Interactive Supercomputing for State-of-the-art Biomolecular Simulation

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

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

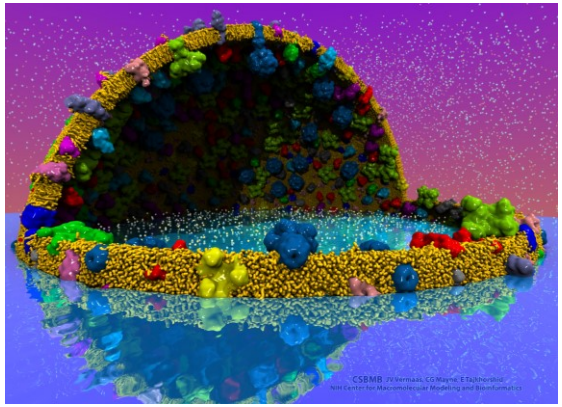
Interactivity in Supercomputing BoF,

12:15pm-1:15pm, Rooms 503-504, Colorado Convention Center

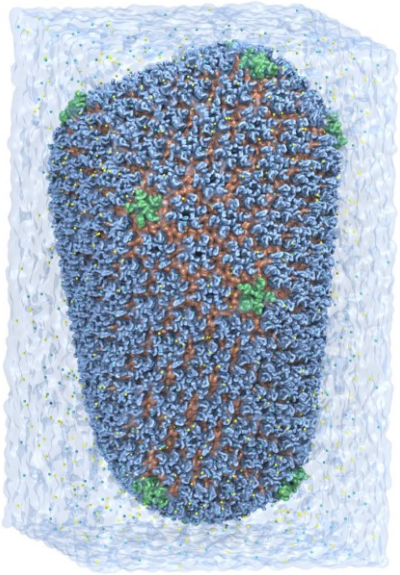
Denver, CO, Tuesday Nov 14th, 2017

VMD – “Visual Molecular Dynamics”

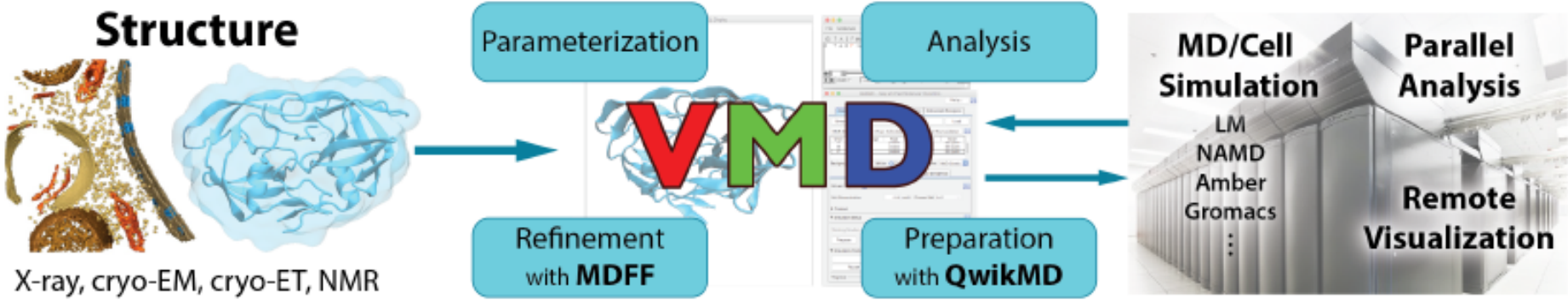
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Sequence information
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



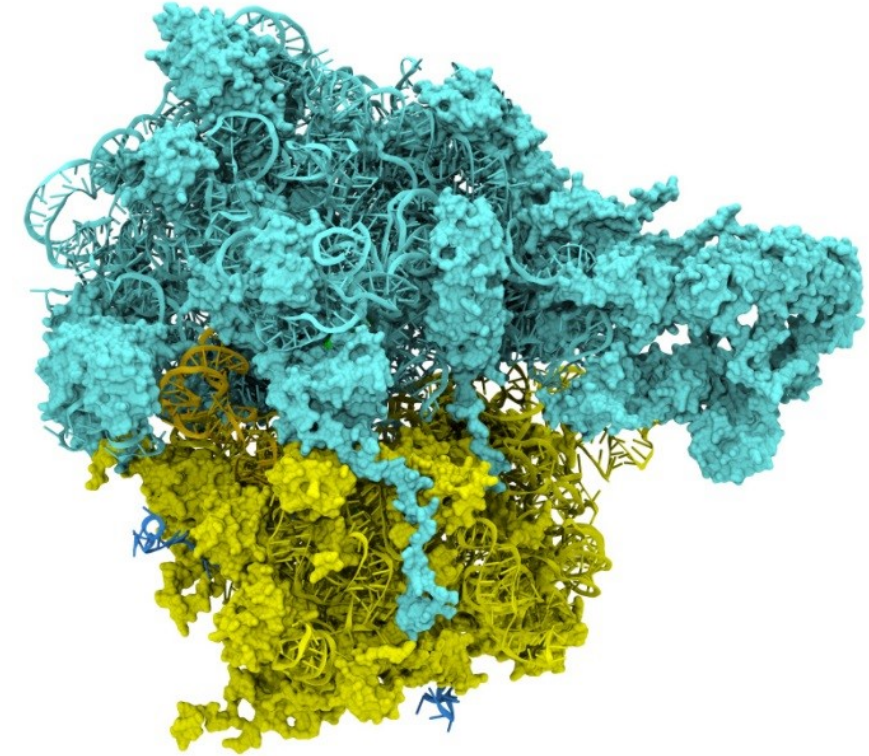
MD Simulation



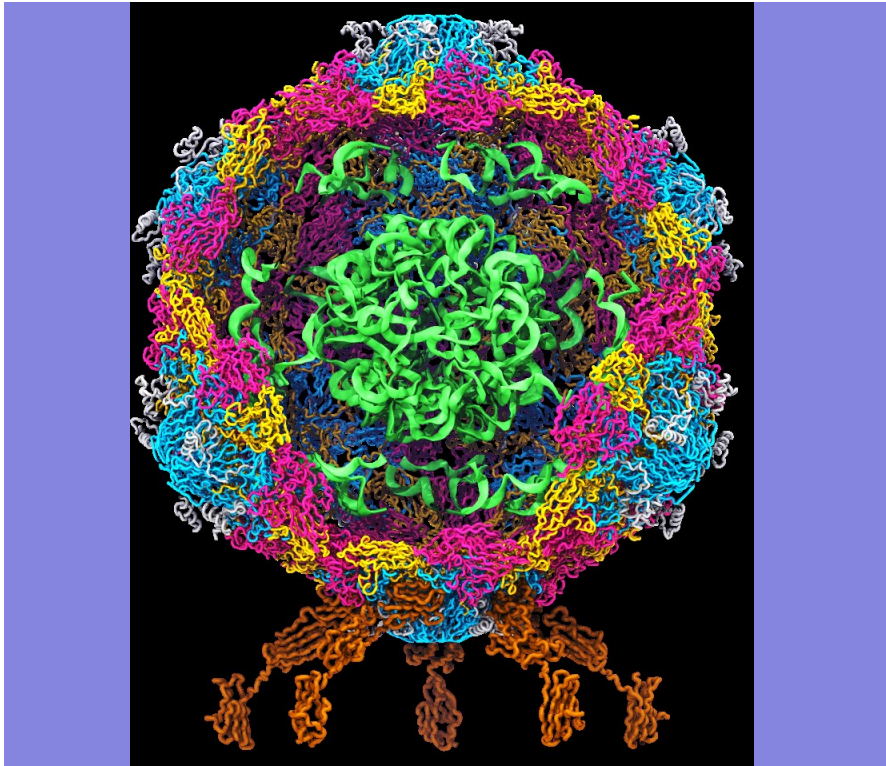
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

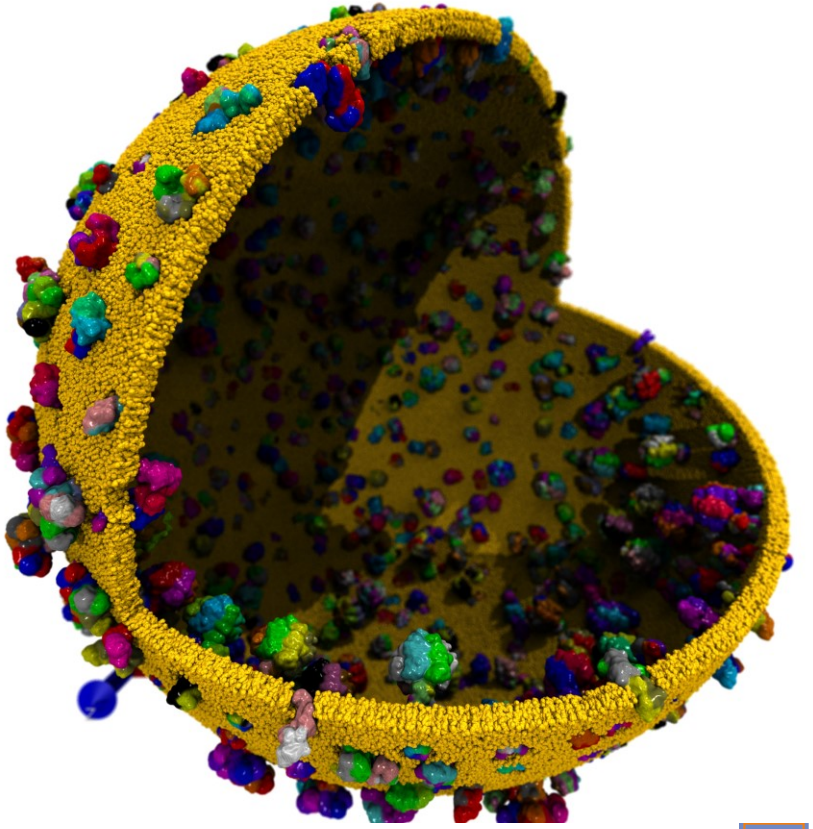


How Does Interactivity in HPC Benefit Scientific Productivity

- Until 2008, MD simulation performance was the major limiting factor on biomolecular modeling productivity, maybe 95% factor
- **In 2017: Batch MD sim code performance is likely only a 50% factor on overall scientific productivity**
- **An extremely simplified outline:**
  - Months or years of science team effort go into preparing state-of-the-art biomolecular simulations w/ experimental structures before MD sims begin
  - **During the initial and early phases of a simulation campaign, hundreds of modeling problems must be identified and addressed**
  - **Interactivity is a fundamental requirement during these phases**
  - After sim campaign has produced required outputs, extensive analytical work begins, and science teams then make key decisions about outcomes, potentially conducting further sim studies, developing manuscripts with detailed analyses, figures, and movies of dynamics of systems under study

Proto-Cell Modeling Project

- Initial model of minimal cell membrane and proteins
- Candidate for our ORNL Summit early science project
- **~1 billion atoms** presently with explicit water, ions, etc.
- Main structure file used for modeling and simulation tasks is currently **~60GB**
- Initial simulation preparation requires **many repeated build / viz / measure / simulate cycles…**
- MD trajectory output : **~12GB/frame**
- **Need to run all tools required for science campaign at remote supercomputer sites:**
  - **Optimize work-efficiency of science team**
  - **Not just NAMD and VMD, but also other tools**
- **Old approach** of repeatedly transferring files back and forth between UIUC lab and remote supercomputers **is untenable at this scale!!!**



What Do We Need?

- **Science campaign "Bullpen" interactive compute/viz**
- Interactive resources supporting the **human-intensive** parts of science team activities
- Specific examples:
  - **Interactive remote visualization** supporting use **of arbitrary science tools**, including those that are **not traditional HPC tools** (e.g. CryoEM and X-Ray crystallography pkgs)
  - **Special batch queues, or queue policies** that support the initial and early phase of simulation bring-up activities, so that **meso-scale interactive calculations** can be performed **"at a mouse click"** to provide rapid-turnaround of results in interactive modeling sessions to correct flaws in molecular models, simulation parameters, etc.
  - A few (10s or less) HPC systems supporting **very large memory capacities** and d**ense GPU counts**, to run the **interactive supercomputing job "front end"**

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:

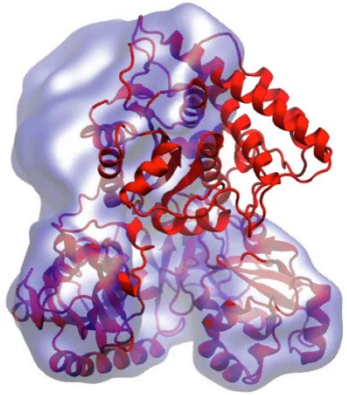
ORNL Titan, NCSA Blue Waters, Indiana Big Red II, CSCS Piz Daint, and similar systems

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

Molecular Dynamics Flexible Fitting (MDFF)

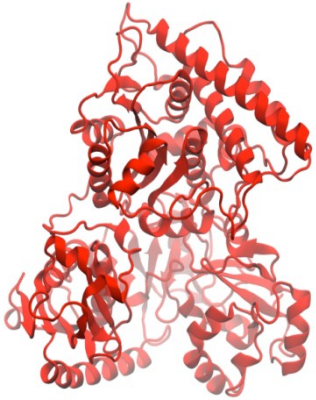
X-ray crystallography → MDFF ← Electron microscopy

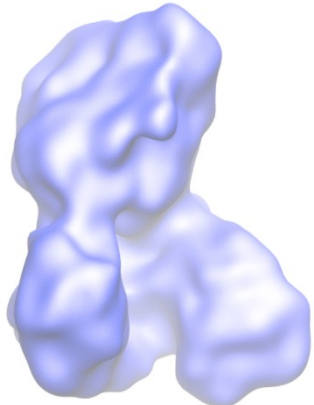
APS at Argonne



FEI microscope

ORNL Titan



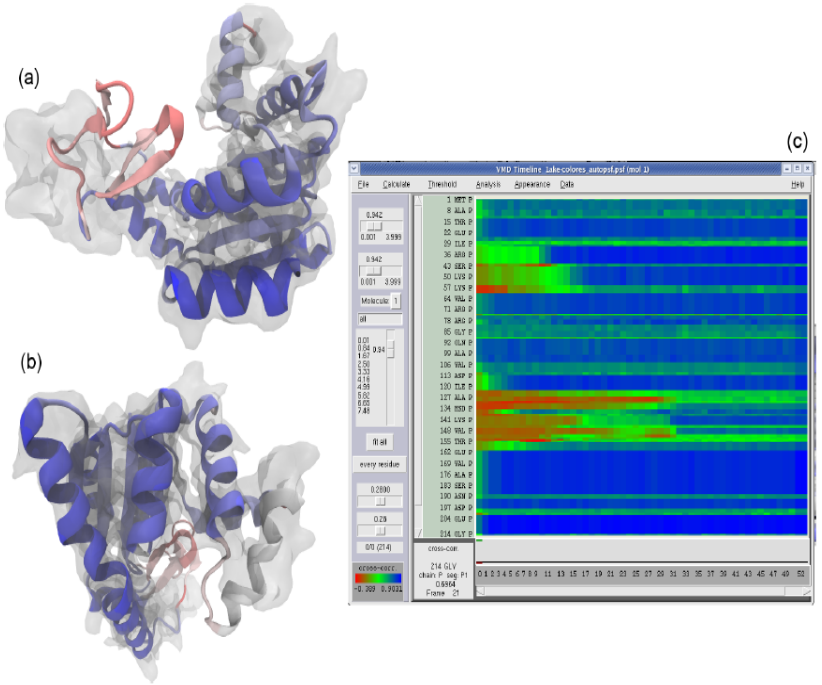


Molecular dynamics-based refinement and validation for sub-5Å cryo-electron microscopy maps. A. Singharoy, I. Teo, R. McGreevy, J. E. Stone, J. Zhao, and K. Schulten. eLife 2016;10.7554/eLife.16105

GPUs Can Reduce MDFF Trajectory Analysis Runtimes from Hours to Minutes

GPUs enable laptops and desktop workstations to handle tasks that would have previously required a cluster, or a *very long wait*…

GPU-accelerated petascale supercomputers enable analyses that were previously impractical, allowing detailed study of very large structures such as viruses

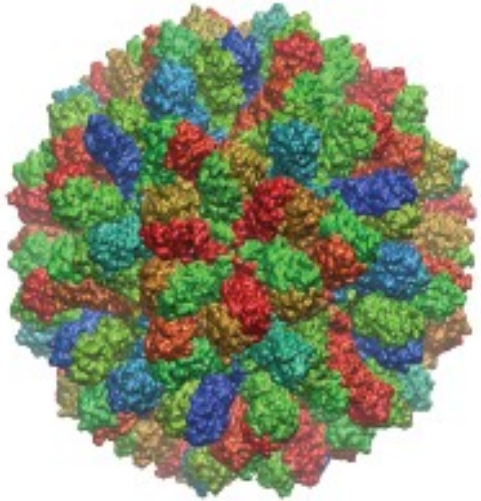


GPU-accelerated MDFF Cross Correlation Timeline

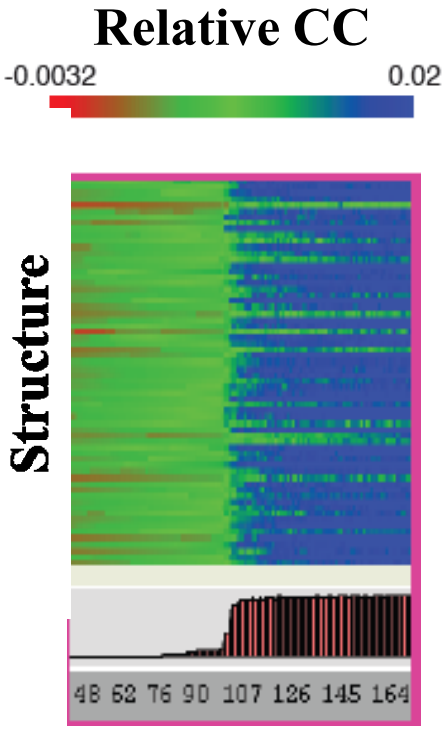
Regions with poor fit **Regions with good fit**

Parallel MDFF Cross Correlation Analysis on Cray XK7

Rabbit Hemorrhagic Disease Virus (RHDV)	
Traj. frames	10,000
Structure component selections	720
Single-node XK7 (projected)	336 hours (14 days)
128-node XK7	3.2 hours 105x speedup
2048-node XK7	19.5 minutes 1035x speedup



RHDV colored by relative CC



Calculation of 7M CCs would take **5 years** using serial CPU algorithm!

Stone et al., Faraday Discuss., 169:265-283, 2014.

VMD Tesla P100+V100 Cross Correlation Performance

Rabbit Hemorrhagic Disease Virus: 702K atoms, 6.5Å resolution

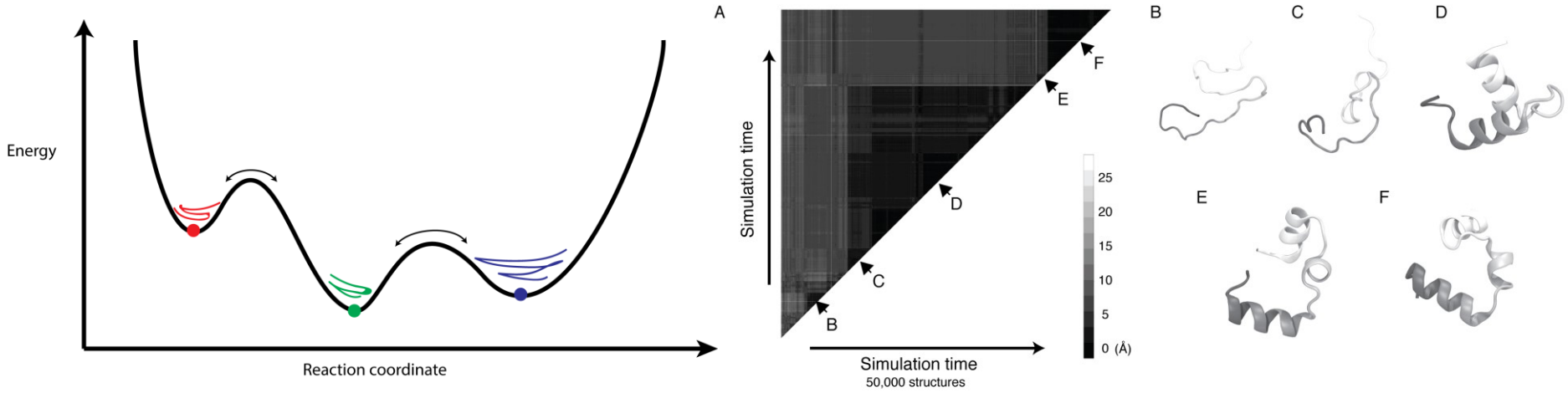
Latest results on Pascal P100, first runs on Volta V100

Hardware platform	Runtime, Speedup vs. Chimera,	VMD+GPU
Chimera Xeon E5-2687W (2 socket) [1]	15.860s, 1x	
VMD-CUDA IBM Power8 + 1x Tesla K40 [2]	0.488s, 32x	**0.9x**
VMD-CUDA Intel Xeon E5-2687W + 1x Quadro K6000 [1,2]	0.458s, 35x	**1.0x**
VMD-CUDA Intel Xeon E5-2698v3 + 1x Tesla P100	**0.090s,** 176x	**5.1x**
VMD-CUDA IBM Power8 "Minsky" + 1x Tesla P100	**0.080s,** 198x	**5.7x**
VMD-CUDA Intel Xeon E5-2697Av4 + 1x Tesla V100	**0.050s,** 317x	**9.2x**

[1] 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.

[2] 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, K. Schulten. International Workshop on OpenPOWER for HPC (IWOPH'16), LNCS 9945, pp. 188-206, 2016.

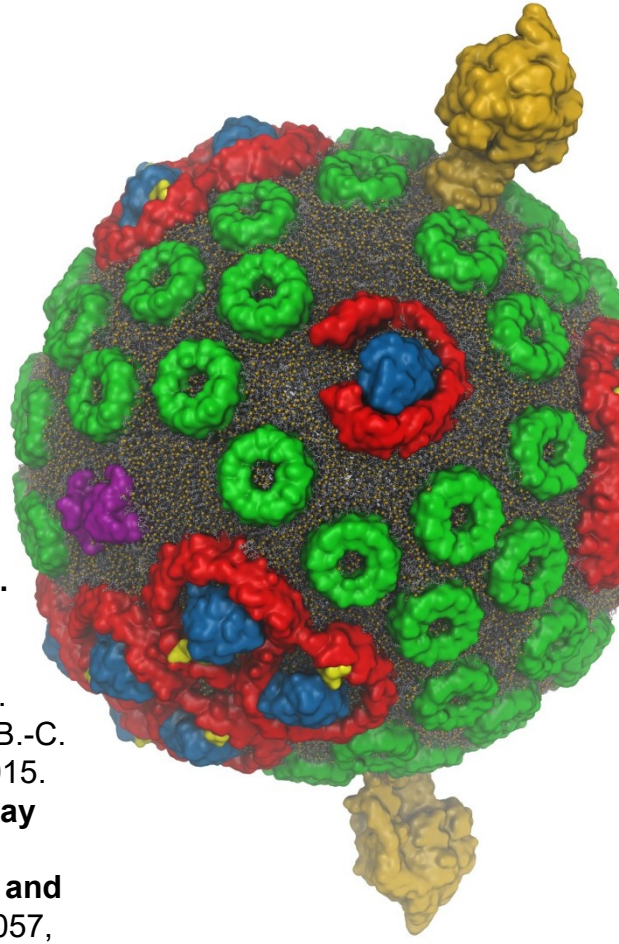
Clustering Analysis of Molecular Dynamics Trajectories



GPU-Accelerated Molecular Dynamics Clustering Analysis with OpenACC. J.E. Stone, J.R. Perilla, C. K. Cassidy, and K. Schulten. In, Robert Farber, ed., Parallel Programming with OpenACC, Morgan Kaufmann, Chapter 11, pp. 215-240, 2016.

Interactive Ray Tracing

- Remote visualization tasks on very large macromolecular complexes
- Large-scale parallel rendering: in situ or post hoc visualization tasks



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.

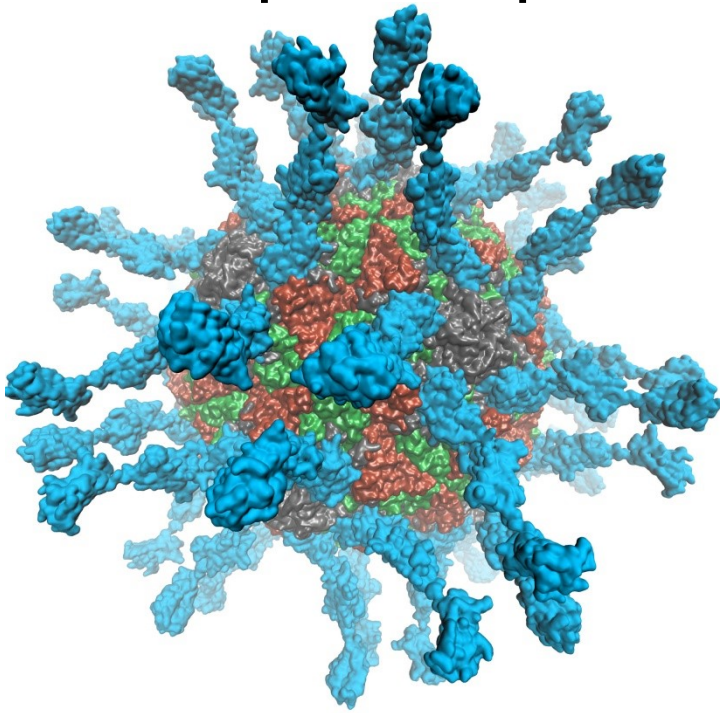
Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

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.

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

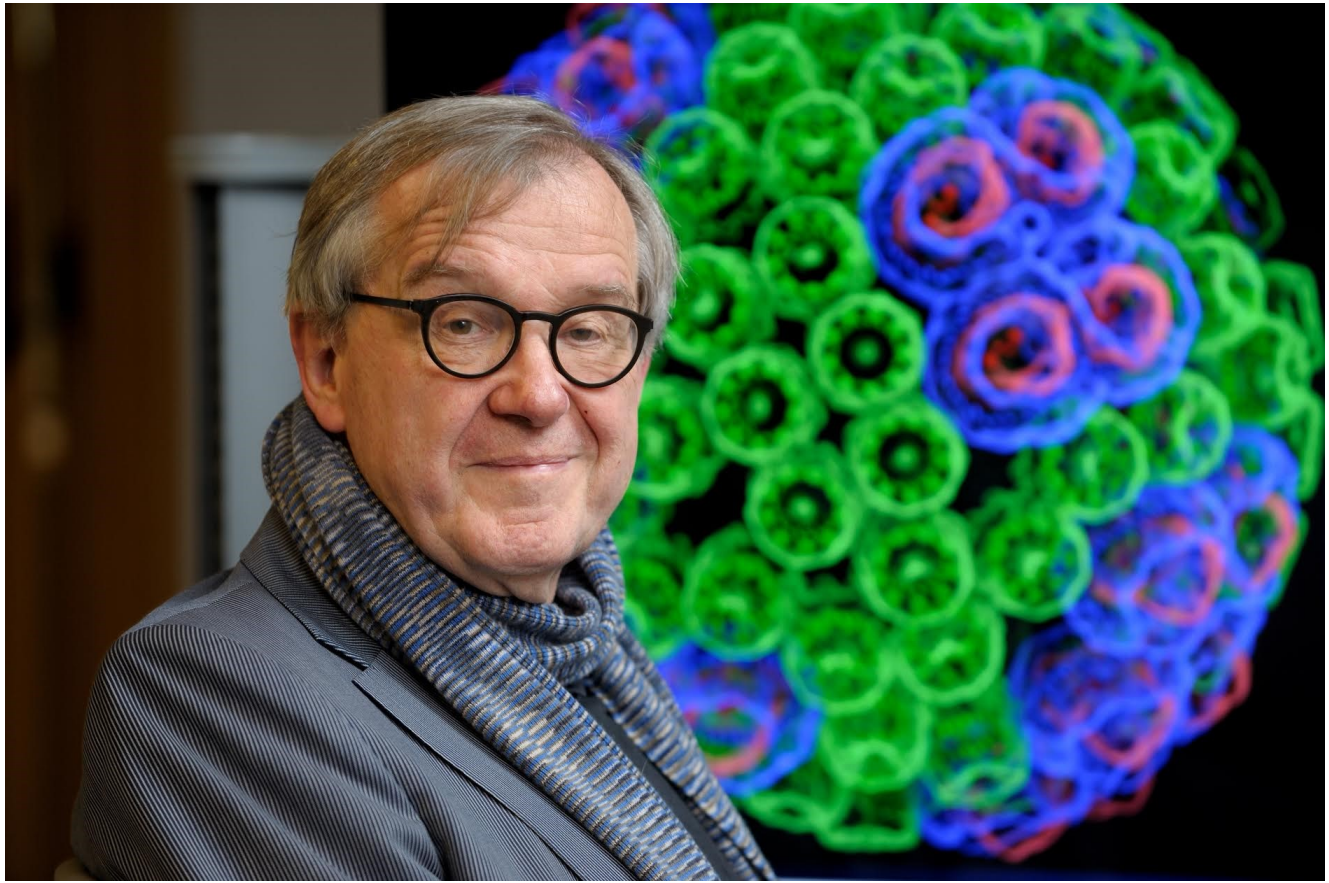
- Eliminate dependency on windowing systems
- Simplified deployment of parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features
- Support high-quality vendor-supported commercial OpenGL implementations in HPC systems that were previously limited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



Poliovirus

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



“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

Acknowledgements

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