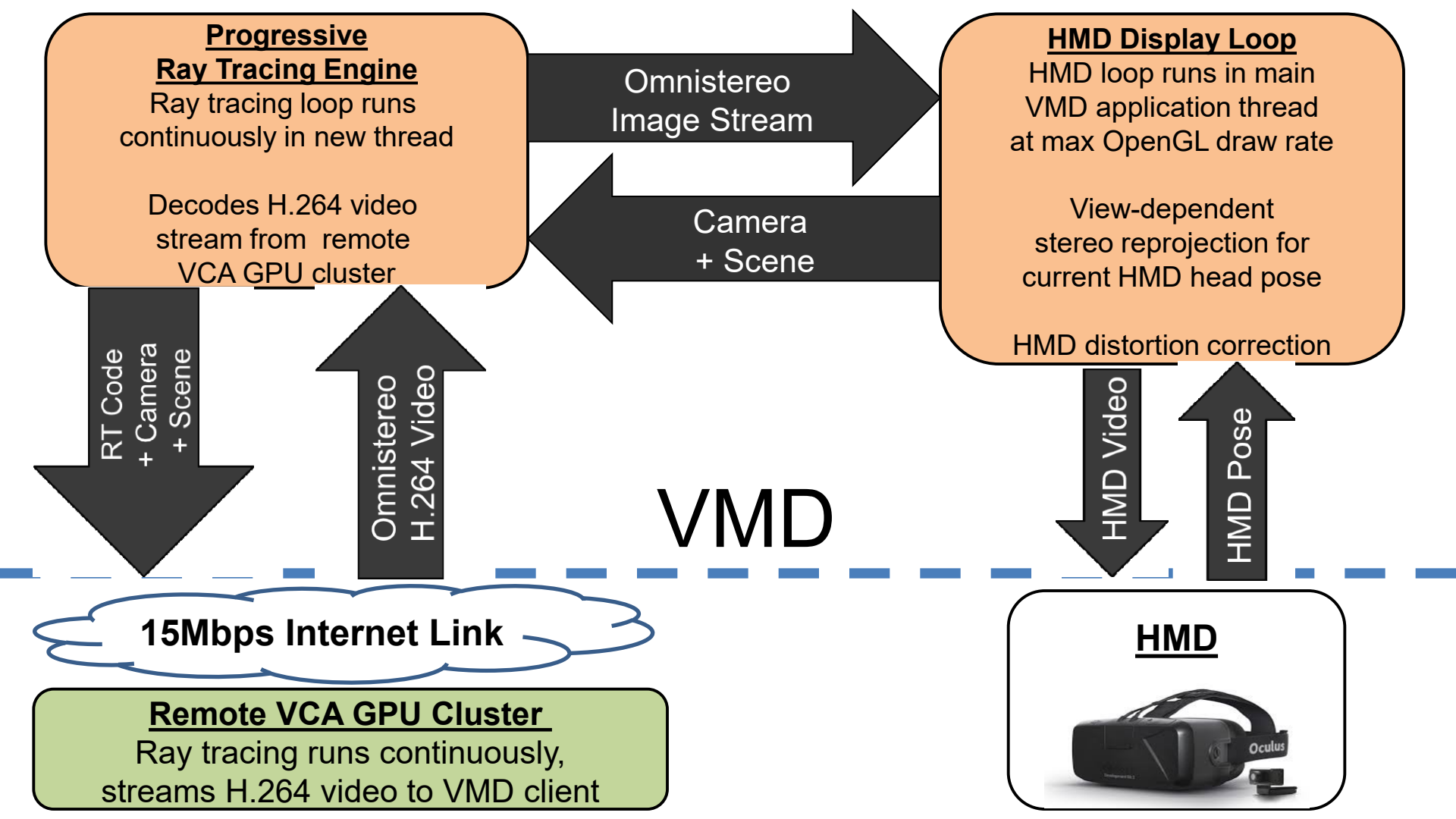


Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …



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
HMD Video
HMD Pose
VMD
15Mbps Internet Link
Remote VCA GPU Cluster
Ray tracing runs continuously, streams H.264 video to VMD client
HMD
Oculus

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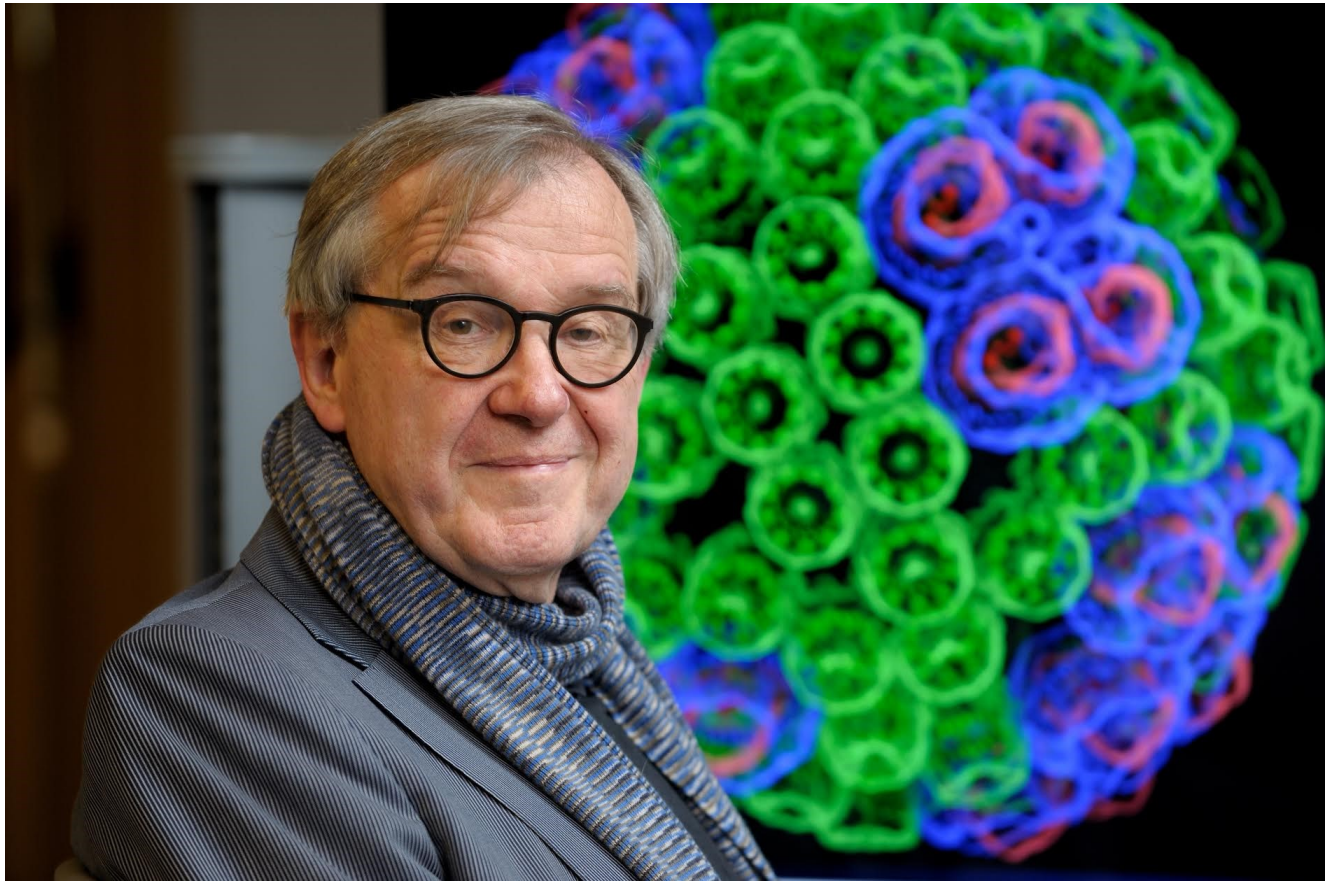
Ongoing VR Work

- 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, …

Acknowledgements

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



“When I was a young man, my goal was to look with mathematical and computational means at the inside of cells, one atom at a time, to decipher how living systems work. That is what I strived for and I never deflected from this goal.” – Klaus Schulten