S6253—VMD: Petascale Molecular Visualization and Analysis with Remote Video Streaming

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

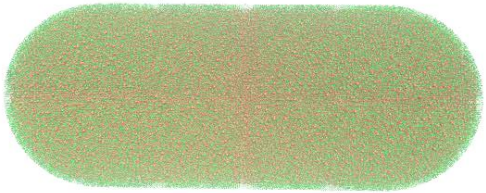
S6253, GPU Technology Conference

1:00pm-1:50pm, Room LL21D, San Jose Convention Center,

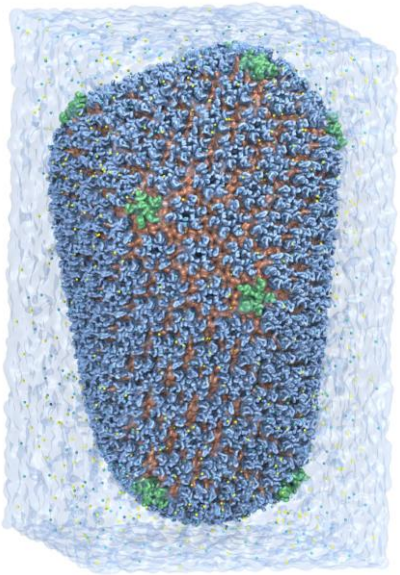
San Jose, CA, Tuesday April 5th, 2016

VMD – “Visual Molecular Dynamics”

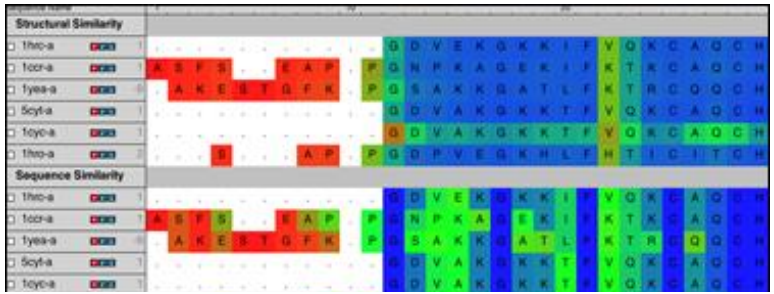
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



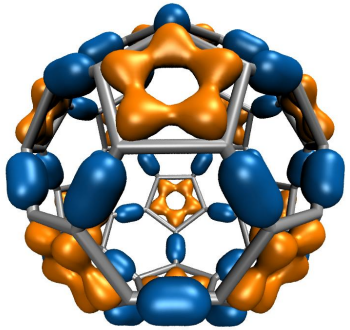
Whole Cell Simulation



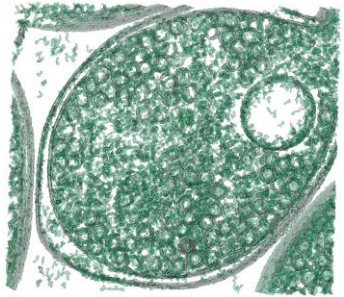
MD Simulations



Sequence Data



Quantum Chemistry

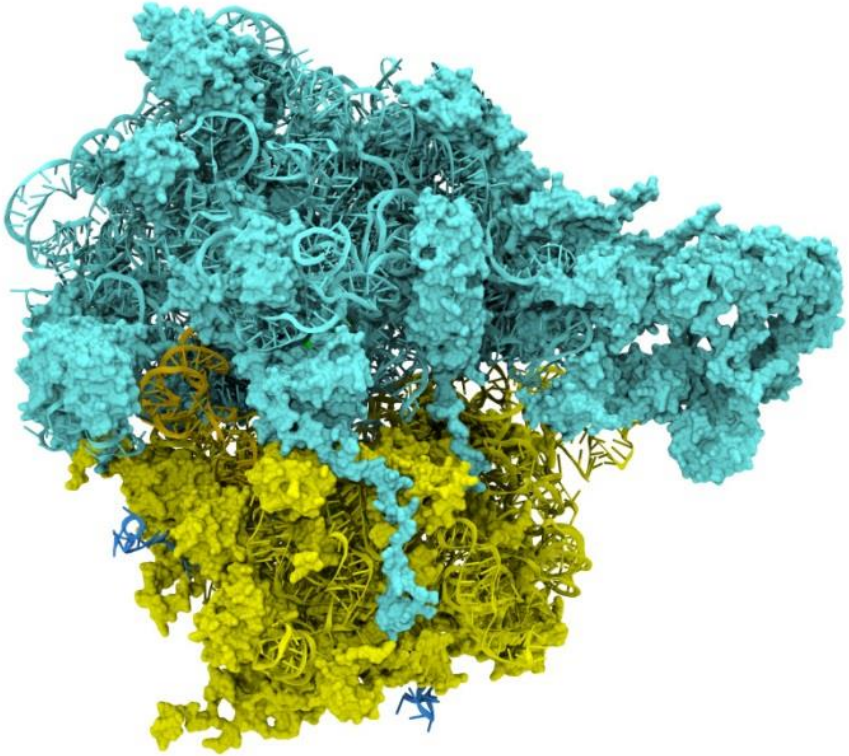


CryoEM, Cellular Tomography

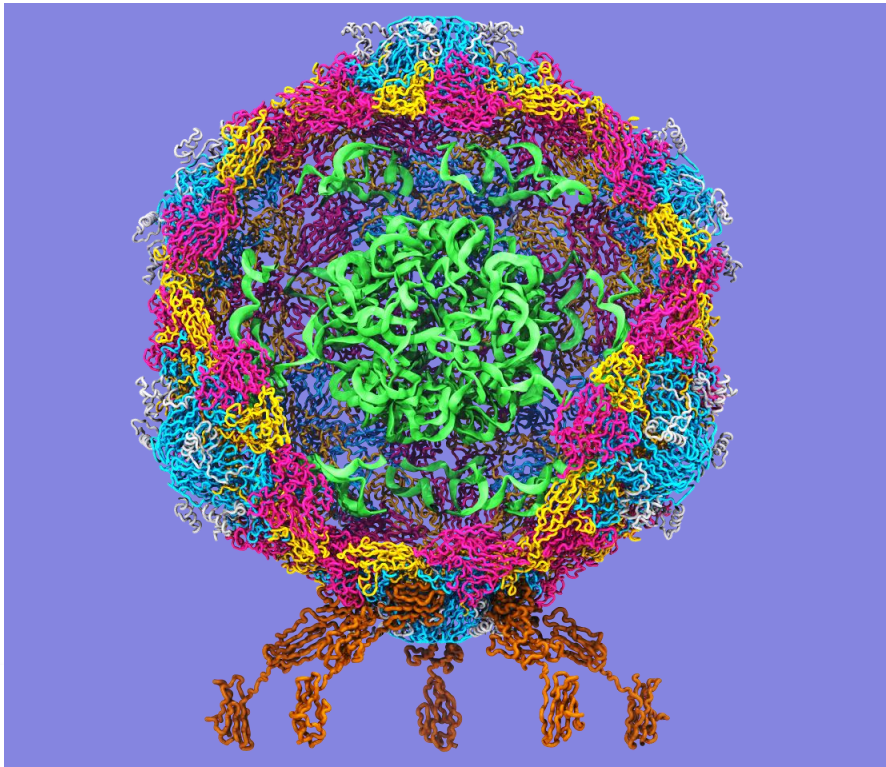
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

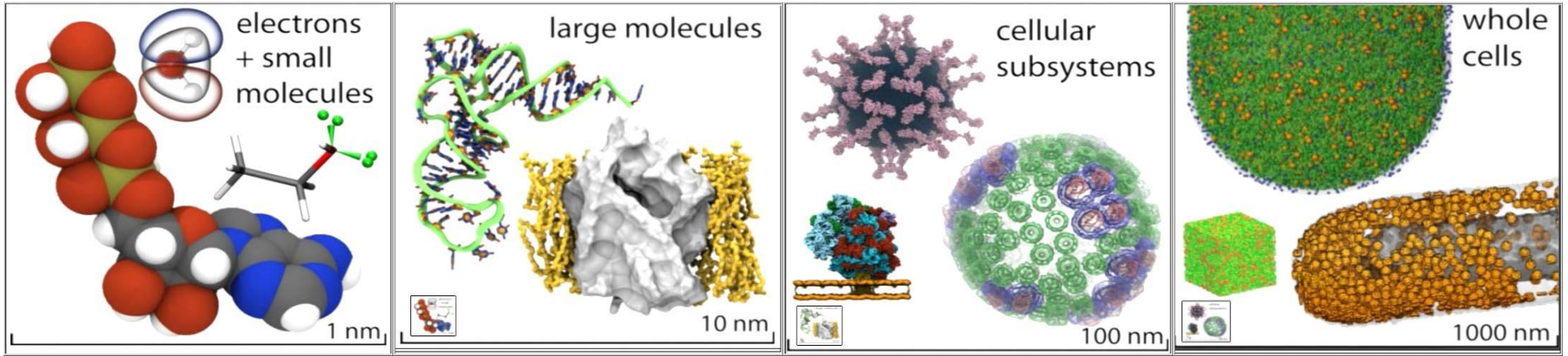


Poliovirus

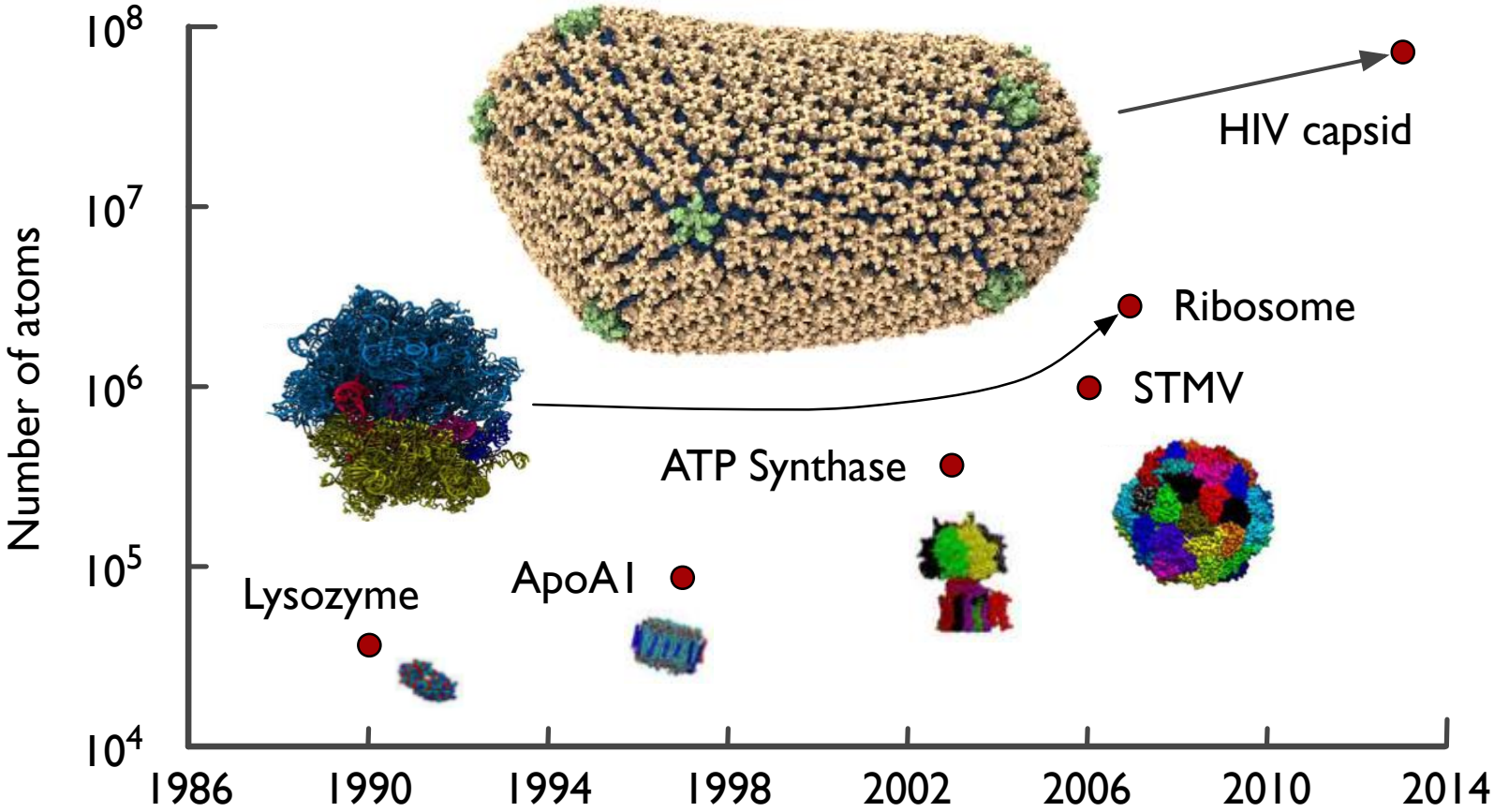


VMD Interoperability Serves Many Communities

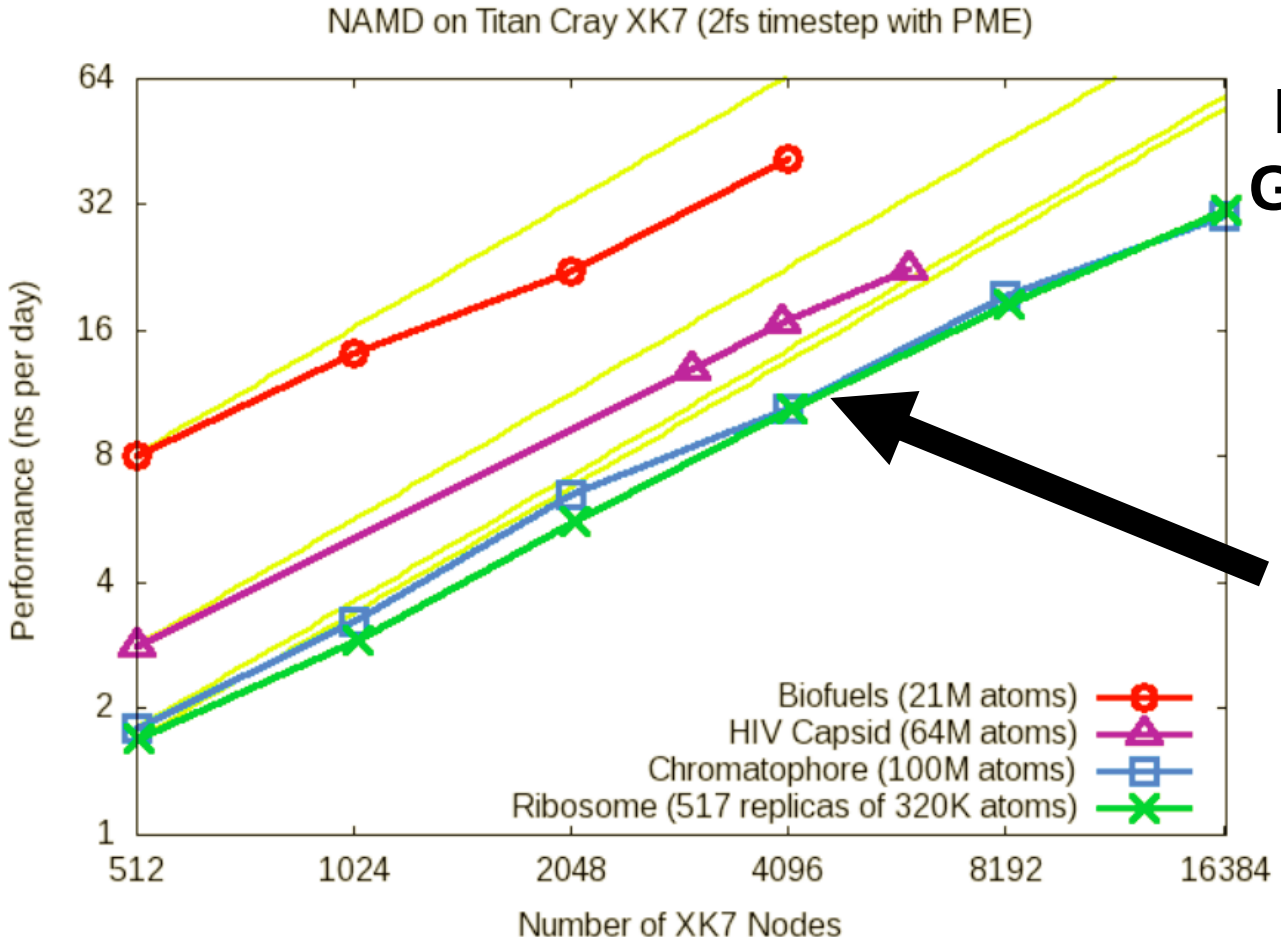
- Uniquely interoperable with a broad range of tools:
  - AMBER, CHARMM, CPMD, DL_POLY, GAMESS, GROMACS, HOOMD, LAMMPS, NAMD, and many more …
- Supports key data types, file formats, and databases
- Incorporates tools for simulation preparation, visualization, and analysis



NAMD and VMD Use GPUs and Petascale Computing to Meet Computational Biology's Insatiable Demand for Processing Power



NAMD Titan XK7 Performance August 2013



NAMD XK7 vs. XE6 GPU Speedup: 2x-4x

HIV-1 Trajectory: ~1.2 TB/day @ 4096 XK7 nodes

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!**

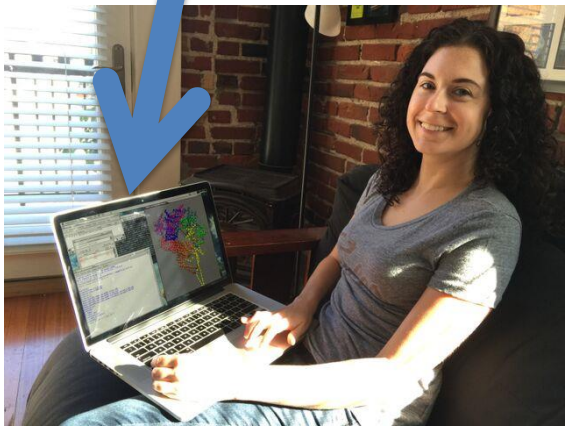
Parallel VMD currently available on:

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



Interactive Collaboration

- Enable interactive VMD sessions with multiple-endpoints
- Enable collaboration features that were previously impractical:
  - Remote viz. overcomes local computing and visualization limitations for interactive display

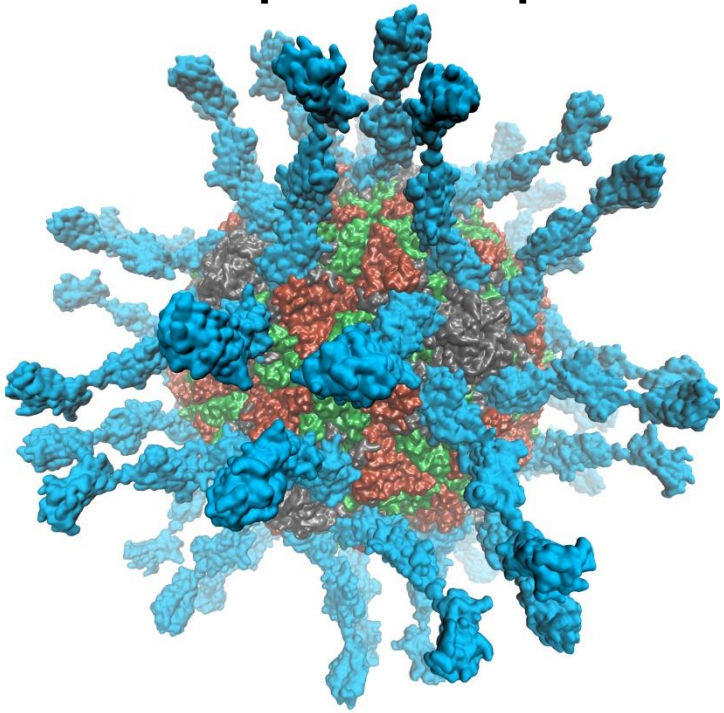
Supercomputer, MD Simulation

Experimentalist Collaborators Pittsburgh, PA

Urbana, IL

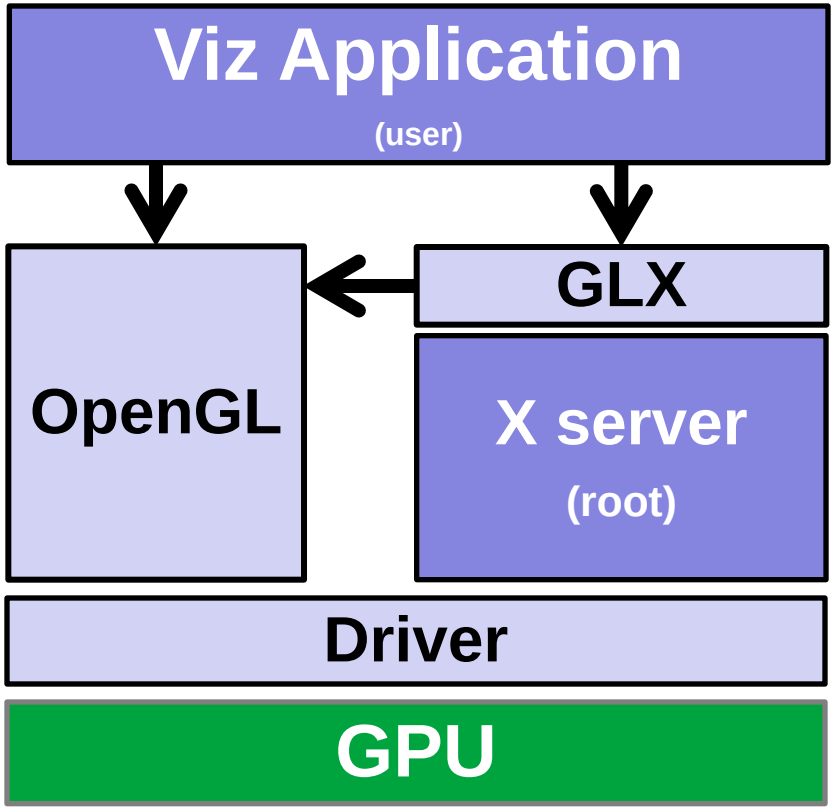
Adaptation of VMD to EGL for in-situ and parallel rendering on clouds, clusters, and supercomputers

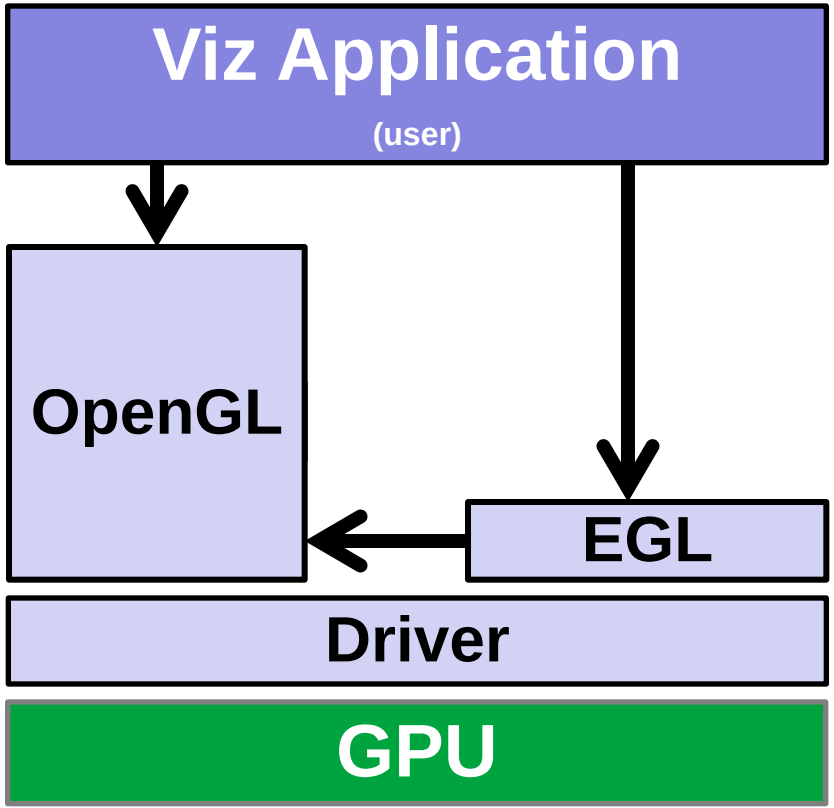
- Eliminate dependency on windowing systems
- Simplified deployment of parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features
- Support high-quality vendor-supported commercial OpenGL implementations in HPC systems that were previously limited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



Poliovirus

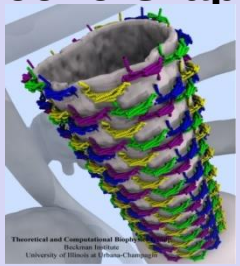
OpenGL: GLX vs. EGL





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”

Display Subsystem

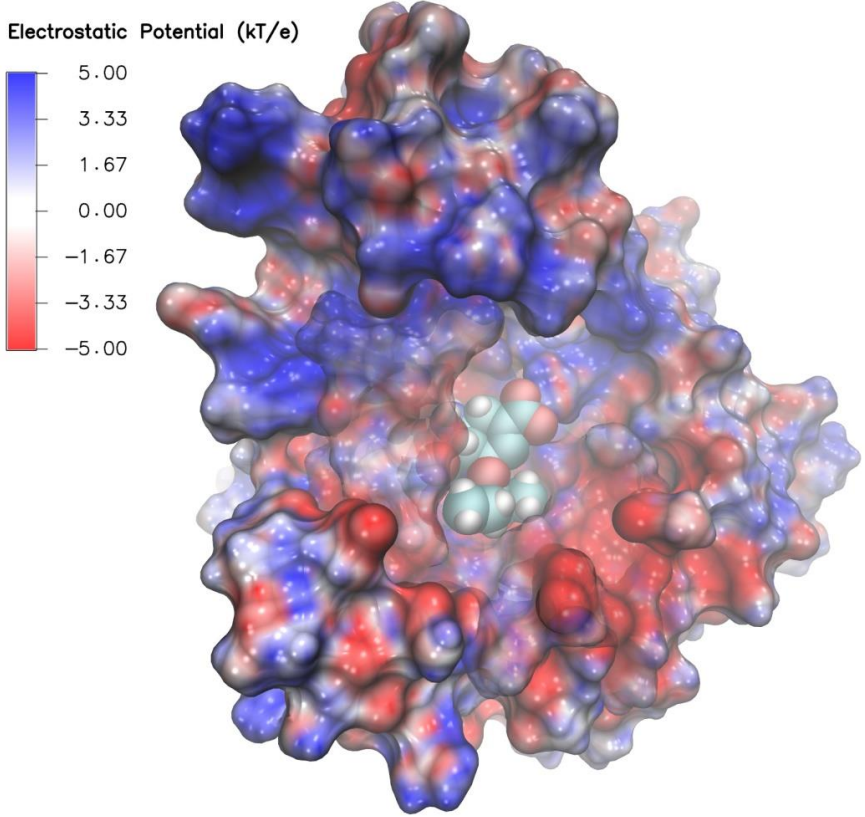
- VMDDisplayList
- DisplayDevice
- OpenGLRenderer

GLX+X11+Drv

- OpenGL Pbuffer/FBO
- Windowed OpenGL

EGL+Drv

- OpenGL Pbuffer/FBO

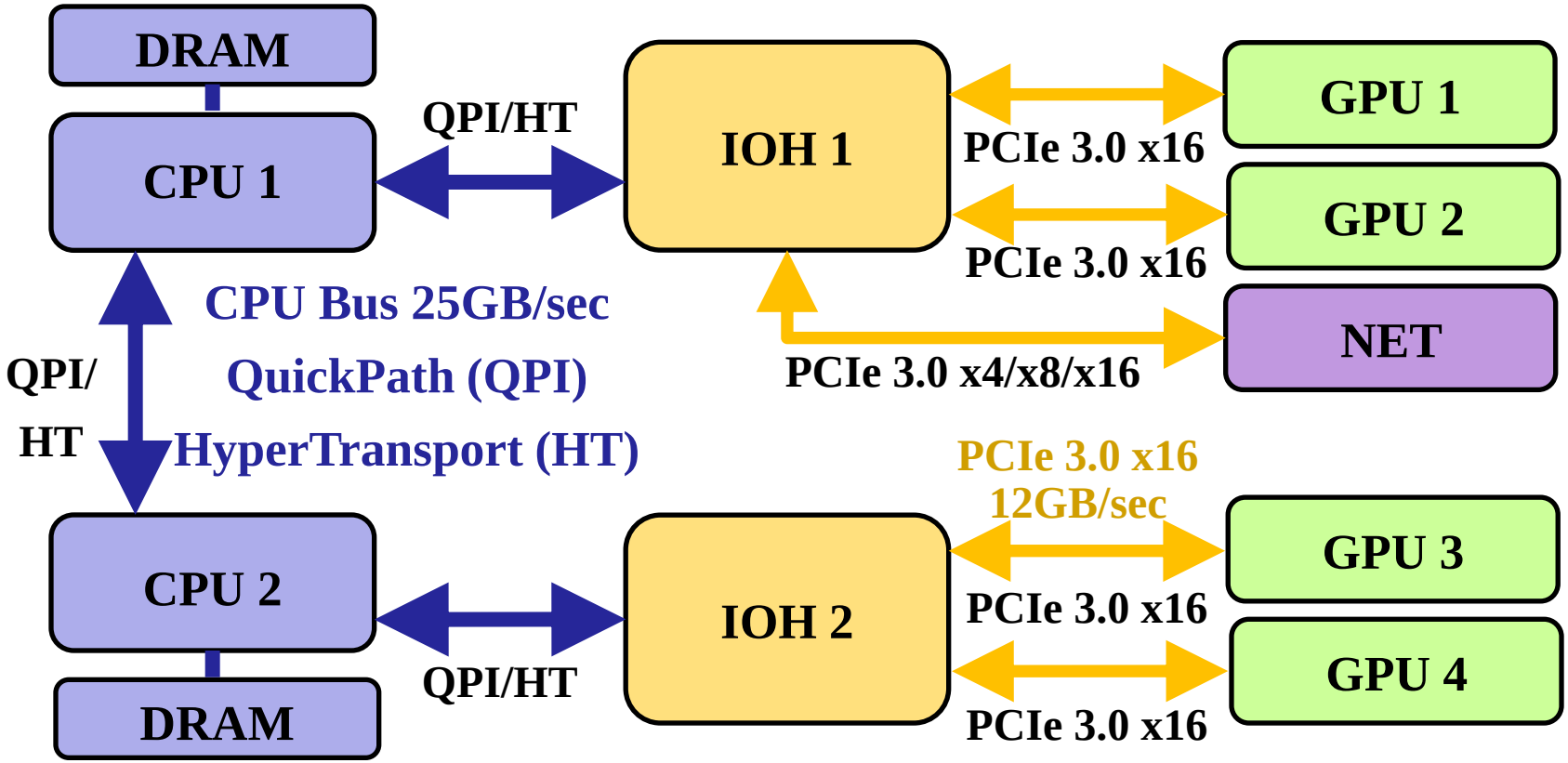


Swine Flu A/H1N1 neuraminidase bound to Tamiflu: VMD EGL rendering demonstrating full support for all VMD shaders and OpenGL features, multisample antialiasing, ray cast spheres, 3-D texture mapping, ...

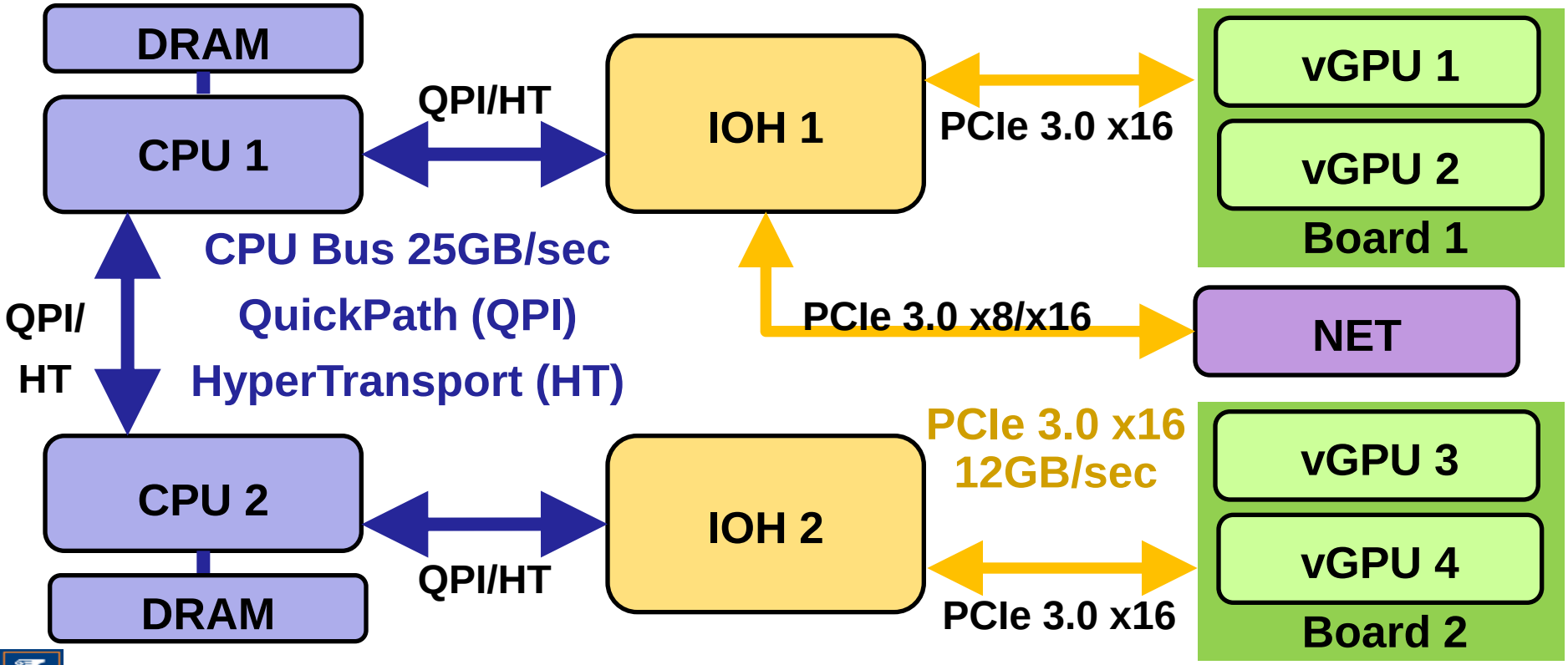
Benefits of EGL Platform Interfaces

- Minor similarity to OpenCL's platform interfaces
- Enumerate and select among available implementations, potentially supporting multiple vendors in the same 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
  - High-perf. multi-GPU image compositing, video
  - NVIDIA EGL implementation supports multiple indexing schemes, e.g. PCIe ordering
  - EGL plays nicely with MPI, CUDA/OpenCL, OptiX, NVENC, etc

Example Node NUMA Topology



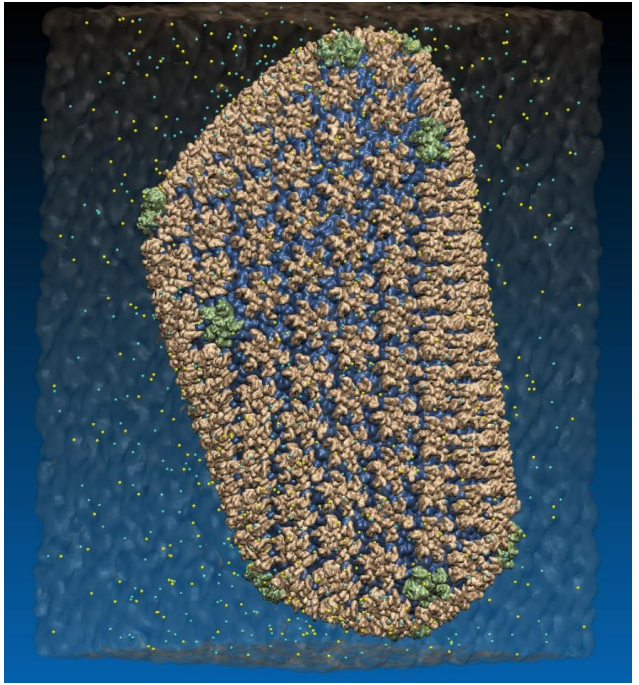
Example Cloud Node NUMA Topology



VMD EGL Performance on Amazon EC2 Cloud

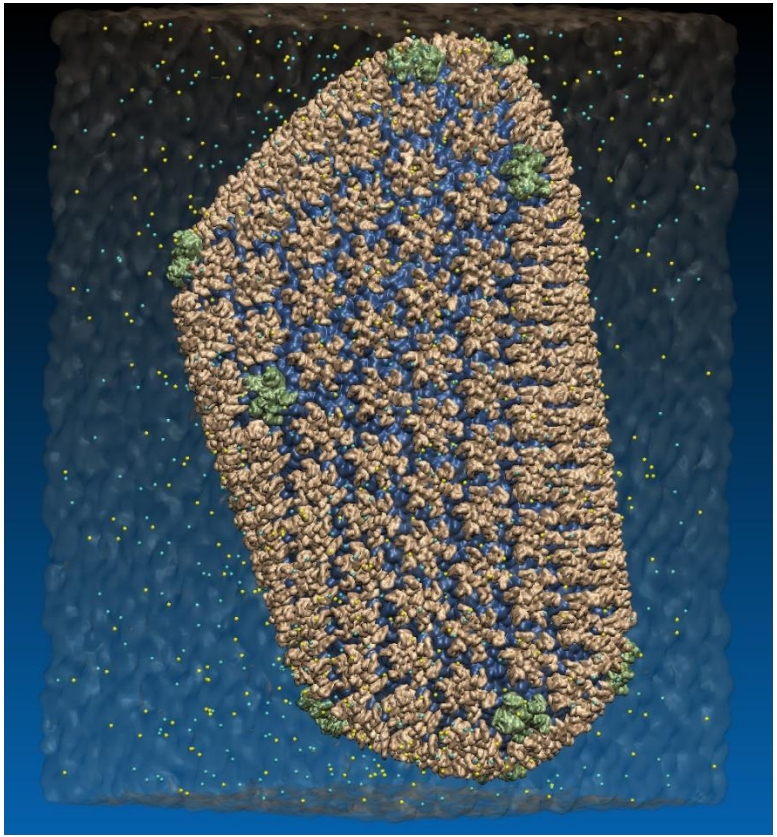
MPI Ranks	EC2 "G2.8xlarge" GPU Instances	HIV-1 movie rendering time (sec), (I/O %) 3840x2160 resolution
1	1	626s (10% I/O)
2	1	347s (19% I/O)
4	1	221s (31% I/O)
8	2	141s (46% I/O)
16	4	107s (64% I/O)
32	8	90s (76% I/O)

Performance at 32 nodes reaches ~48 frames per second

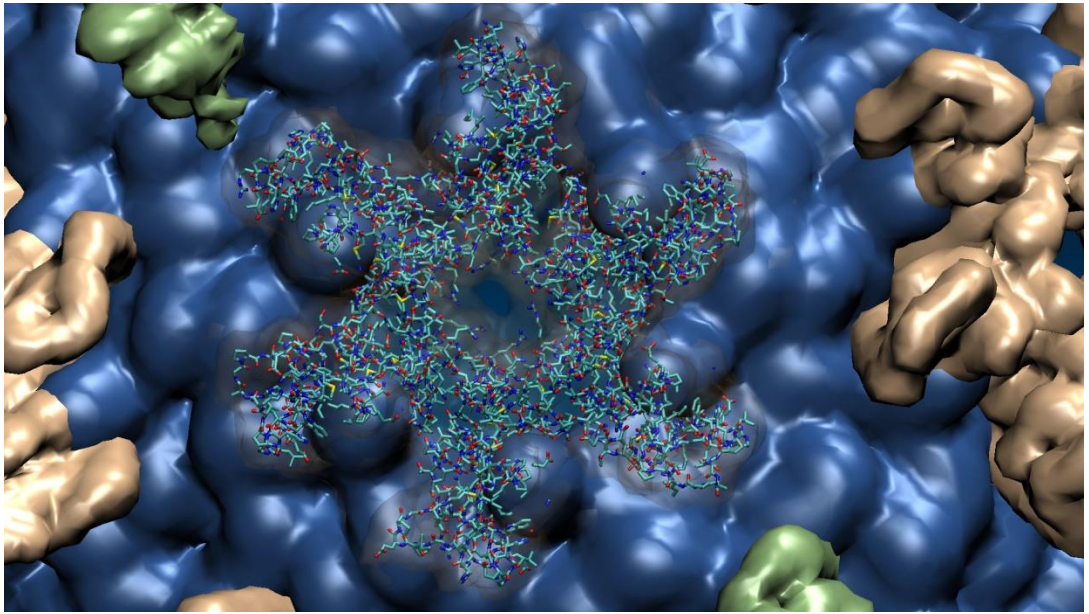


64M atom HIV-1 capsid simulation rendered via EGL

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, 2016.



64M atom HIV-1 capsid simulation rendered via EGL

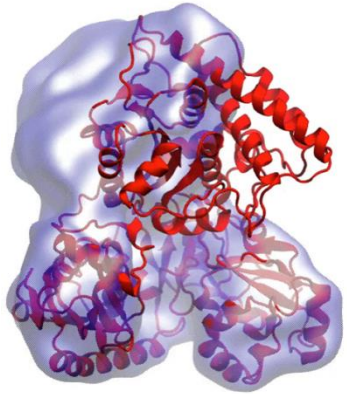


Close-up view of HIV-1 hexamer rendered via EGL

Molecular Dynamics Flexible Fitting (MDFF)

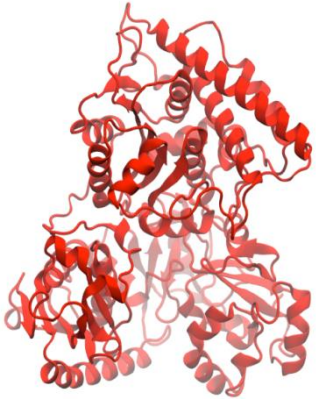
X-ray crystallography → MDFF ← Electron microscopy

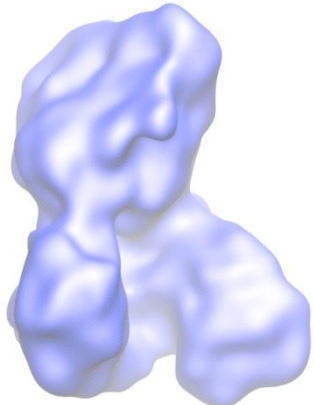
APS at Argonne



ORNL Titan

FEI microscope





Flexible fitting of atomic structures into electron microscopy maps using molecular dynamics.
L. Trabuco, E. Villa, K. Mitra, J. Frank, and K. Schulten. Structure, 16:673-683, 2008.

Molecular Dynamics Flexible Fitting - Theory

Two terms are added to the MD potential

$$U_{total} = U_{MD} + U_{EM} + U_{SS}$$

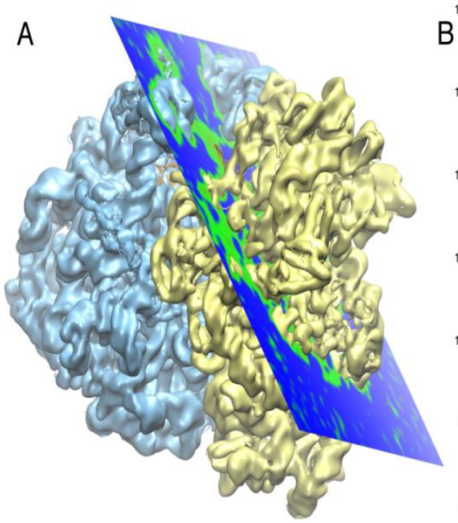
An external potential derived from the EM map is defined on a grid as

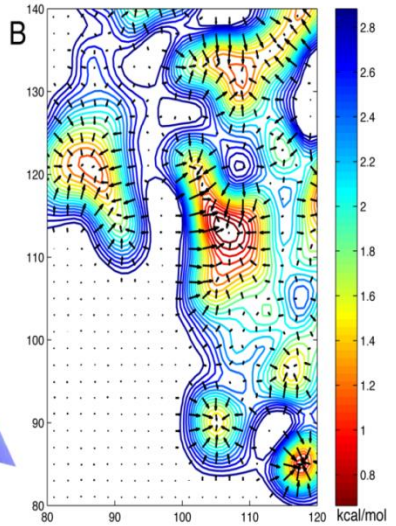
$$U_{EM}(\mathbf{R}) = \sum_j w_j V_{EM}(\mathbf{r}_j)$$

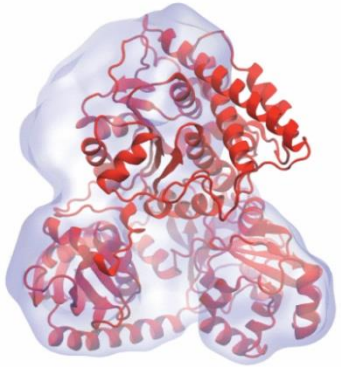
$$V_{EM}(\mathbf{r}) = \begin{cases} \xi \left(1 - \frac{\Phi(\mathbf{r}) - \Phi_{thr}}{\Phi_{max} - \Phi_{thr}}\right) & \text{if } \Phi(\mathbf{r}) \geq \Phi_{thr}, \\ \xi & \text{if } \Phi(\mathbf{r}) < \Phi_{thr}. \end{cases}$$

A mass-weighted force is then applied to each atom

$$\mathbf{f}_i^{EM} = -\nabla U_{EM}(\mathbf{R}) = -w_i \partial V_{EM}(\mathbf{r}_i)/\partial r_i$$

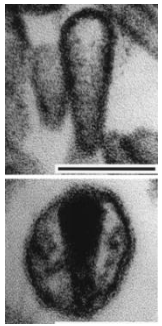


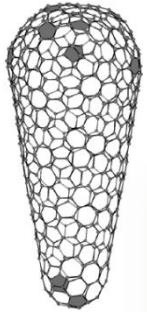


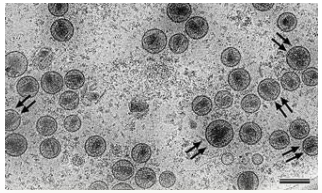


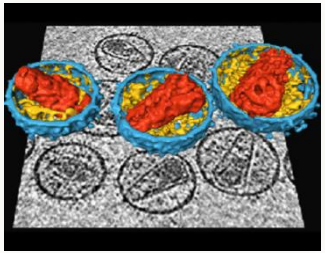
Structural Route to the all-atom HIV-1 Capsid

1st TEM (1999) 1st tomography (2003)



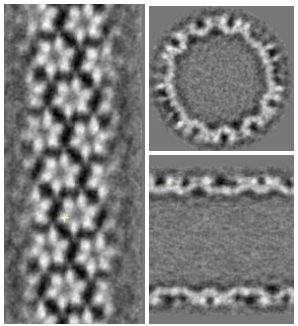






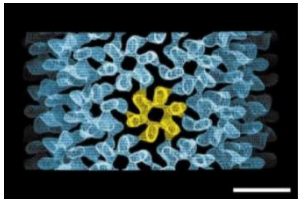
Ganser et al. *Science*, 1999
Briggs et al. *EMBO J*, 2003
Briggs et al. *Structure*, 2006

cryo-ET (2006)



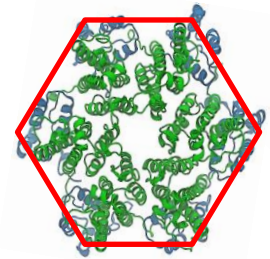
Byeon et al., *Cell* 2009

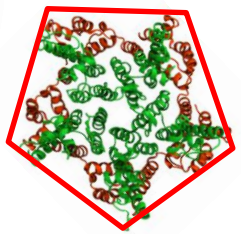
hexameric tubule

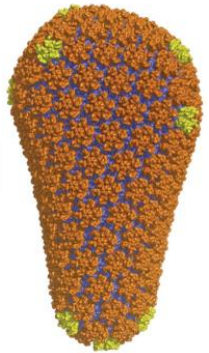


Li et al., *Nature*, 2000

Crystal structures of separated hexamer and pentamer

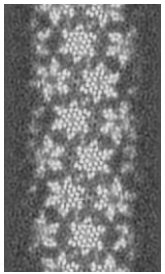


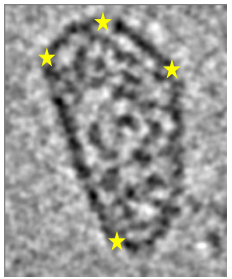


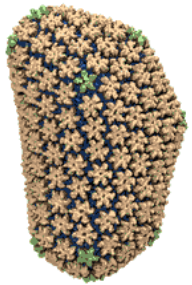


Pornillos et al. , *Cell* 2009, *Nature* 2011

High res. EM of hexameric tubule, tomography of capsid,
all-atom model of capsid by MDFF w/ NAMD & VMD, NSF/NCSA Blue Waters computer at Illinois



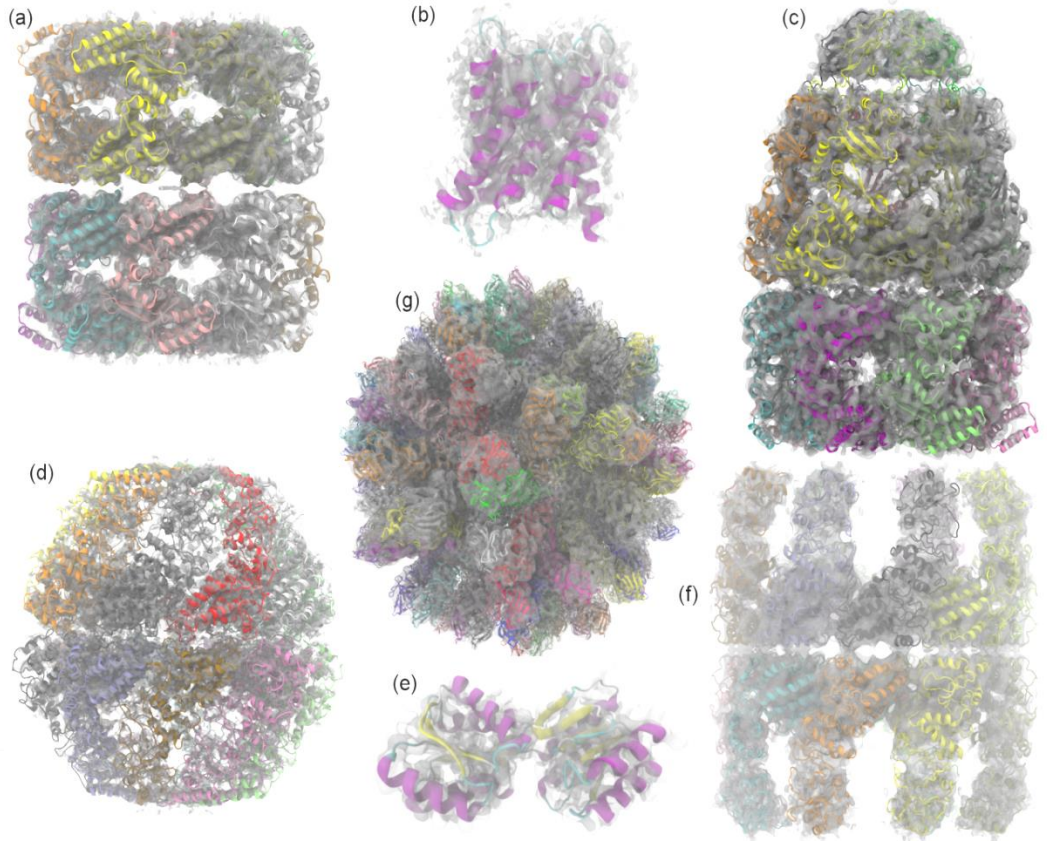




Zhao et al. , *Nature* 497: 643-646 (2013)

Evaluating Quality-of-Fit for Structures Solved by Hybrid Fitting Methods

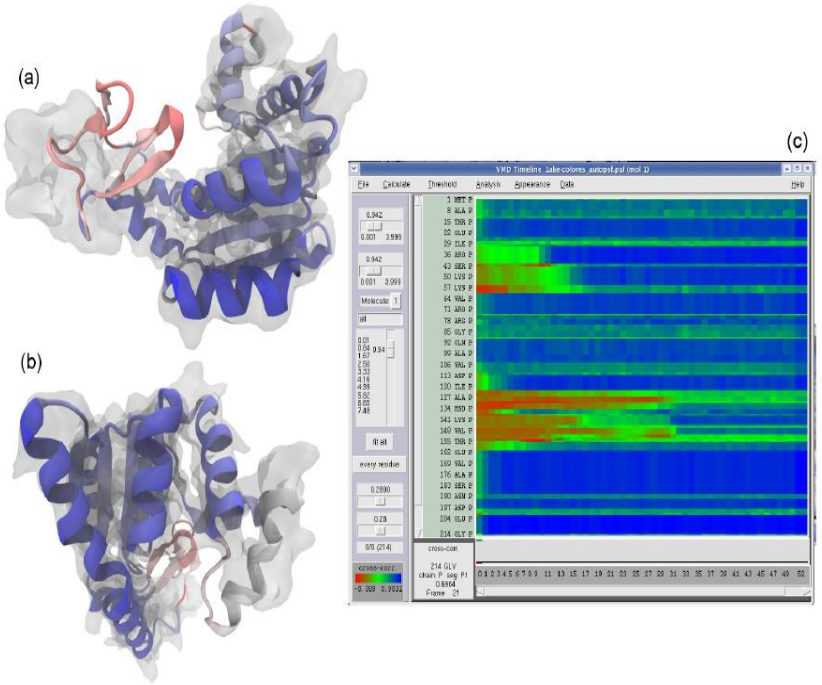
Compute Pearson correlation to evaluate the fit of a reference cryo-EM density map with a **simulated density map** produced from an **all-atom structure**.



GPUs Can Reduce MDFF Trajectory Analysis Runtimes from Hours to Minutes

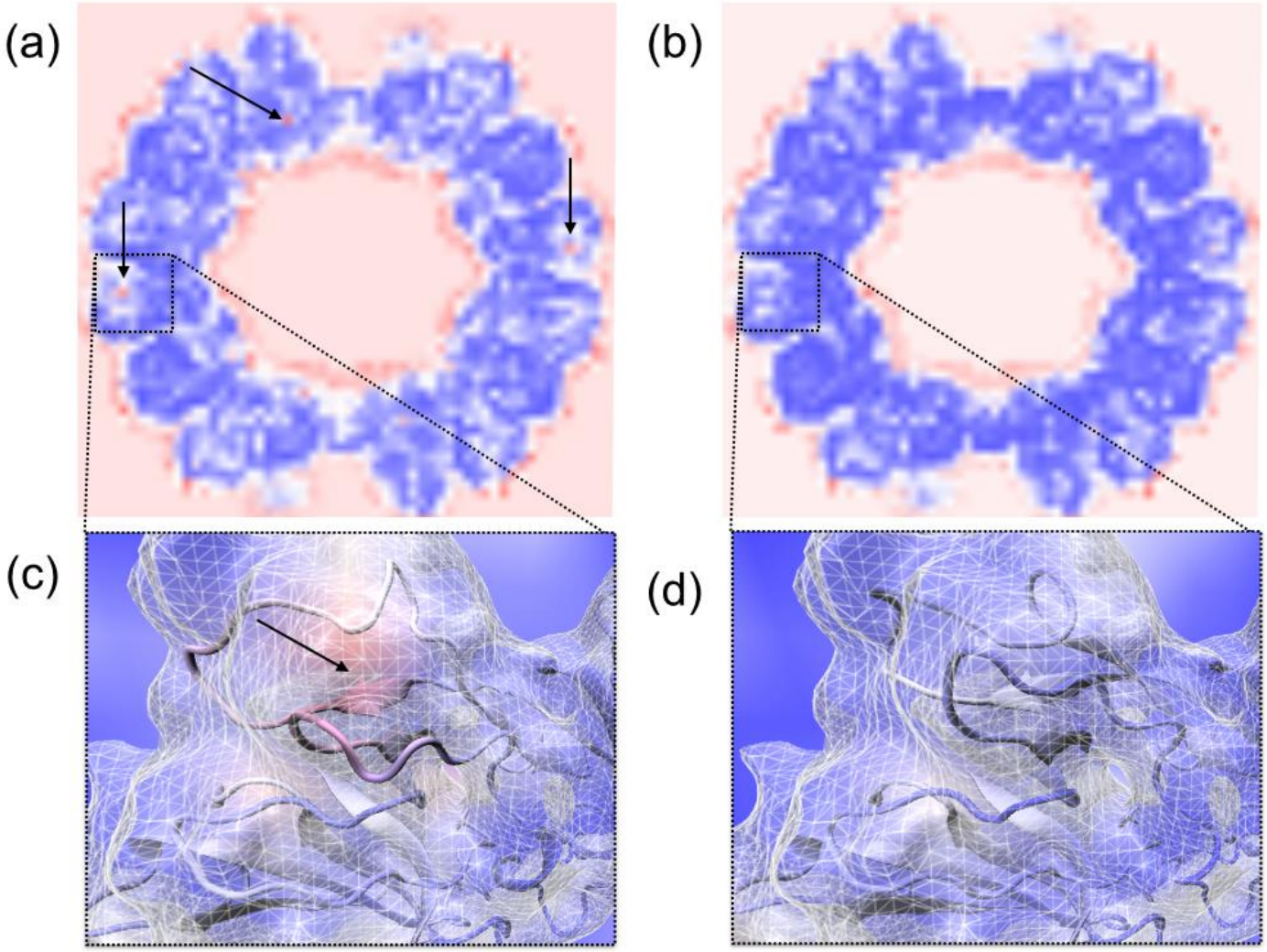
GPUs enable laptops and desktop workstations to handle tasks that would have previously required a cluster, or a *very long wait*…

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**

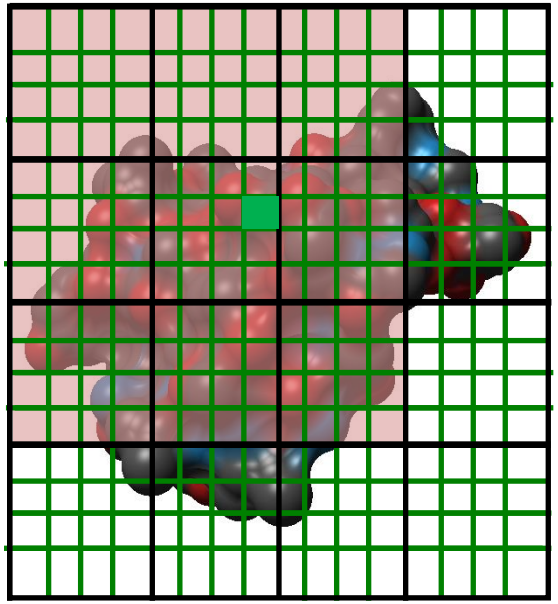

(a)
(b)
(c)
(d)

MDFF Density Map Algorithm

- Build spatial acceleration data structures, optimize data for GPU
- Compute 3-D density map:

$$\rho(\vec{r}; \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} e^{\frac{-|\vec{r}-\vec{r}_i|^2}{2\alpha^2}}$$

- Truncated Gaussian and spatial acceleration grid ensure linear time-complexity



3-D density map lattice point and the neighboring spatial acceleration cells it references

Single-Pass MDFF GPU Cross-Correlation

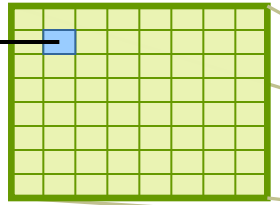
3-D density map decomposes into 3-D grid of 8x8x8 tiles containing CC partial sums and local CC values

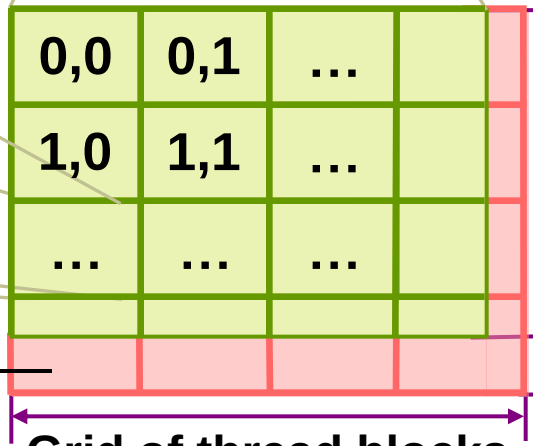
Fusion of density and CC calculations into a single CUDA kernel!!!

Spatial CC map and overall CC value computed in a single pass

Small 8x8x2 CUDA thread blocks afford large per-thread register count, shared memory

Each thread computes 4 z-axis density map lattice points and associated CC partial sums





Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

VMD GPU Cross Correlation Performance

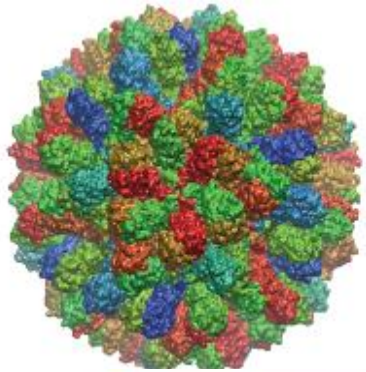
	RHDV	Mm-cpn open	GroEL	Aquaporin
Resolution (Å)	**6.5**	**8**	**4**	**3**
Atoms	**702K**	**61K**	**54K**	**1.6K**
VMD-CUDA Quadro K6000	**0.458s 34.6x**	**0.06s 25.7x**	**0.034s 36.8x**	**0.007s 55.7x**
VMD-CPU-SSE 32-threads, 2x Xeon E5-2687W	**0.779s 20.3x**	**0.085s 18.1x**	**0.159s 7.9x**	**0.033s 11.8x**
Chimera 1-thread Xeon E5-2687W	**15.86s 1.0x**	**1.54s 1.0x**	**1.25s 1.0x**	**0.39s 1.0x**

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.

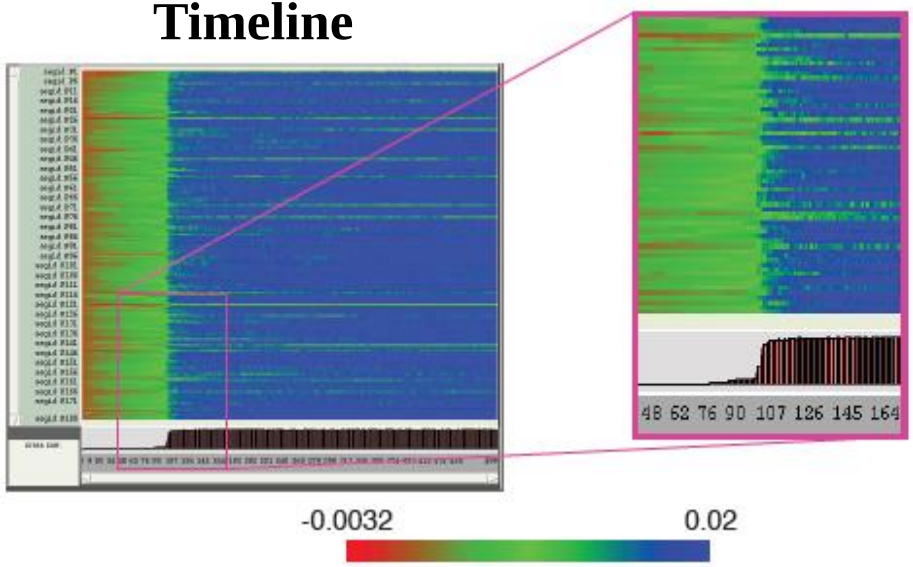
VMD RHDV Cross Correlation Timeline on Cray XK7

	RHDV
Atoms	702K
Traj. Frames	10,000
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

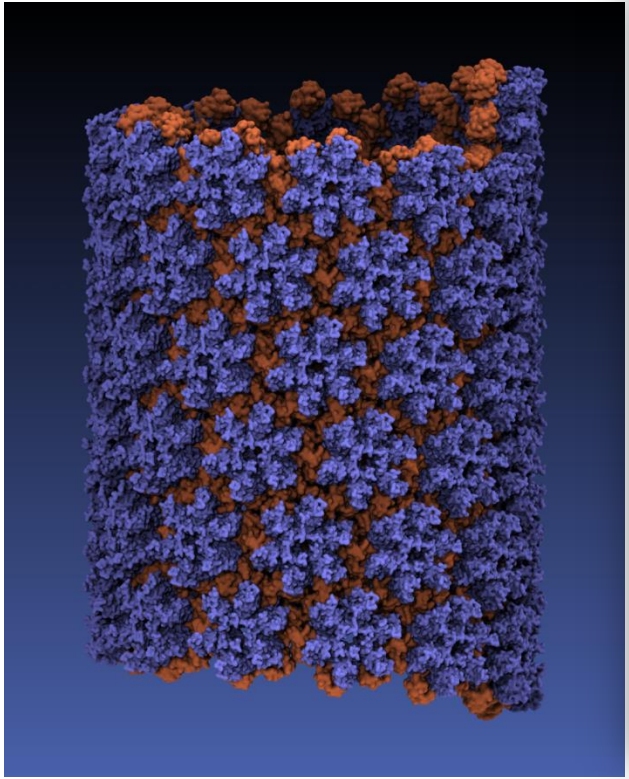
Calculation would take **5 years** using original serial CC calculation on a workstation!

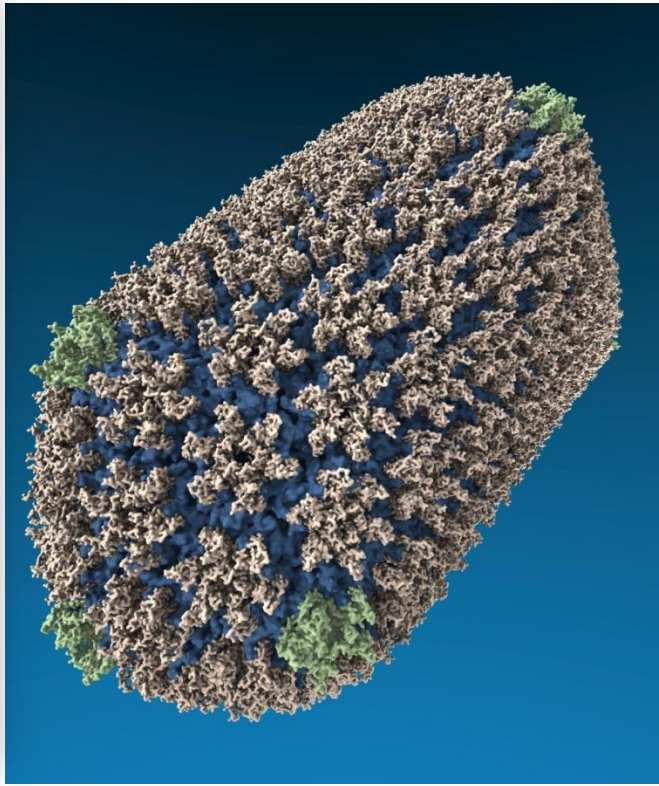


RHDV Group-relative CC Timeline



VMD “QuickSurf” Representation, Ray Tracing





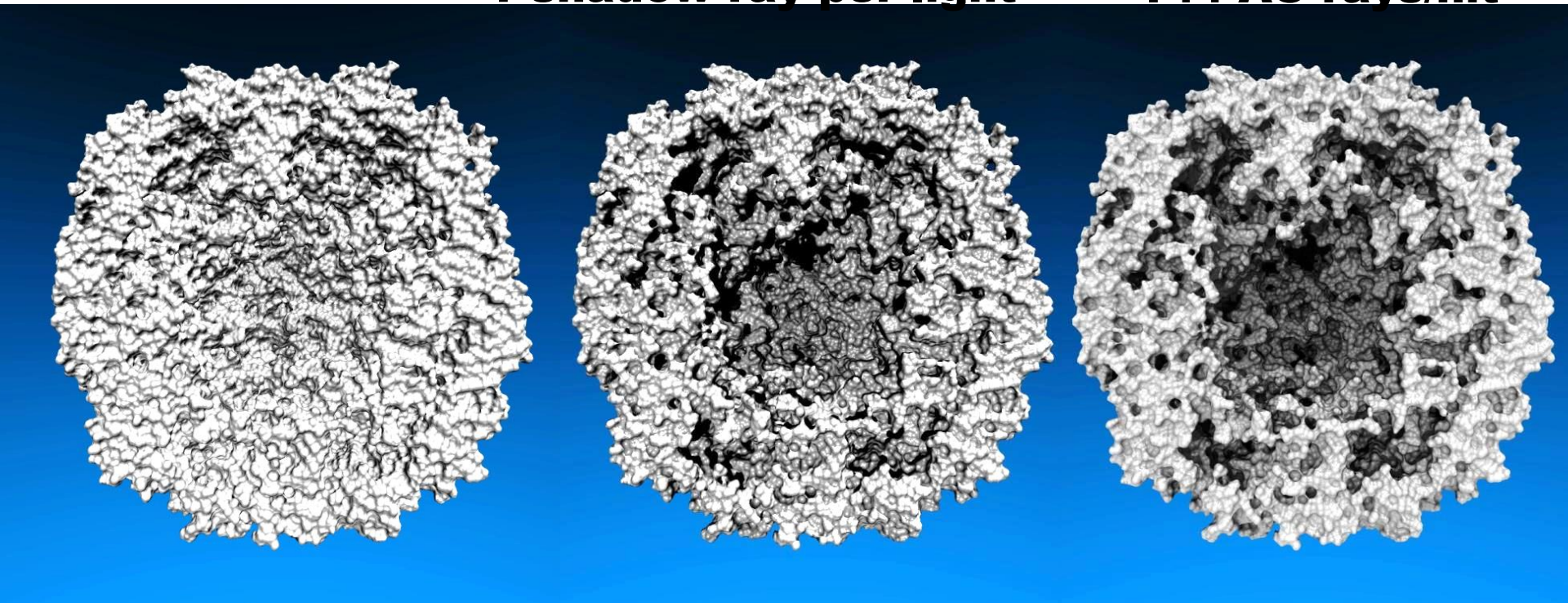
All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

Lighting Comparison, STMV Capsid

Two lights, no shadows

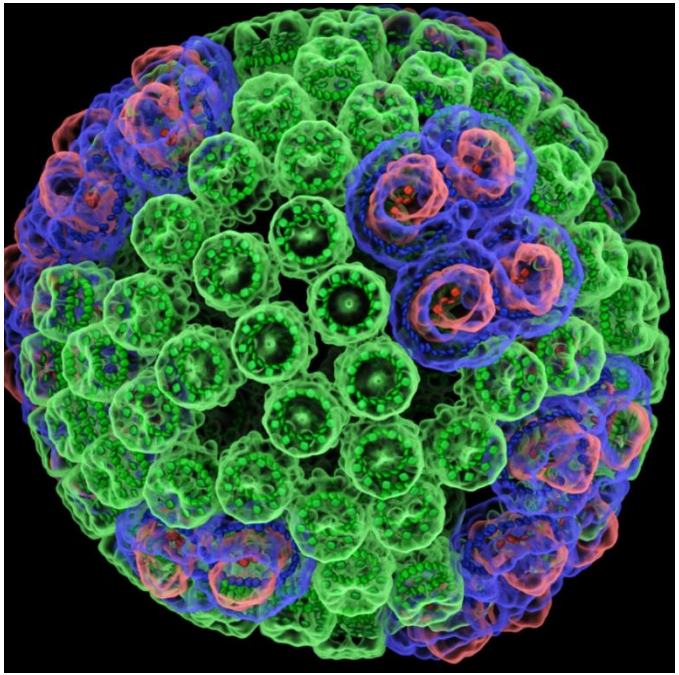
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit



VMD Chromatophore Rendering on Blue Waters

- New representations, GPU-accelerated molecular surface calculations, memory-efficient algorithms for huge complexes
- VMD GPU-accelerated ray tracing engine w/ OptiX+CUDA+MPI+Pthreads
- ***Each revision:*** 7,500 frames render on ~96 Cray XK7 nodes in 290 node-hours, 45GB of images prior to editing

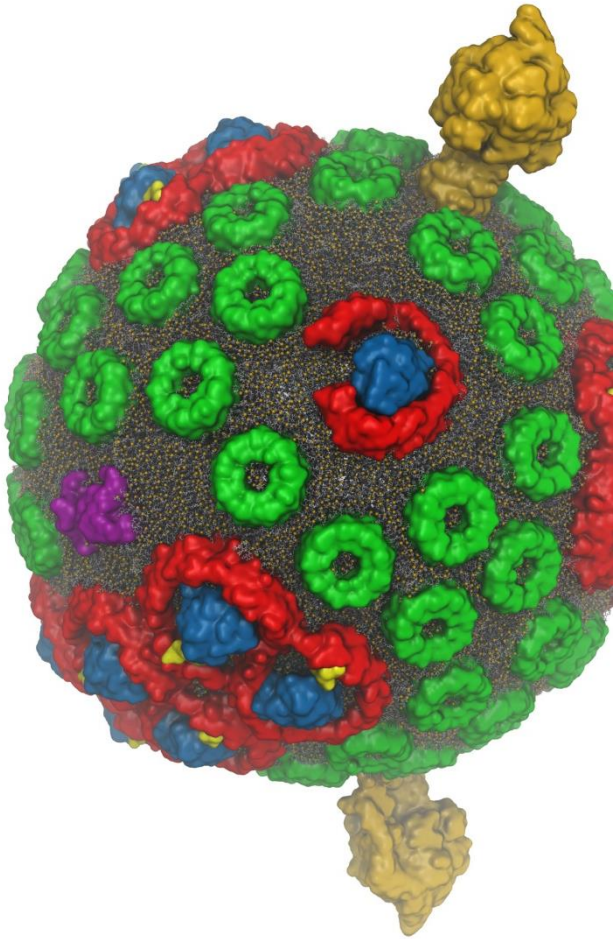


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

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.
*****Winner of the SC'14 Visualization and Data Analytics Showcase**

VMD 1.9.3+OptiX 3.9 – ~1.5x Performance Increase on Blue Waters Supercomputer

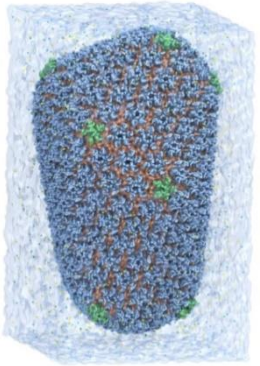
- OptiX GPU-native **"Trbvh" acceleration structure builder** yields substantial perf increase vs. CPU builders running on Opteron 6276 CPUs
- New optimizations in VMD TachyonL-OptiX RT engine:
  - **CUDA C++ Template specialization of RT kernels**
    - **Combinatorial expansion of ray-gen and shading kernels at compile-time: stereo on/off, AO on/off, depth-of-field on/off, reflections on/off, etc…**
    - **Optimal kernels selected from expansions at runtime**
  - **Streamlined OptiX context and state management**
  - **Optimization of GPU-specific RT intersection routines, memory layout**



VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.

Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone et al., J. Parallel Computing, 2016.

VMD 1.9.3 HIV-1 Parallel Movie Rendering on Blue Waters Cray XE6/XK7



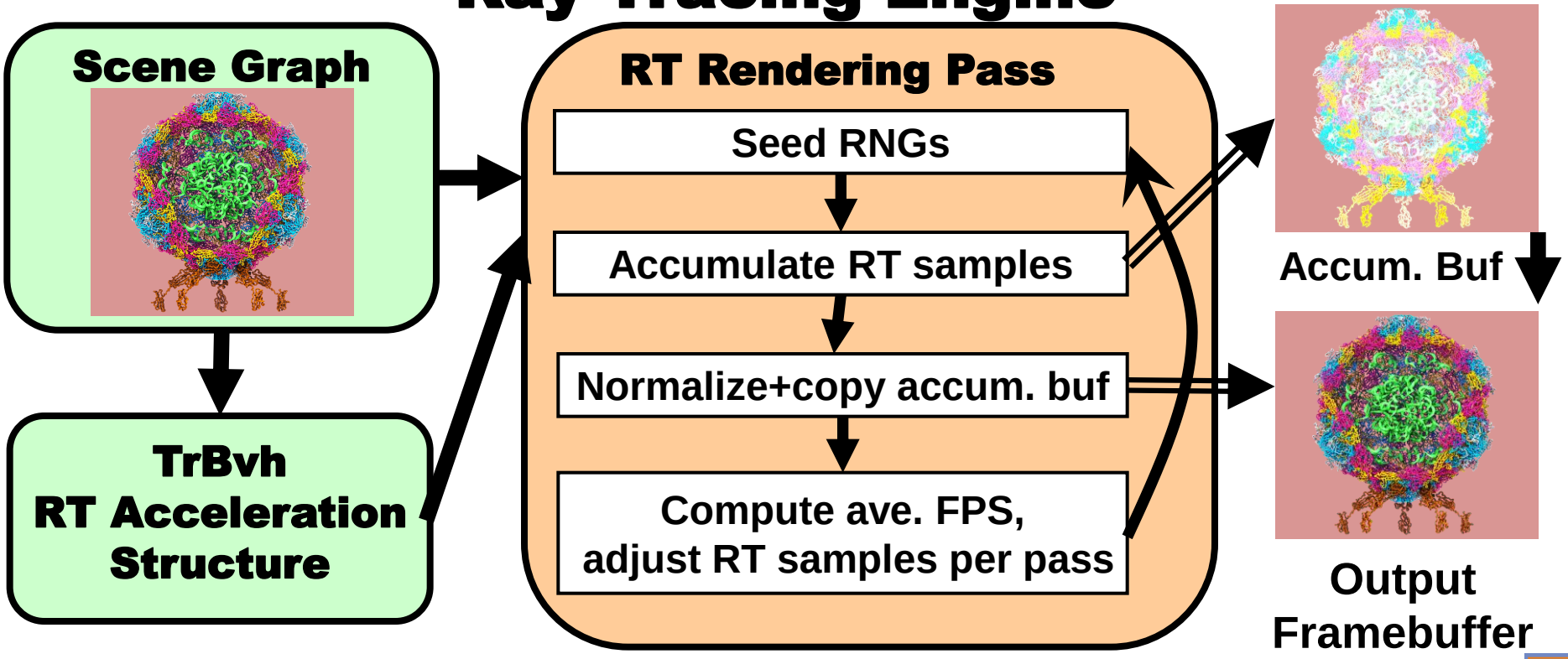
New VMD 1.9.3: TachyonL-OptiX on XK7 vs. Tachyon on XE6, K20X GPUs yield **up to twelve times** geom+ray tracing speedup

Ray Tracer Version	Node Type and Count	Script Load	State Load	Geometry + Ray Tracing	Total Time
New TachyonL-OptiX [2]	64 XK7 Tesla K20X GPUs	2 s	39 s	435 s	476 s
New TachyonL-OptiX [2]	**128 XK7 Tesla K20X GPUs**	**3 s**	**62 s**	**230 s**	**295 s**
TachyonL-OptiX [1]	64 XK7 Tesla K20X GPUs	2 s	38 s	655 s	695 s
TachyonL-OptiX [1]	128 XK7 Tesla K20X GPUs	4 s	74 s	331 s	410 s
TachyonL-OptiX [1]	**256 XK7 Tesla K20X GPUs**	**7 s**	**110 s**	**171 s**	**288 s**
Tachyon [1]	**256 XE6 CPUs**	7 s	160 s	**1,374 s**	**1,541 s**
Tachyon [1]	512 XE6 CPUs	13 s	211 s	808 s	1,032 s

[1] GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms. J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13: Proceedings of the 8th International Workshop on Ultrascale Visualization, pp. 6:1-6:8, 2013.

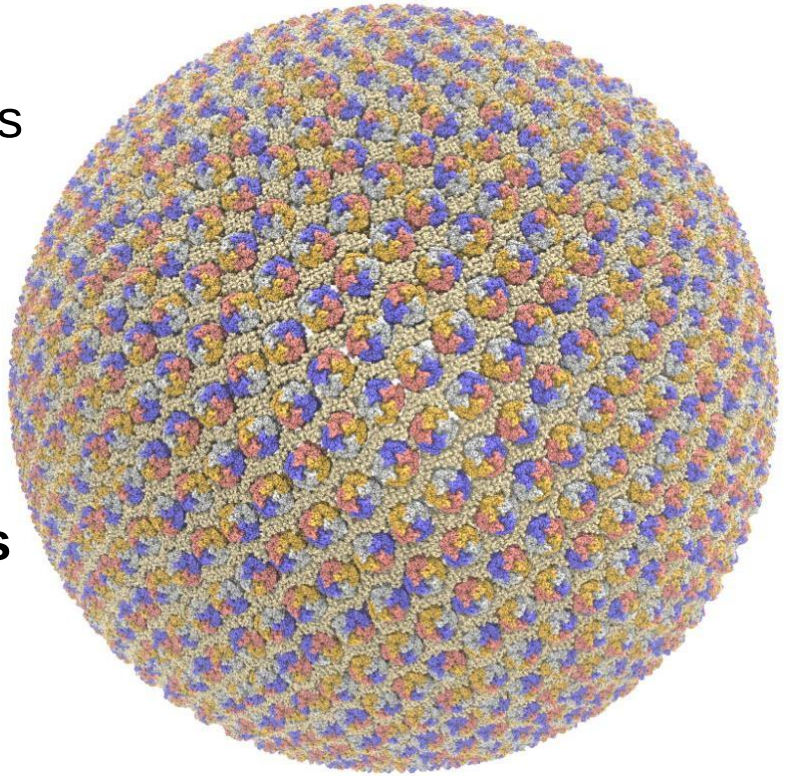
[2] Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing. J. E. Stone et al., J. Parallel Computing, 2016 (in-press)

VMD TachyonL-OptiX Interactive Ray Tracing Engine



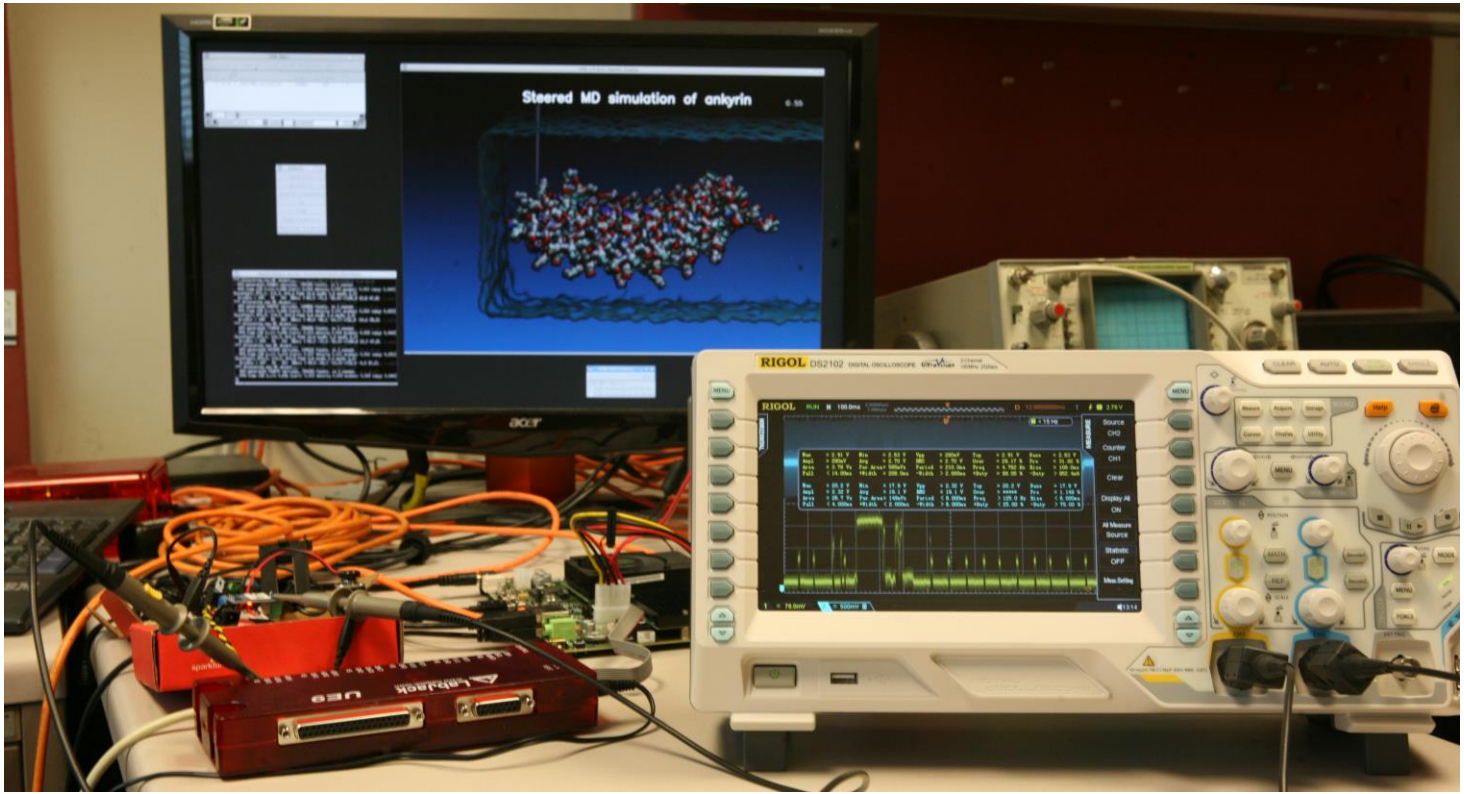
Interactive RT of All-Atom Minimal Cell Envelope

- 200 nm spherical envelope
- Membrane with ~50% occupancy by proteins (2000x Aquaporin channels)
- 42M atoms in membrane
- **Interactive RT w/ 2 dir. lights and AO on GeForce Titan X @ ~12 FPS**
- **Complete model with correct proteins, solvent, etc, will contain billions of atoms**



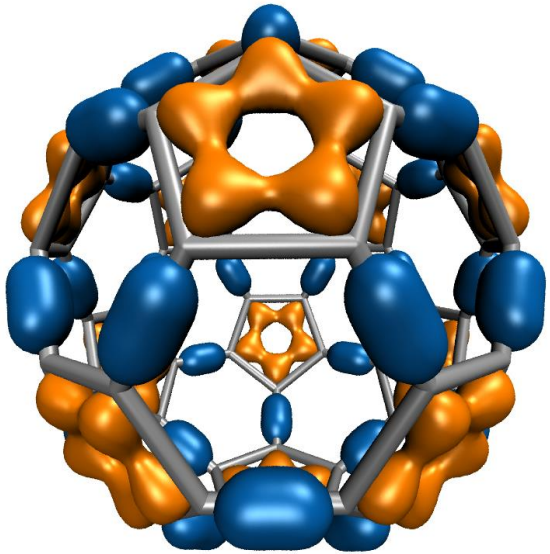
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering. J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and

Optimizing VMD for Speed+Power Consumption



Molecular Orbitals w/ JIT Kernel Generation

- Visualization of MOs aids in understanding the chemistry of molecular system
- MO spatial distribution is correlated with probability density for an electron(s)
- **Animation** of (classical mechanics) molecular dynamics trajectories provides insight into simulation results
  - To do the same for QM or QM/MM simulations MOs must be computed at **10 FPS** or more
  - **Large GPU speedups (up to 30x vs. 4-core CPU)** over existing tools makes this possible!
- **Run-time code generation** (JIT) and compilation via **CUDA 7.0 NVRTC** enable further optimizations and the **highest performance to date: 1.8x faster than previous best result**



C_{60}

High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs. J. E. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Processing Units (GPGPU-2), ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.

```
for (shell=0; shell < maxshell; shell++)  {
  float contracted_gto = 0.0f;

  // Loop over the Gaussian primitives of CGTO
  int maxprim = const_num_prim_per_shell[shell_counter];
  int shell_type = const_shell_symmetry[shell_counter];
  for (prim=0; prim < maxprim;  prim++) {
    float exponent         = const_basis_array[prim_counter      ];
    float contract_coeff = const_basis_array[prim_counter + 1];
    contracted_gto += contract_coeff  * expf(-exponent*dist2);
    prim_counter += 2;
  }
```

General loop-based data-dependent MO CUDA kernel

Runtime-generated data-specific MO CUDA kernel compiled via **CUDA 7.x NVRTC** JIT…

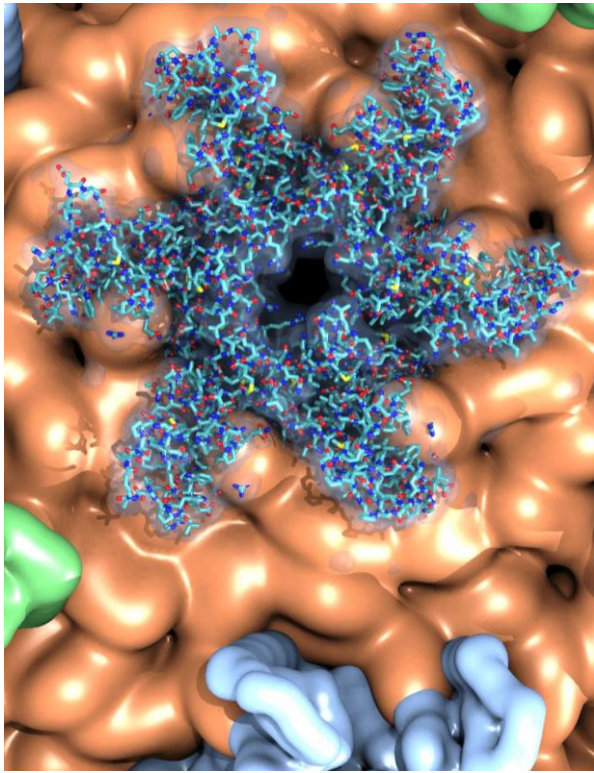
```
contracted_gto = 1.832937 * expf(-7.868272*dist2);
contracted_gto += 1.405380 * expf(-1.881289*dist2);
contracted_gto += 0.701383 * expf(-0.544249*dist2);
```

1.8x Faster

VMD-Next: Coming Soon

- Improved structure building tools
- Many new and updated user-contributed plugins
- Further integration of interactive ray tracing into VMD
  - Seamless interactive RT in main VMD display window
  - Support trajectory playback in interactive RT
  - Enable multi-node interactive RT on HPC systems

- Improved movie making tools, off-screen OpenGL movie rendering, parallel movie rendering:
  - EGL for parallel graphics w/o X11 server
  - Built-in (basic) interactive remote visualization on HPC clusters and supercomputers
- Much work to do on VR user interfaces, multi-user collaborative visualization, …



GPU Ray Tracing of HIV-1 Capsid Detail

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
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- **Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering.** John E. Stone, William R. Sherman, and Klaus Schulten.High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
- **High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL.** John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten.High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
- **Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads.** John E. Stone, Michael J. Hallock, James C. Phillips, Joseph R. Peterson, Zaida Luthey-Schulten, and Klaus Schulten.25th International Heterogeneity in Computing Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2016. **(In-press)**
- **Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.** J. E. Stone, M. Sener, K. L. Vandivort, A. Barragan, A. Singharoy, I. Teo, J. V. Ribeiro, B. Isralewitz, B. Liu, B.-C. Goh, J. C. Phillips, C. MacGregor-Chatwin, M. P. Johnson, L. F. Kourkoutis, C. Neil Hunter, and K. Schulten. J. Parallel Computing, 2016. **(In-press)**
- **Chemical Visualization of Human Pathogens: the Retroviral Capsids.** Juan R. Perilla, Boon Chong Goh, John E. Stone, and Klaus SchultenSC'15 Visualization and Data Analytics Showcase, 2015.

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- **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.
  ***Winner of the SC'14 Visualization and Data Analytics Showcase**
- **Runtime and Architecture Support for Efficient Data Exchange in Multi-Accelerator Applications.** J. Cabezas, I. Gelado, J. E. Stone, N. Navarro, D. B. Kirk, and W. Hwu. IEEE Transactions on Parallel and Distributed Systems, 2014. **(In press)**
- **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.
- **Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations**. M. J. Hallock, J. E. Stone, E. Roberts, C. Fry, and Z. Luthey-Schulten. Journal of Parallel Computing, 40:86-99, 2014.

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- **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.
- **Lattice Microbes: High-performance stochastic simulation method for the reaction-diffusion master equation.** E. Roberts, J. Stone, and Z. Luthey-Schulten. J. Computational Chemistry 34 (3), 245-255, 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.
- **Fast Analysis of Molecular Dynamics Trajectories with Graphics Processing Units – Radial Distribution Functions.** B. Levine, J. Stone, and A. Kohlmeyer. *J. Comp. Physics*, 230(9):3556-3569, 2011.

Related Publications

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- **Quantifying the Impact of GPUs on Performance and Energy Efficiency in HPC Clusters.** J. Enos, C. Steffen, J. Fullop, M. Showerman, G. Shi, K. Esler, V. Kindratenko, J. Stone, J Phillips. *International Conference on Green Computing,* pp. 317-324, 2010.
- **GPU-accelerated molecular modeling coming of age.** J. Stone, D. Hardy, I. Ufimtsev, K. Schulten. *J. Molecular Graphics and Modeling,* 29:116-125, 2010.
- **OpenCL: A Parallel Programming Standard for Heterogeneous Computing.** J. Stone, D. Gohara, G. Shi. *Computing in Science and Engineering,* 12(3):66-73, 2010.
- **An Asymmetric Distributed Shared Memory Model for Heterogeneous Computing Systems**. I. Gelado, J. Stone, J. Cabezas, S. Patel, N. Navarro, W. Hwu. *ASPLOS '10: Proceedings of the 15th International Conference on Architectural Support for Programming Languages and Operating Systems,* pp. 347-358, 2010.

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

- **GPU Clusters for High Performance Computing**. V. Kindratenko, J. Enos, G. Shi, M. Showerman, G. Arnold, J. Stone, J. Phillips, W. Hwu. *Workshop on Parallel Programming on Accelerator Clusters (PPAC),* In Proceedings IEEE Cluster 2009, pp. 1-8, Aug. 2009.
- **Long time-scale simulations of in vivo diffusion using GPU hardware**. E. Roberts, J. Stone, L. Sepulveda, W. Hwu, Z. Luthey-Schulten. In *IPDPS'09: Proceedings of the 2009 IEEE International Symposium on Parallel & Distributed Computing*, pp. 1-8, 2009.
- **High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs**. J. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Pricessing Units (GPGPU-2), ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.
- **Probing Biomolecular Machines with Graphics Processors**. J. Phillips, J. Stone. *Communications of the ACM,* 52(10):34-41, 2009.
- **Multilevel summation of electrostatic potentials using graphics processing units**. D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

Related Publications

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

- **Adapting a message-driven parallel application to GPU-accelerated clusters**. J. Phillips, J. Stone, K. Schulten. *Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, IEEE Press, 2008.
- **GPU acceleration of cutoff pair potentials for molecular modeling applications**. C. Rodrigues, D. Hardy, J. Stone, K. Schulten, and W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.
- **GPU computing**. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.
- **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.
- **Continuous fluorescence microphotolysis and correlation spectroscopy**. A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.