VMD: Immersive Molecular Visualization and Interactive Ray Tracing for Domes, Panoramic Theaters, and Head Mounted Displays

John E. Stone

Theoretical and Computational Biophysics Group

Beckman Institute for Advanced Science and Technology

University of Illinois at Urbana-Champaign

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

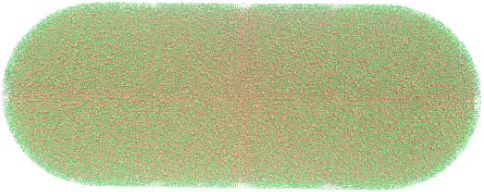
9:00am, Monday August 10, 2015

BOF: Immersive Visualization for Science and Research

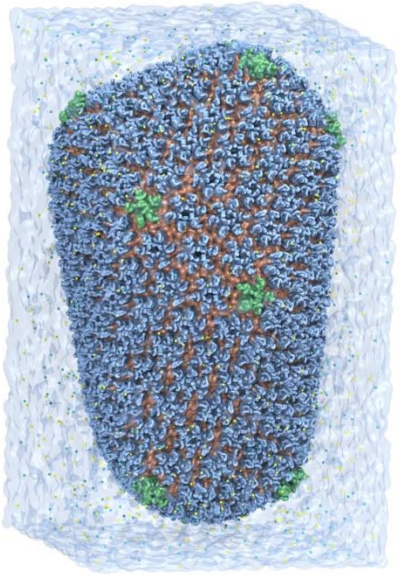
Siggraph 2015, Los Angeles, CA

VMD – “Visual Molecular Dynamics”

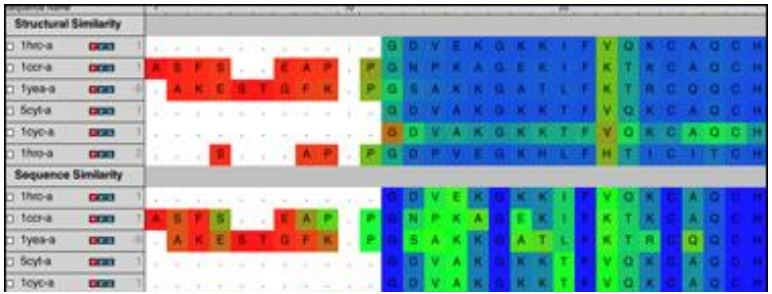
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



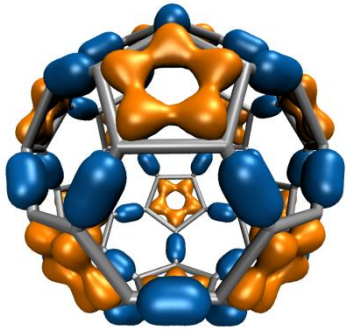
Whole Cell Simulation



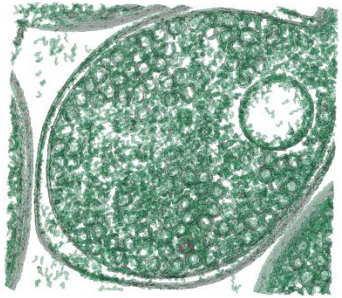
MD Simulations



Sequence Data



Quantum Chemistry

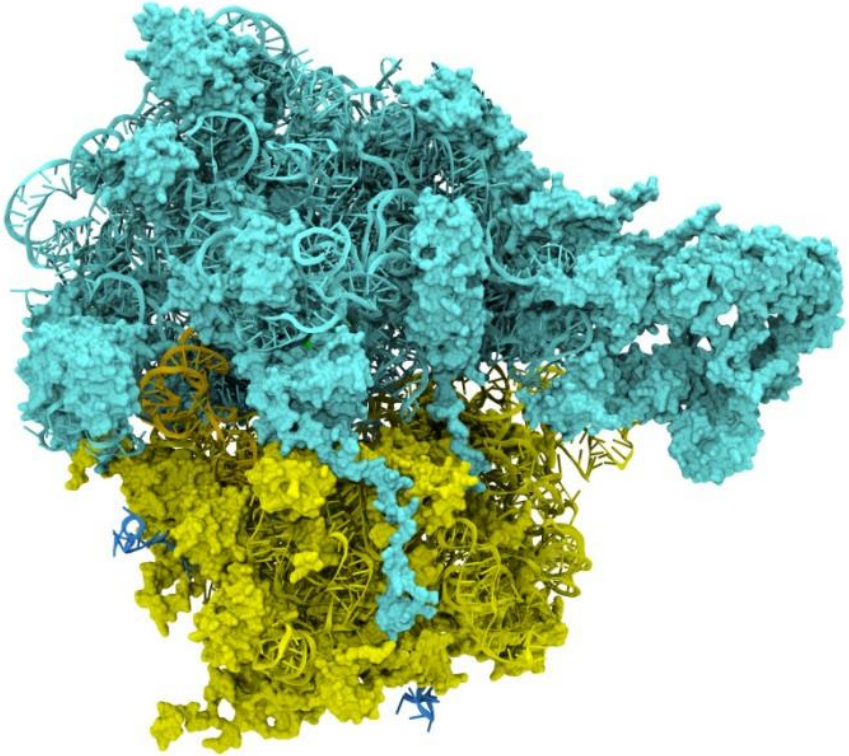


CryoEM, Cellular Tomography

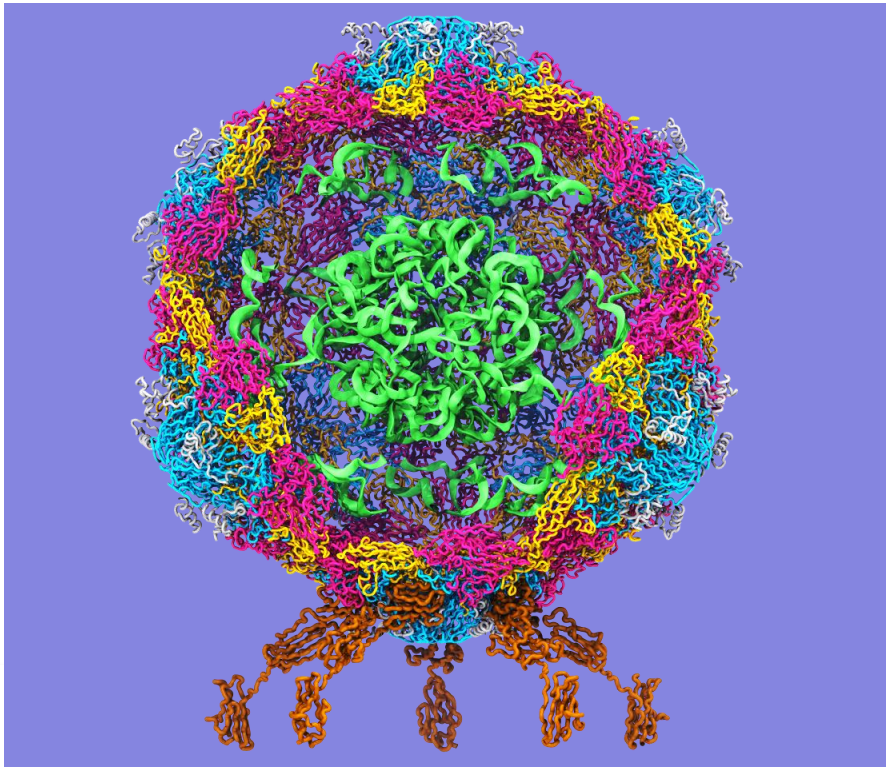
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus



VMD GPU-Accelerated Ray Tracing Engine

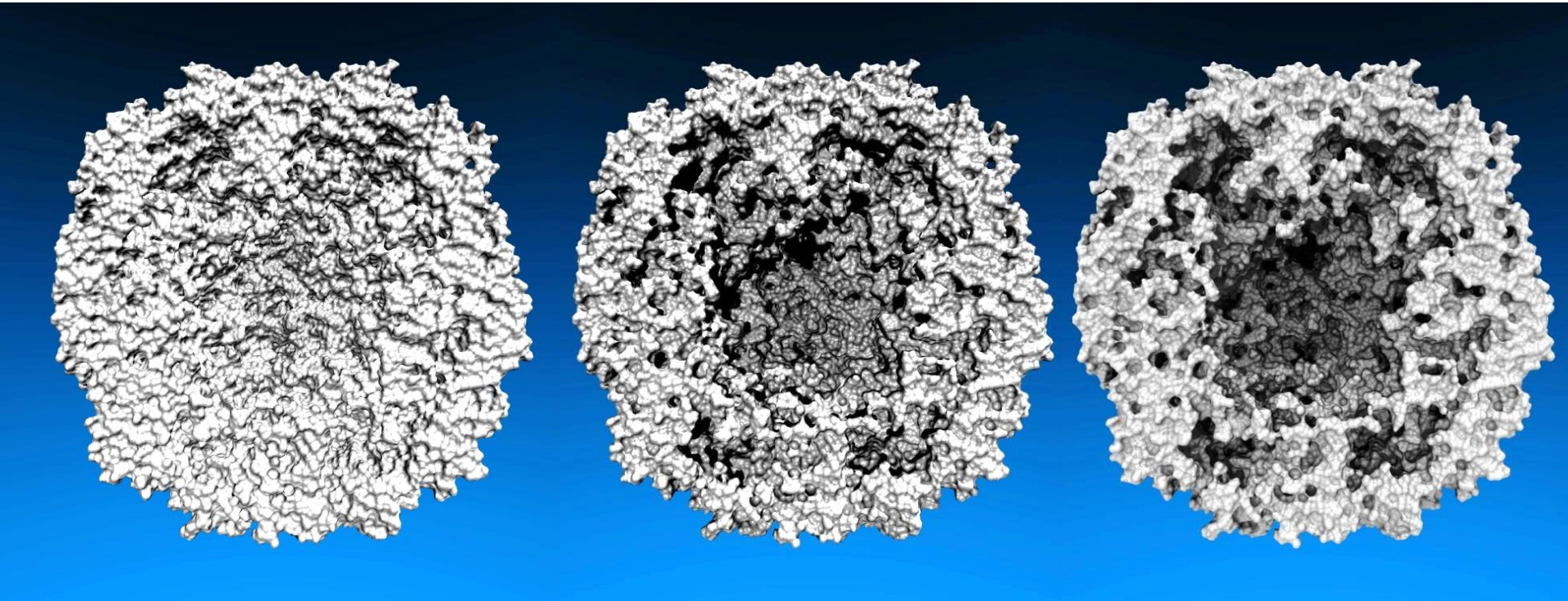
- Complementary to VMD OpenGL GLSL renderer
- Key ray tracing benefits:
  - Ambient occlusion lighting and shadows
  - High quality transparent surfaces
  - Depth of field focal blur and similar optical effects
  - Mirror reflection
  - Single-pass stereoscopic rendering
  - Special panoramic and 360° cameras:
    - Planetarium dome master format
    - Equirectangular spheremap projections
    - Cubemap projections

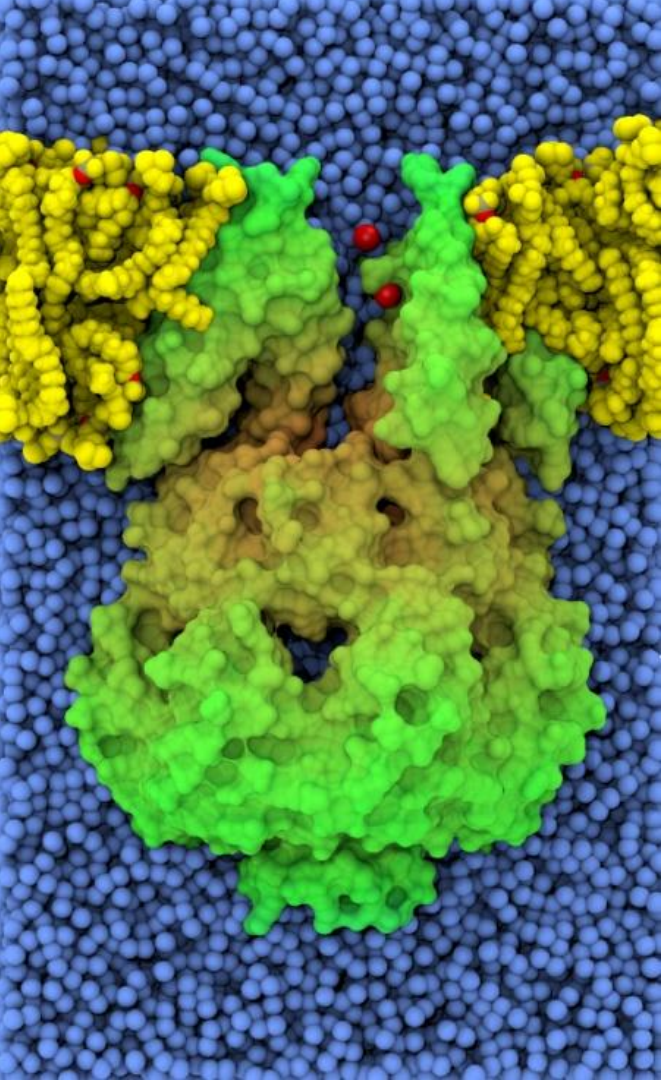
Lighting Comparison

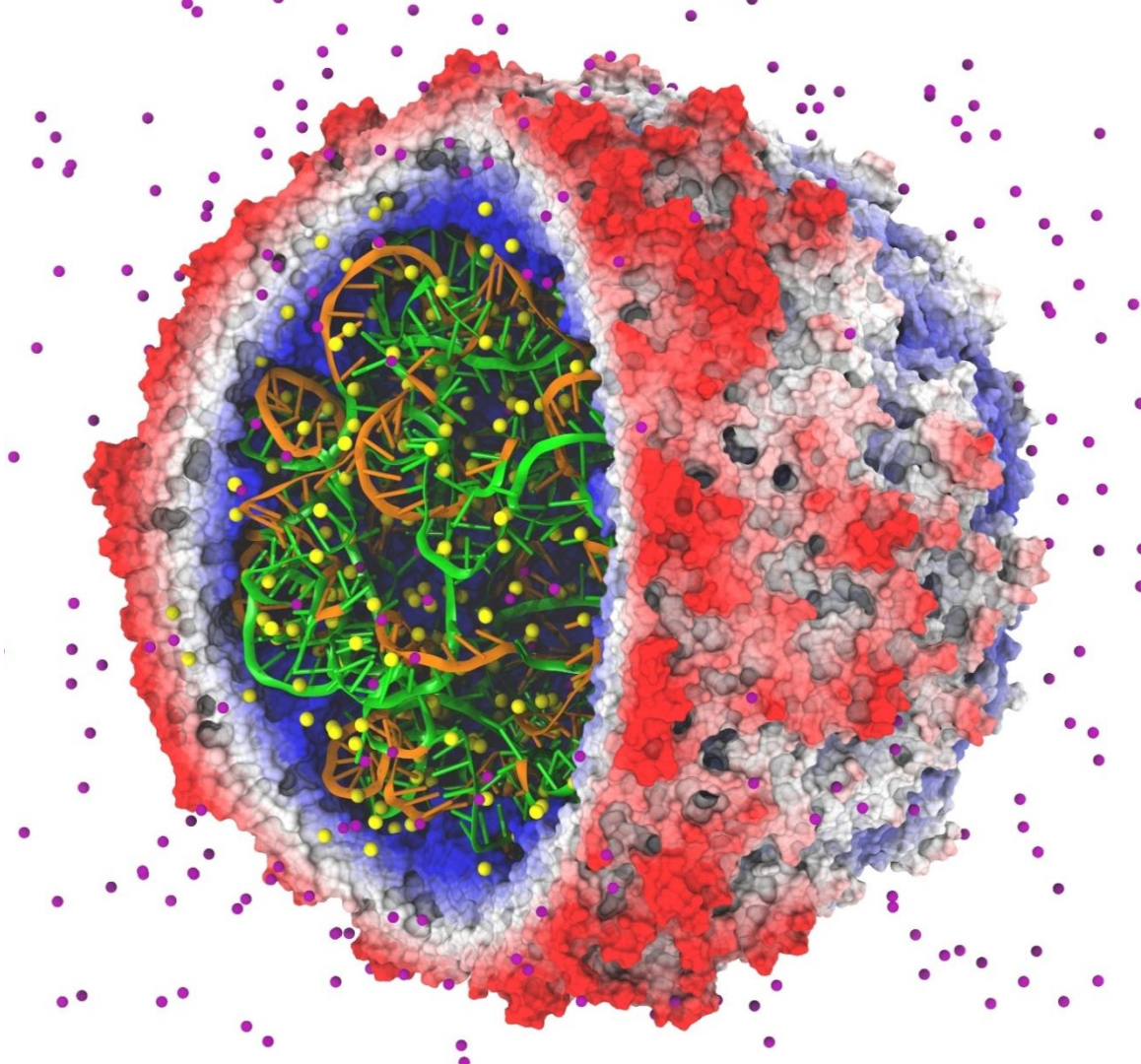
Two lights, no shadows

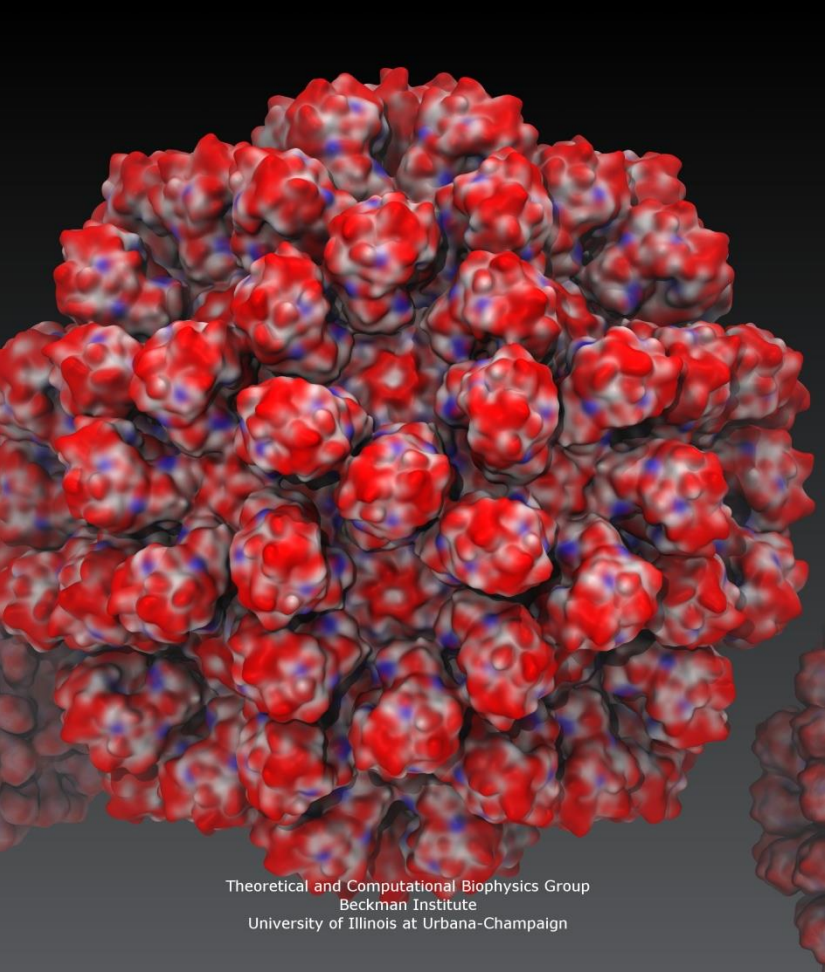
Two lights, hard shadows, 1 shadow ray per light

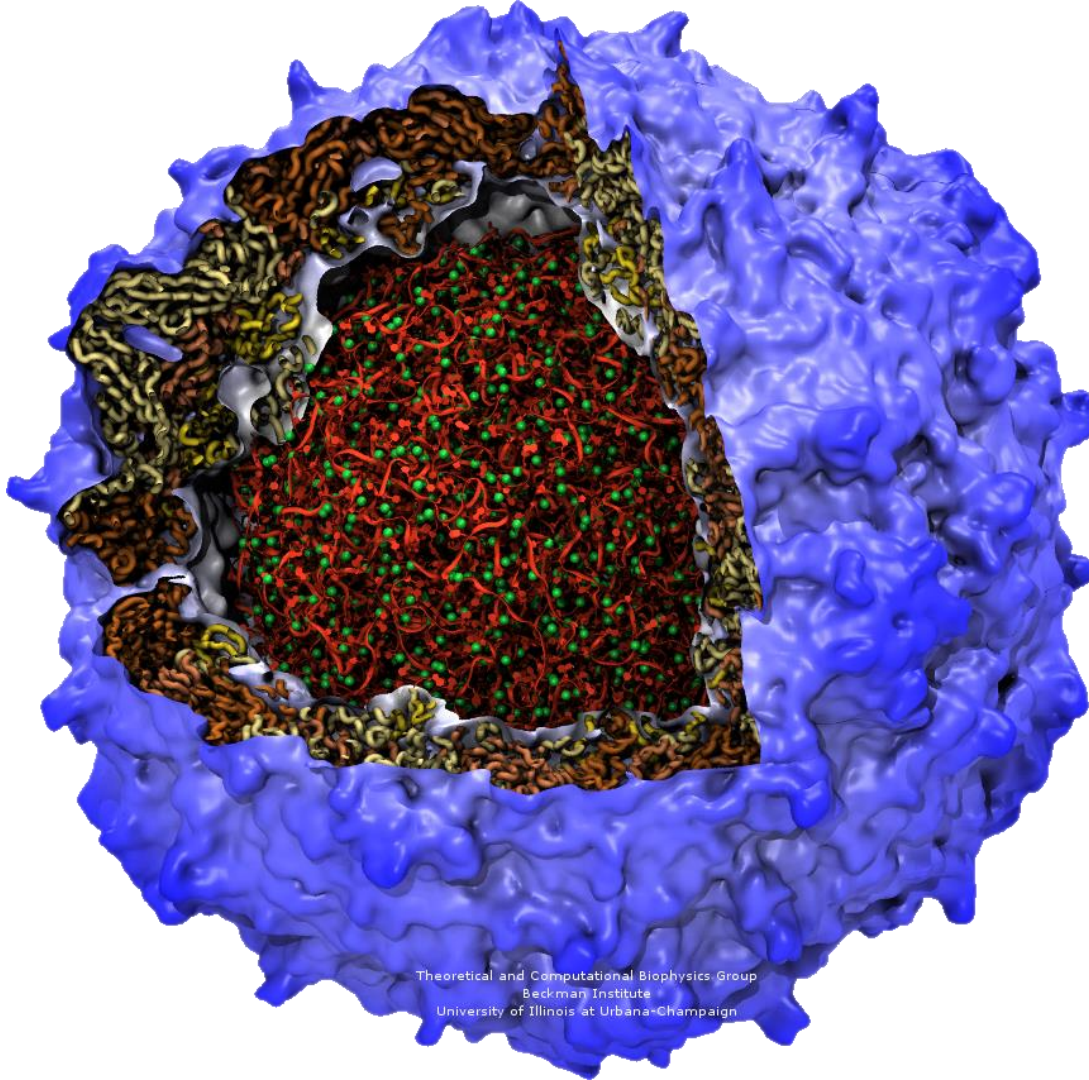
Ambient occlusion + two lights, 144 AO rays/hit

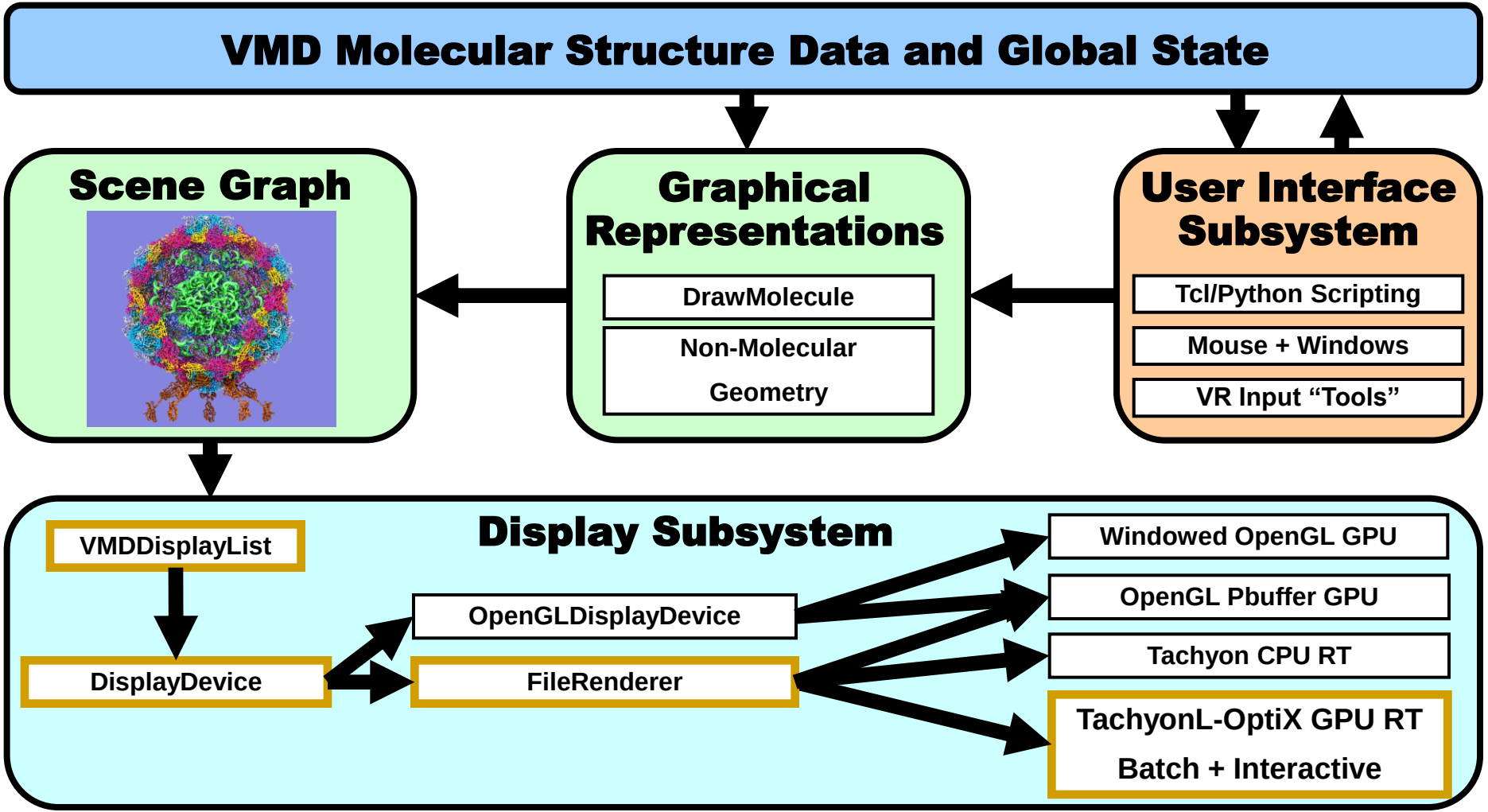






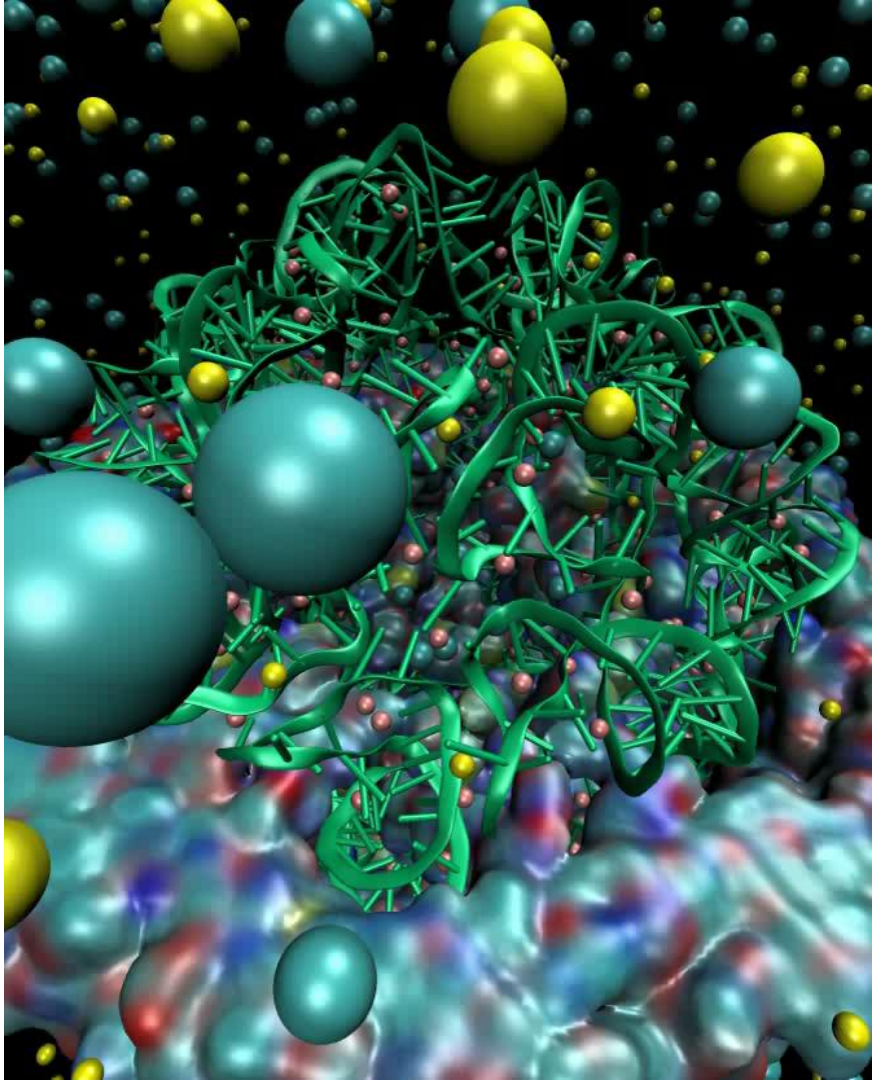

Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign


Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

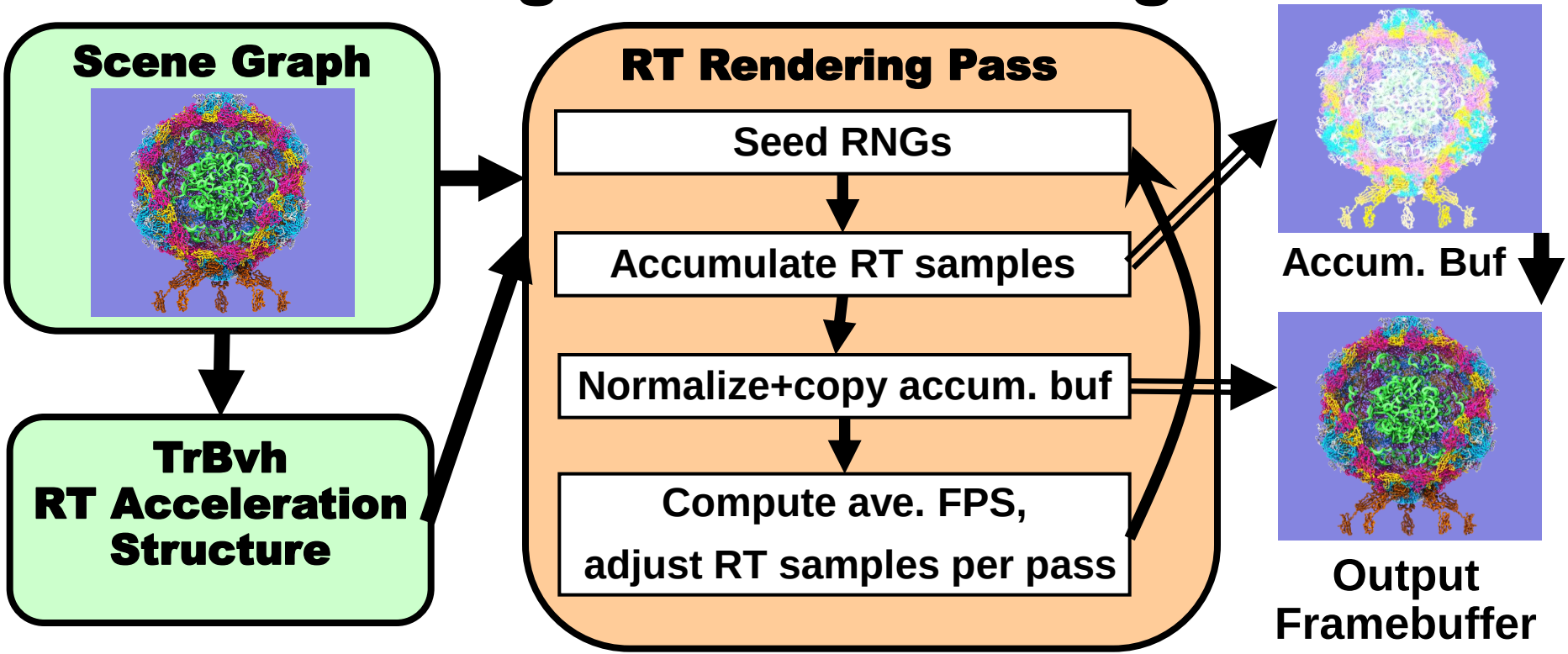

VMD Molecular Structure Data and Global State
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR Input “Tools”
Display Subsystem
VMDDisplayList
DisplayDevice
OpenGLDisplayDevice
FileRenderer
Windowed OpenGL GPU
OpenGL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

VMD Interactive GPU Ray Tracing

- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides – ***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers
- **Movie was recorded live while using remote visualization**

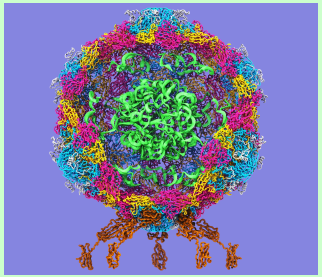


VMD TachyonL-OptiX Interactive RT w/ Progressive Rendering



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

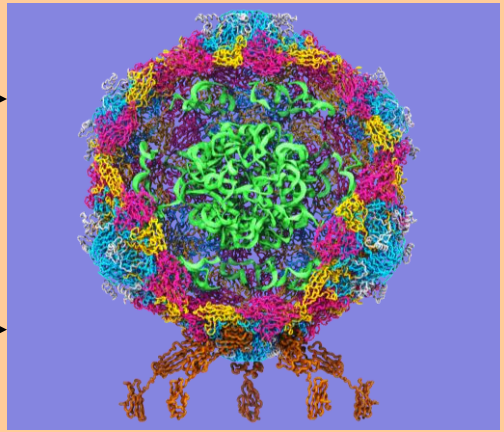
VMD Scene



Scene Data Replicated, Image Space / Sample Space Parallel Decomposition onto GPUs

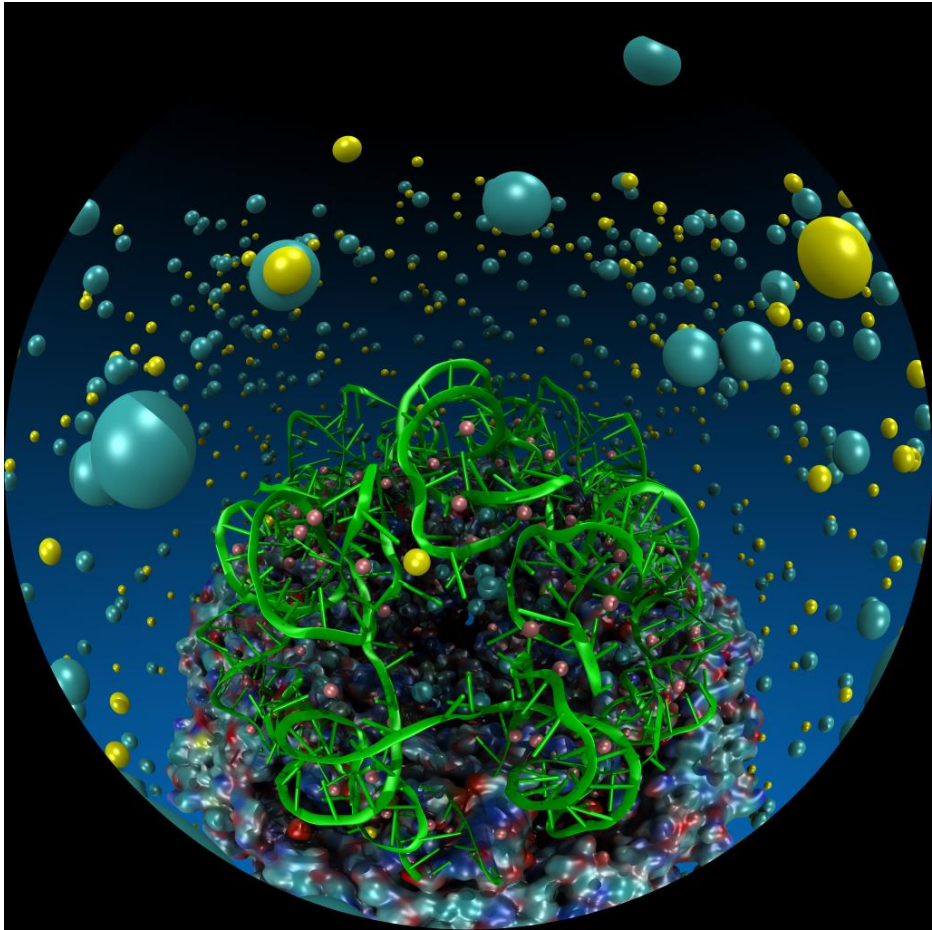
VCA 0:
8 K6000 GPUs

VCA N:
8 K6000 GPUs

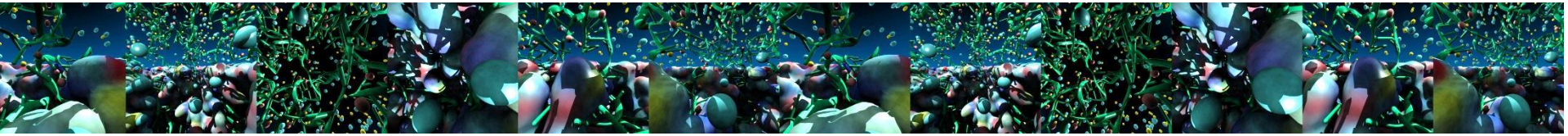


VMD Planetarium Dome Master Camera

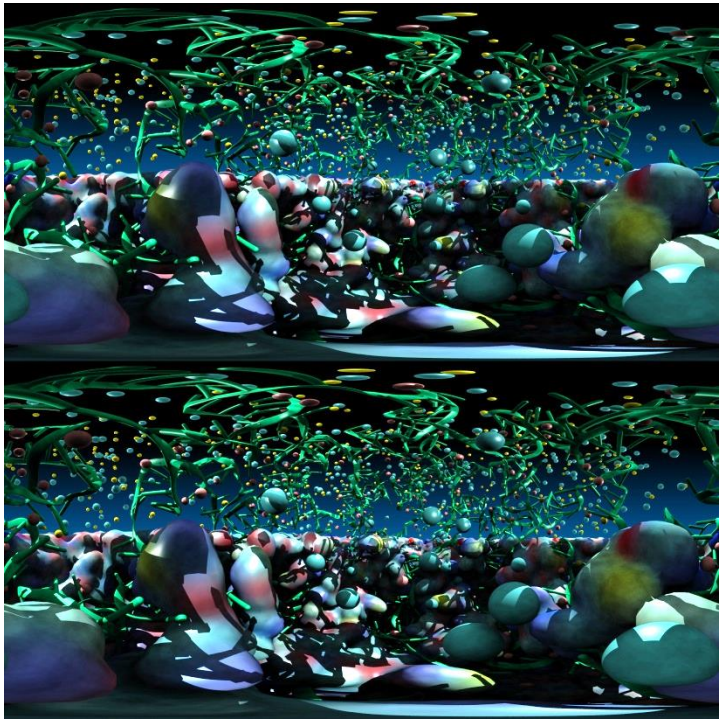
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required



Stereoscopic Panorama Ray Tracing w/ OptiX

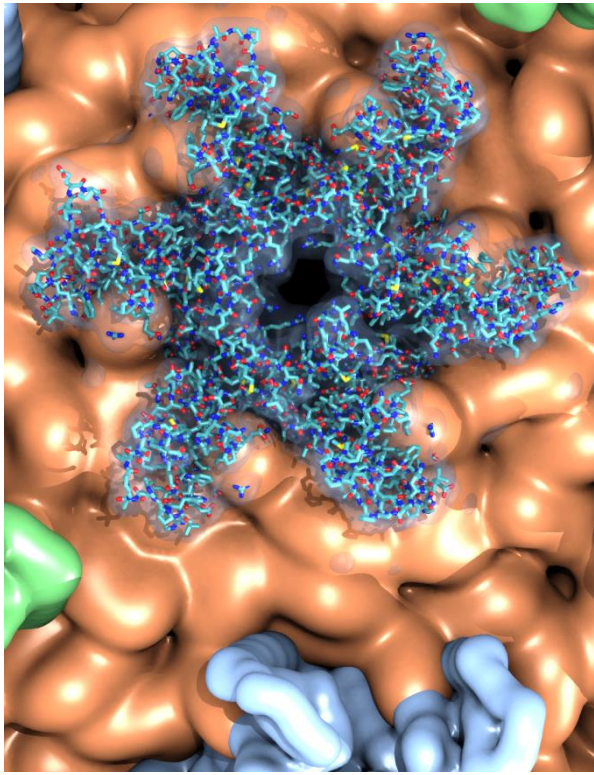


- Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard
- Ray trace panoramic stereo spheremaps, cubemaps that are displayed on to VR headset via OpenGL texturing
- Stereo requires spherical camera projection not well suited to rasterization
- Benefits from OptiX multi-GPU rendering, and load balancing



Future Work

- Further integration of interactive ray tracing into VMD
  - Seamless interactive RT in main VMD display
  - Support trajectory playback in interactive RT
  - Multi-node interactive RT on HPC systems
- Improved performance / quality trade-offs in interactive RT stochastic sampling strategies
- Optimize GPU scene DMA and BVH regen speed for time-varying geometry, e.g. MD trajectories
- Optimization of GPU-specific RT intersection routines, memory layout
- GPU-accelerated movie encoder back-end
- Interactive RT combined with remote viz on HPC systems, much larger data sizes



GPU Ray Tracing of HIV-1 Capsid Detail

Acknowledgements

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

Research Publications

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

- **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.
- **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.
- **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.
- **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.

NIH BTRC for Macromolecular Modeling and Bioinformatics
1990-2017
Beckman Institute
University of Illinois at
Urbana-Champaign