Harnessing GPUs to Probe Biomolecular Machines at Atomic Detail

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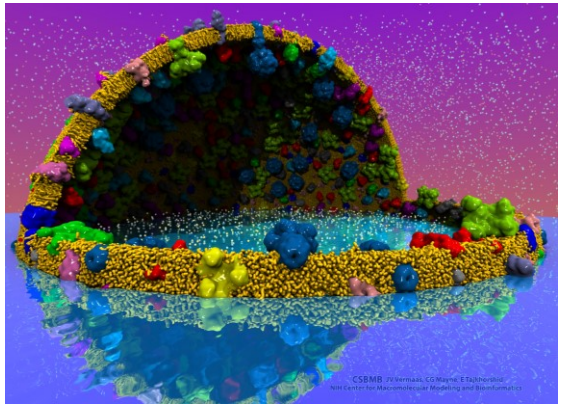
http://www.ks.uiuc.edu/Research/gpu/

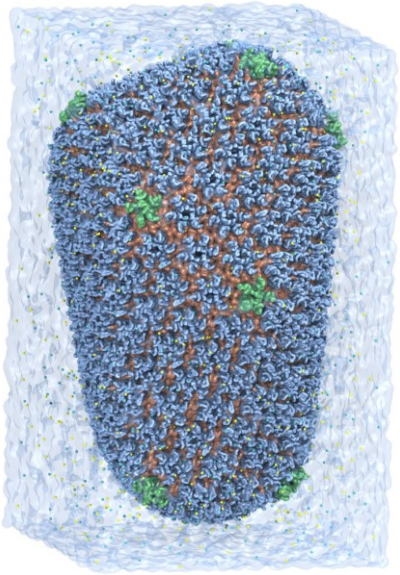
NVIDIA GPU Technology Theater
4:30pm, Salt Palace Convention Center,
Salt Lake City, UT, Wednesday Nov 16th, 2016

VMD – “Visual Molecular Dynamics”

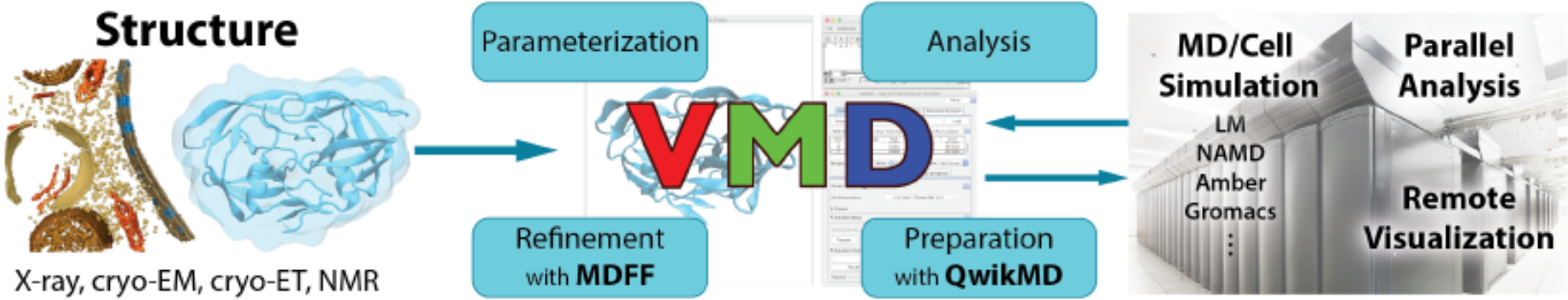
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Sequence information
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling

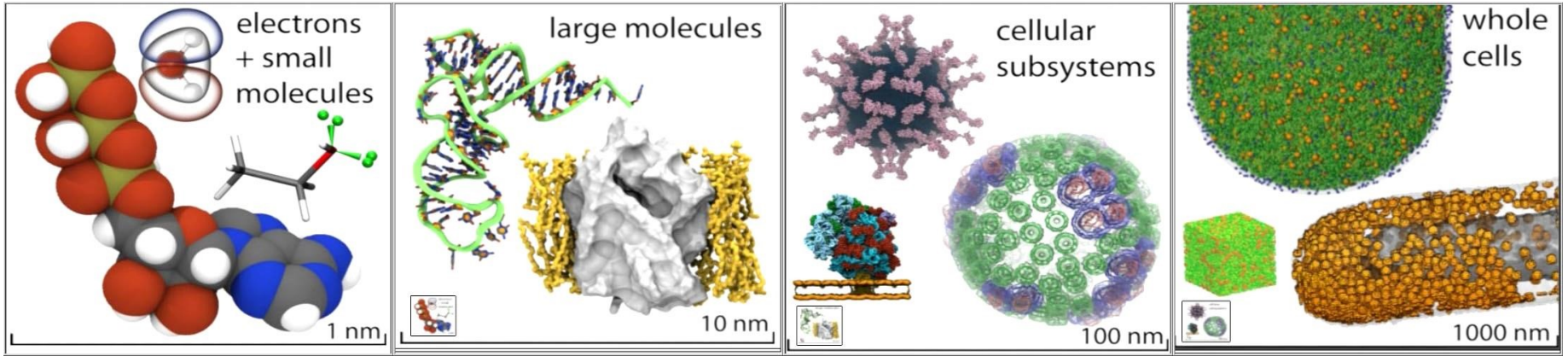


MD Simulation



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



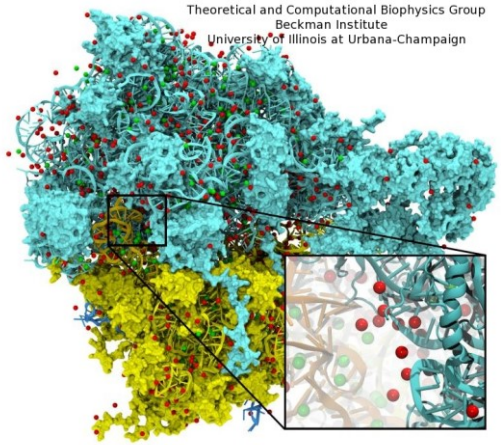
9.5 Years of GPU Computing in VMD

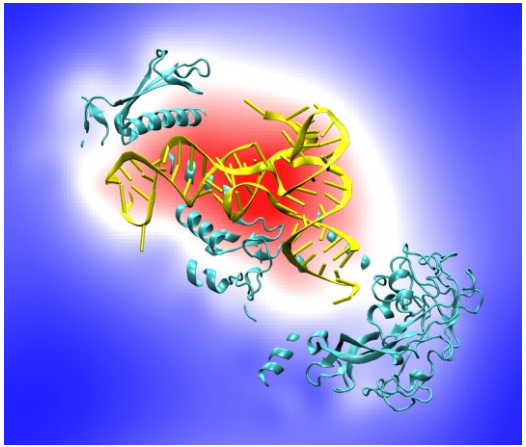
- Has stood the test of time
- Modeling, Visualization, Rendering, and Analysis

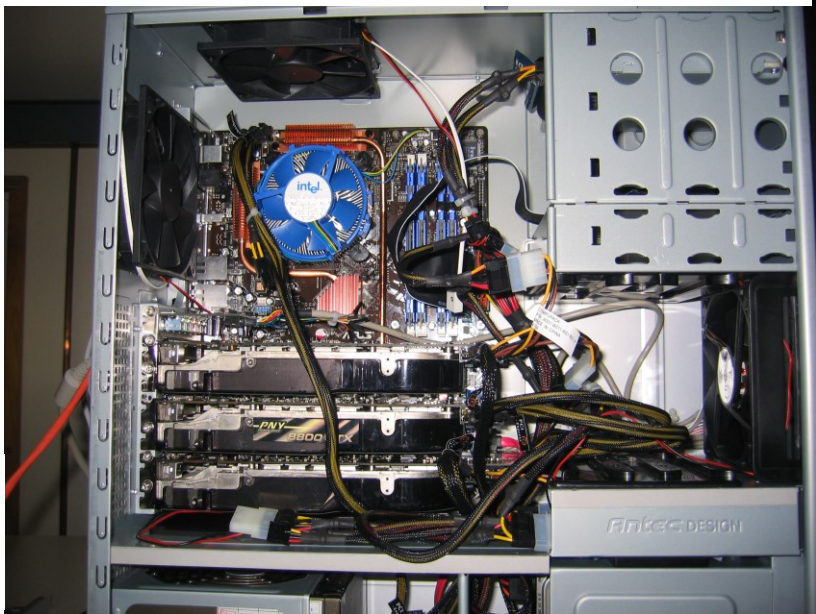
Blast from the past:

CUDA starting with version 0.7 !!!

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



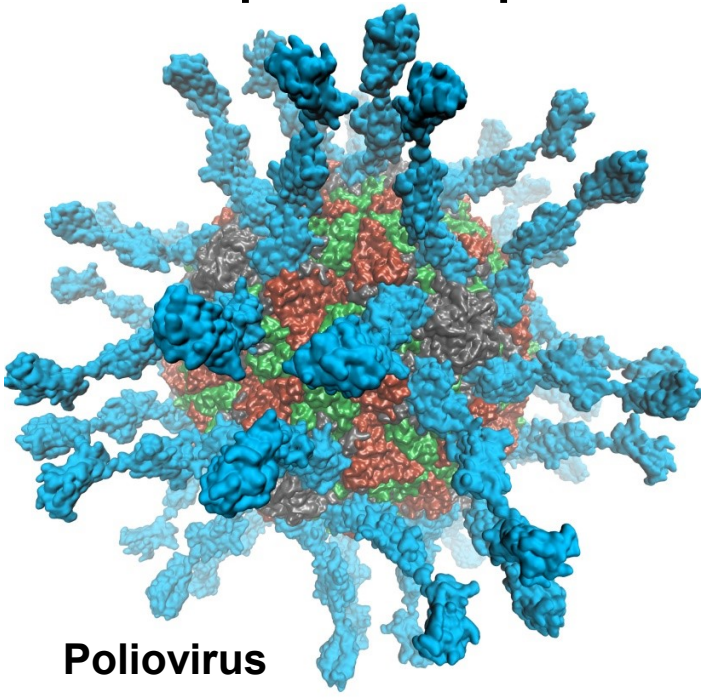




Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.

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

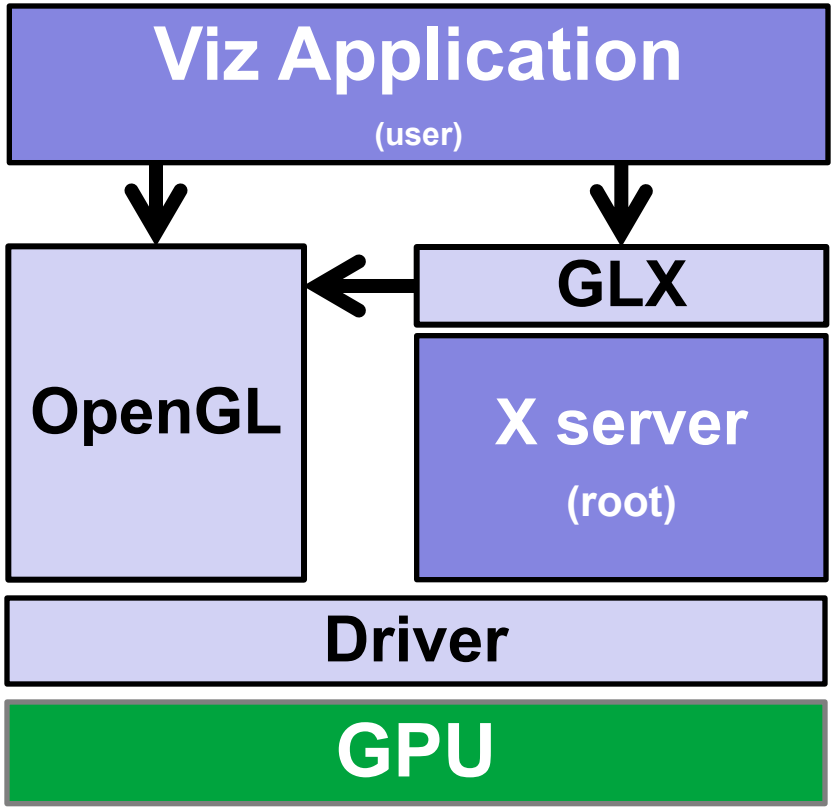
- Eliminate dependency on windowing systems
- Easy deployment of parallel VMD builds w/ off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features
- High-quality commercial OpenGL implementations in HPC systems
- Easier management of multi-GPU nodes and NUMA affinity issues

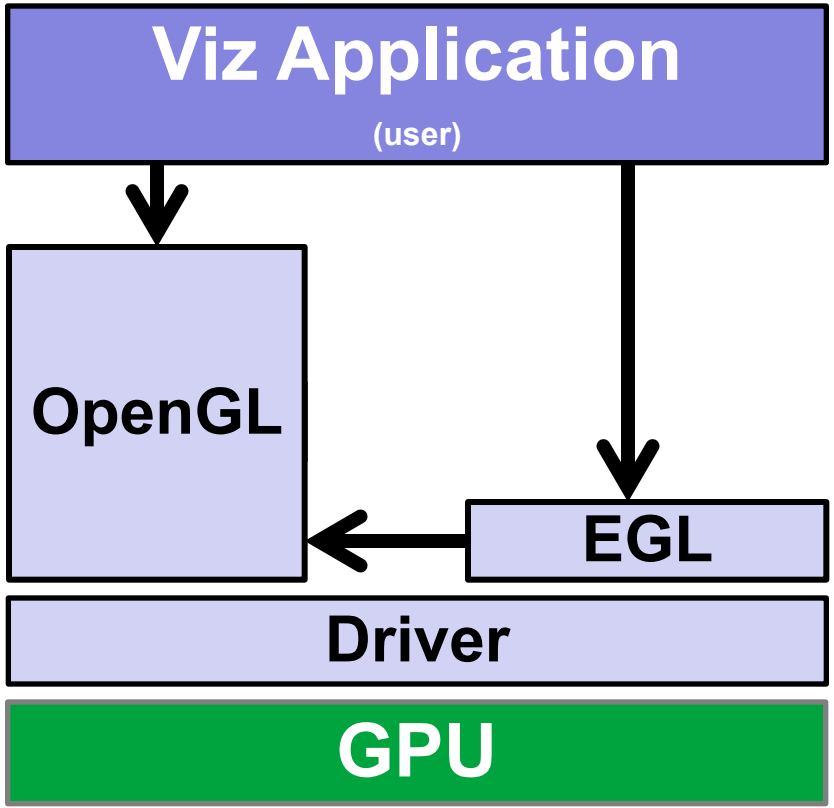


Poliovirus

High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL
J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. HPDAV, IEEE IPDPS, pp. 1014-1023, 2016.

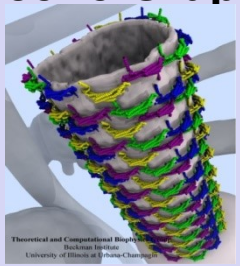
OpenGL: GLX vs. EGL





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

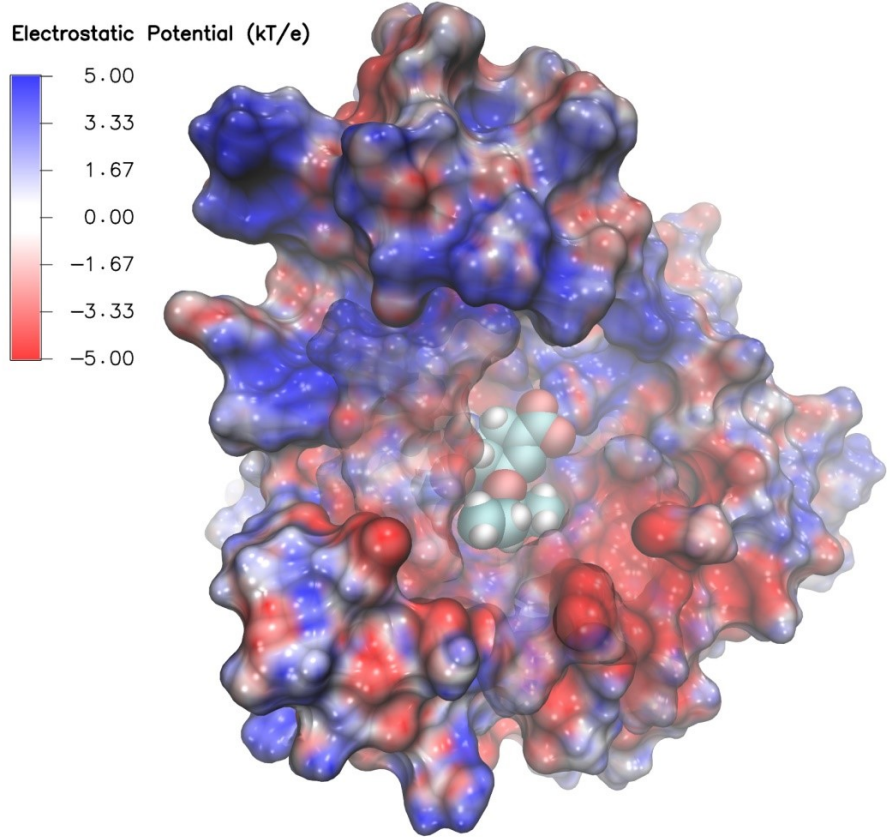
- OpenGL Pbuffer/FBO
- Windowed OpenGL

EGL+Drv

- OpenGL Pbuffer/FBO

VMD EGL rendering:

- Supports all VMD shaders and associated OpenGL features:
  - Pixel-rate lighting
  - Ray-cast spheres w/ GLSL
  - 3-D texture mapping
  - Text rendering
  - Multisample antialiasing
  - And much more...



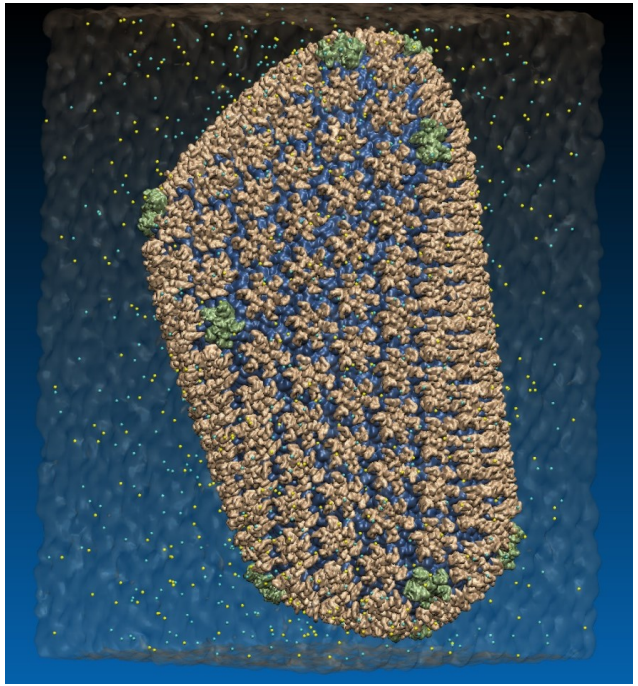
Tamiflu bound to Swine Flu A/H1N1

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.

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

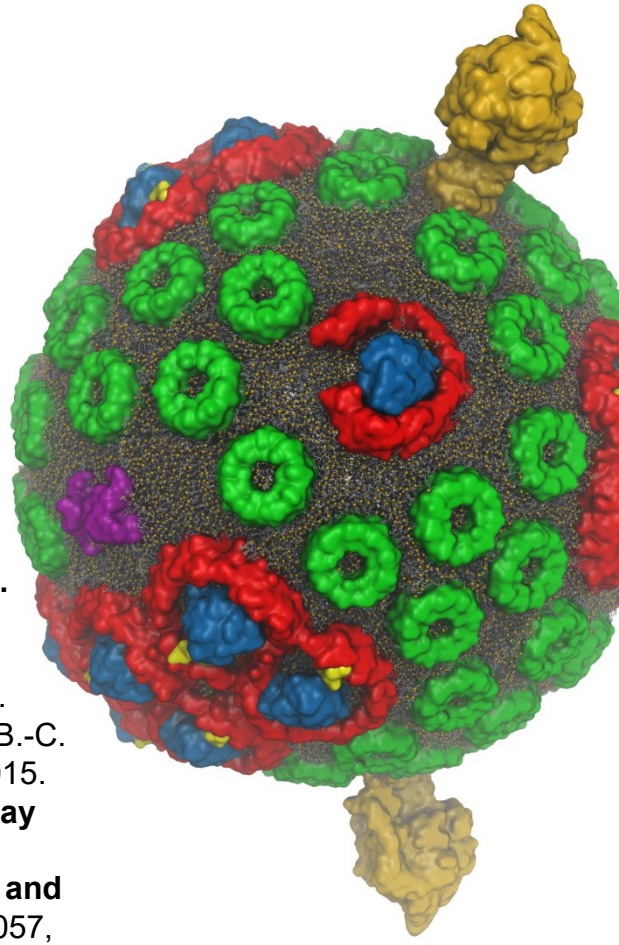


64M atom HIV-1 capsid simulation rendered via EGL

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.

VMD 1.9.3+OptiX 4.0

- 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



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, 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.

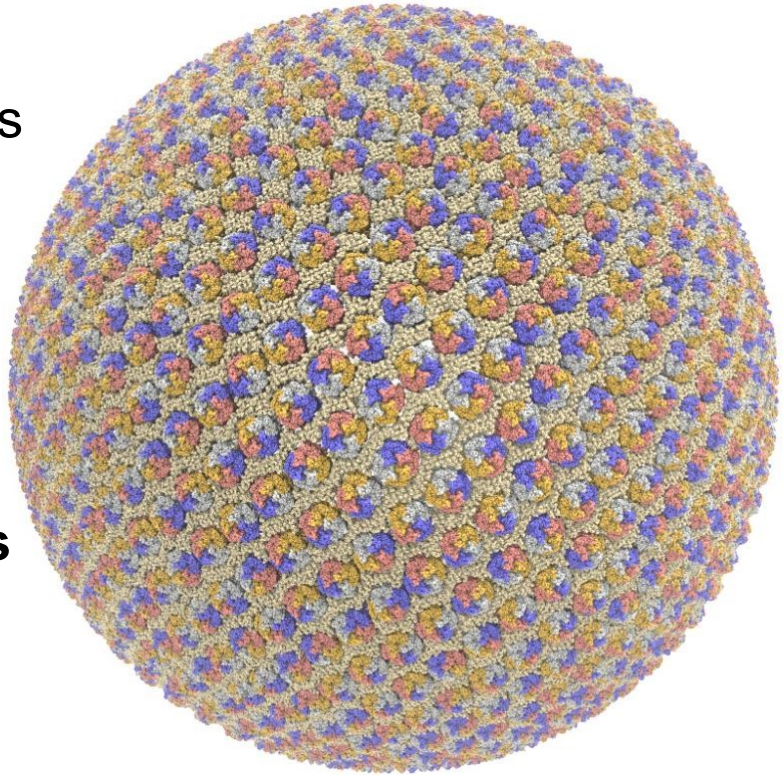
Chemical Visualization of Human Pathogens: the Retroviral Capsids. J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

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.

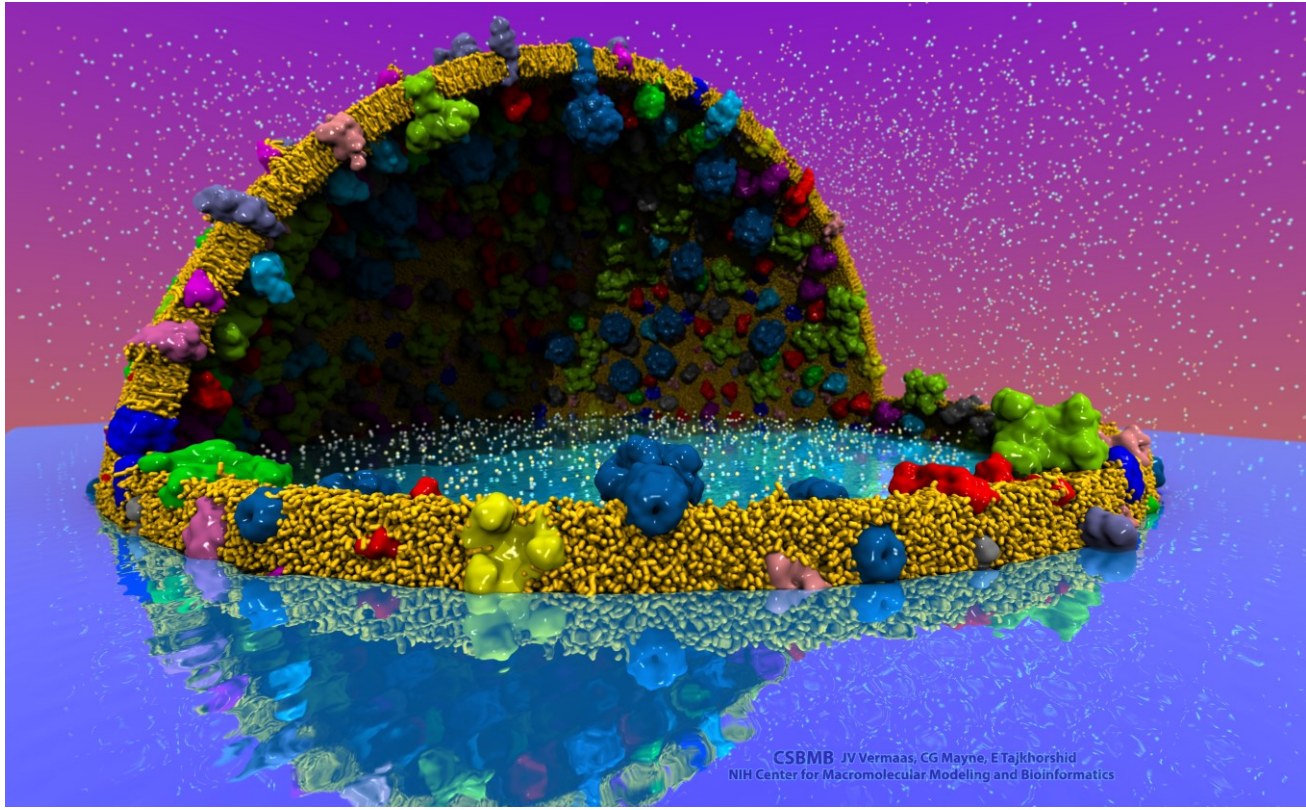
Interactive RT of All-Atom Minimal Cell Envelope

- 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 Kepler GeForce Titan X @ ~12 FPS**
- **Complete model with correct proteins, solvent, etc, will contain billions of atoms**

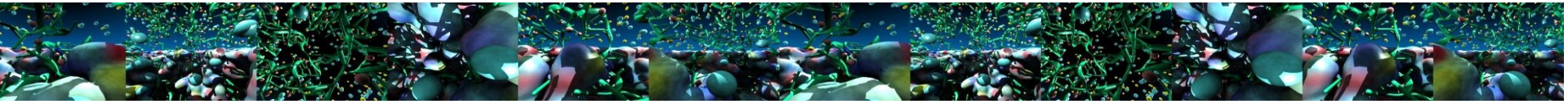


Proto-Cell Rendered with VMD+OptiX

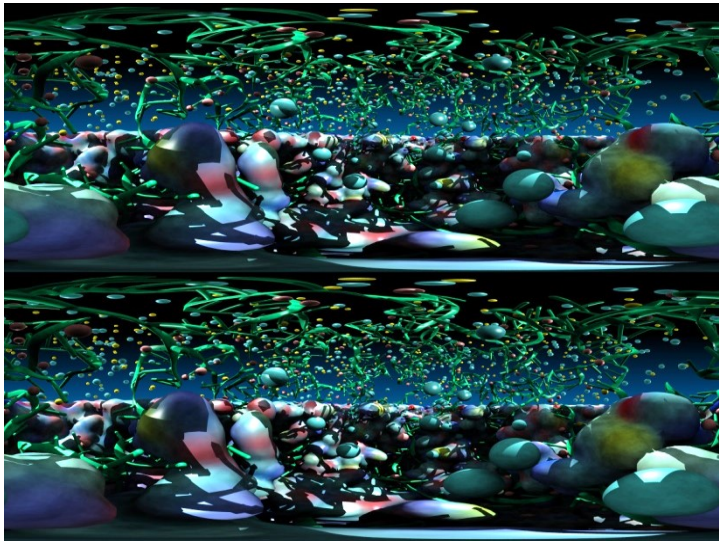
- 113M particles
- 1,397 copies of 14 different membrane proteins
- Preparing for simulations on pre-exascale computers

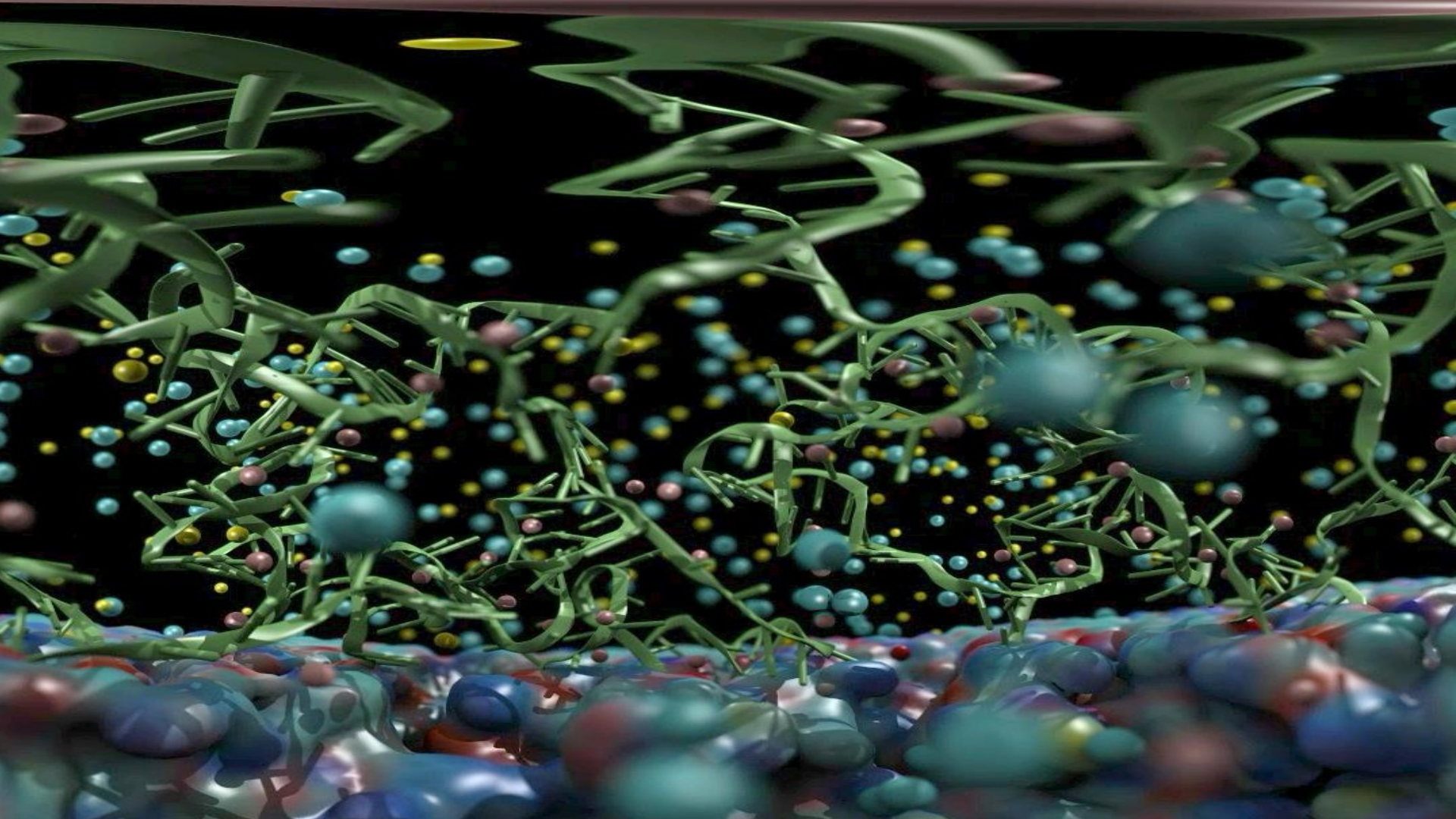


Stereoscopic Panorama Ray Tracing w/ OptiX



- **Render 360° images and movies for VR headsets such as Oculus, Vive, GearVR, Google Cardboard, and YouTube VR**
- 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**





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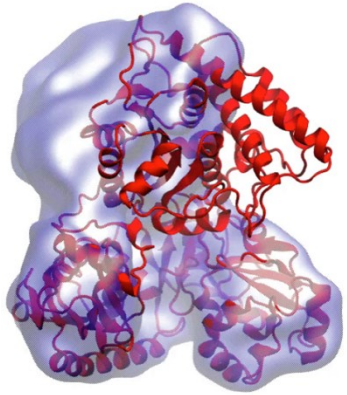
J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE IPDPSW, pp. 1048-1057, 2016.

Molecular Dynamics Flexible Fitting (MDFF)

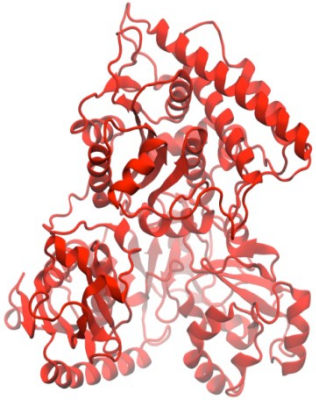
X-ray crystallography → MDFF ← Electron microscopy

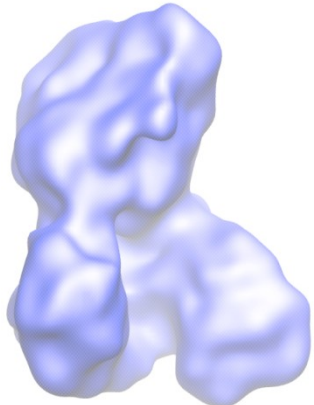
APS at Argonne



FEI microscope

ORNL Titan

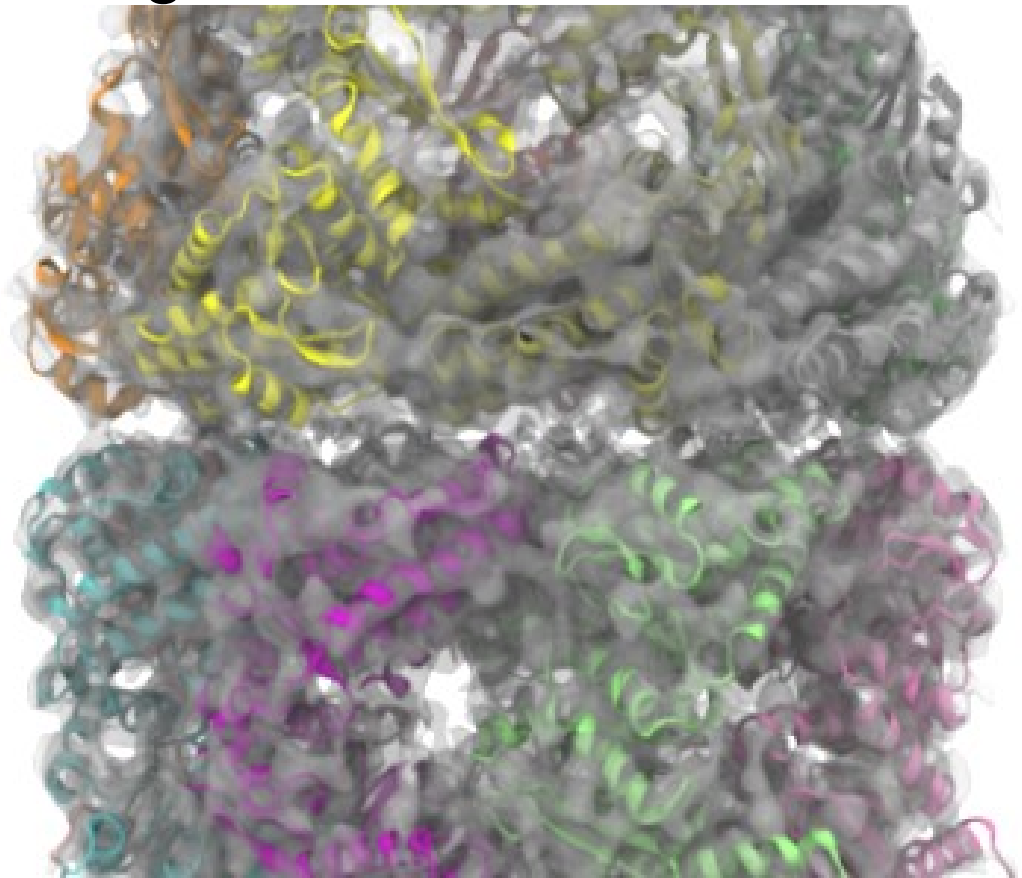




Molecular dynamics-based refinement and validation for sub-5Å cryo-electron microscopy maps. A. Singharoy, I. Teo, R. McGreevy, J. E. Stone, J. Zhao, and K. Schulten. eLife 2016;10.7554/eLife.16105

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

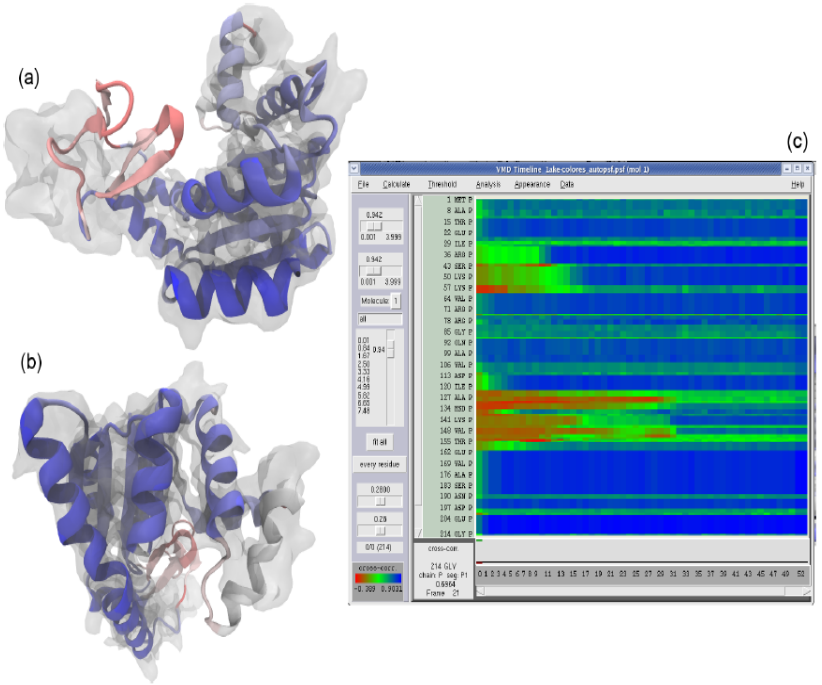
Compute Pearson correlation to evaluate quality-of-fit between a reference **cryo-EM density map** and a **simulated density map** produced from an **all-atom structure**.



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**

Single-Pass MDFF GPU Cross-Correlation

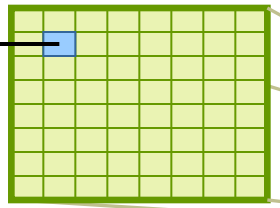
3-D density map decomposes into 3-D grid of 8x8x8 tiles containing CC partial sums and local CC values

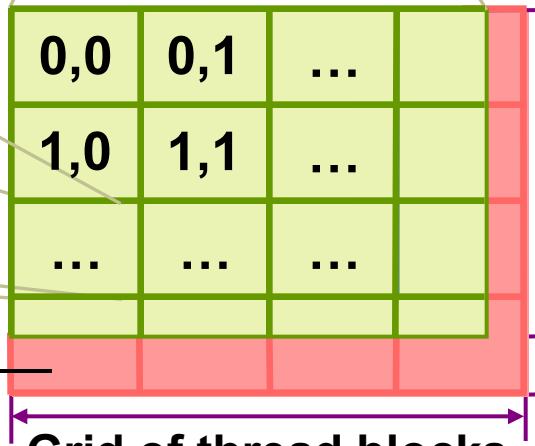
Fusion of density and CC calculations into a single CUDA kernel!!!

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 Tesla P100 Cross Correlation Performance

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

P100 Die-Stacked Mem Accelerates Bandwidth Intensive Calculation

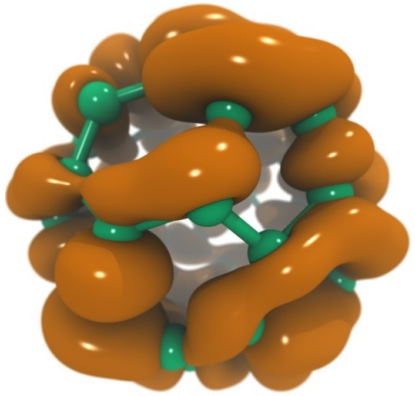
Hardware platform	Runtime, Speedup vs. Chimera,	VMD+GPU
Chimera Xeon E5-2687W (2 socket) [1]	15.860s, 1x	
VMD-CPU IBM Power8 (2 socket) [2]	1.334s, 12x	
VMD-CPU Intel Xeon E5-2660v3 (2 socket) [2]	0.905s, 17x	
VMD-CUDA IBM Power8 + 1x Tesla K40 [2]	0.488s, 32x	**0.9x**
VMD-CUDA Intel Xeon E5-2687W + 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**

[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.

NIH

VMD Tesla P100 Performance for C_{60} Molecular Orbitals, 516x519x507 grid



Hardware platform	Runtime,	Speedup
IBM Power8 (2 socket) (ORNL 'crest') [1]	8.03s,	0.4x
Intel Xeon E5-2660v3 (2 socket) [1]	7.14s,	0.5x
IBM Power8 (ORNL 'crest') + 1x Tesla K40 [1]	3.49s,	**1.0x**
Intel Xeon E5-2698v3 + 1x Tesla P100	**1.35s,**	**2.5x**
IBM Power8 "Minsky" + 1x Tesla P100	**1.09s,**	**3.3x**
IBM Power8 (ORNL 'crest') + 4x Tesla K40 [1]	0.91s,	3.8x
Intel Xeon E5-2698v3 + 4x Tesla P100	**0.37s,**	**9.4x**
IBM Power8 "Minsky" + 4x Tesla P100	**0.30s,**	**11.6x**

NVLink perf. boost w/ no code tuning

[1] 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.

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Come See the VMD+Unreal Chromatophore VR Demo in the NVIDIA VR Room!

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- CUDA Center of Excellence, University of Illinois at Urbana-Champaign
- NVIDIA CUDA, OptiX, GL/EGL teams, and PSG cluster admins
- IBM and NVIDIA for access to “Minsky” Power8+P100 hardware
- NCSA Blue Waters Team, ORNL Titan Team, ORNL CAAR
- 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


NIH BTRC for Macromolecular Modeling and Bioinformatics
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Urbana-Champaign

Related Publications

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

- **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),pp. 1048-1057, 2016.
- **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), pp. 1014-1023, 2016.
- **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), pp. 89-100, 2016.
- **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, 55:17-27, 2016.
- **Chemical Visualization of Human Pathogens: the Retroviral Capsids.** Juan R. Perilla, Boon Chong Goh, John E. Stone, and Klaus Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

Related Publications

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

- **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.

Related Publications

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

- **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.
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