

# Putting High-Octane GPU-Accelerated Molecular Modeling Tools in the Hands of Scientists

John E. Stone

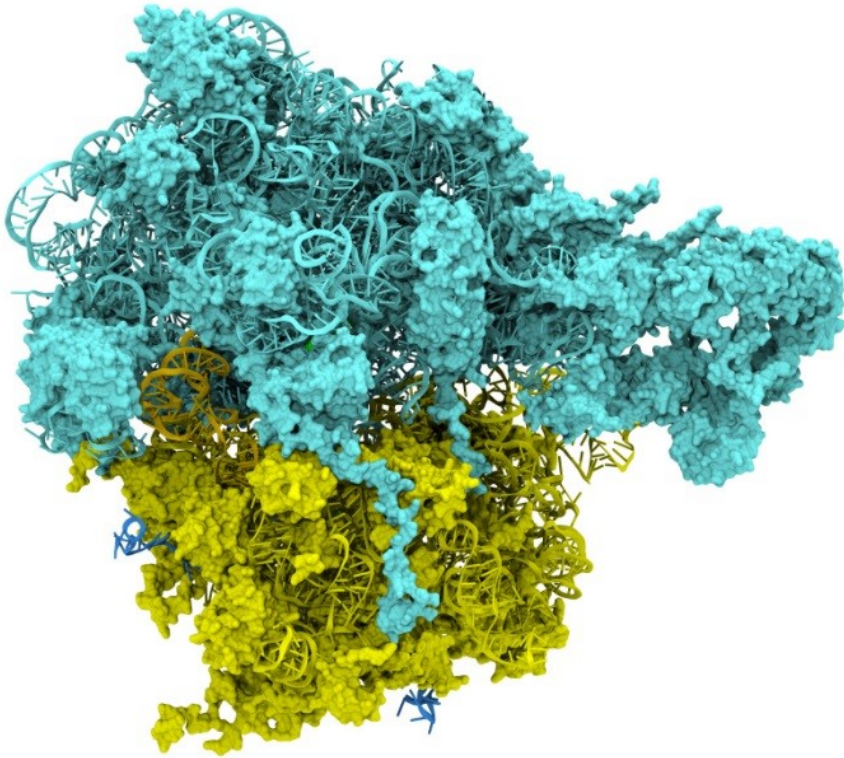
Theoretical and Computational Biophysics Group  
Beckman Institute for Advanced Science and Technology  
University of Illinois at Urbana-Champaign  
**<http://www.ks.uiuc.edu/Research/cloud/>**

10:30am-10:55am, NVIDIA Theater, Supercomputing 2018,  
Dallas, TX, Tuesday, November 13<sup>th</sup>, 2018

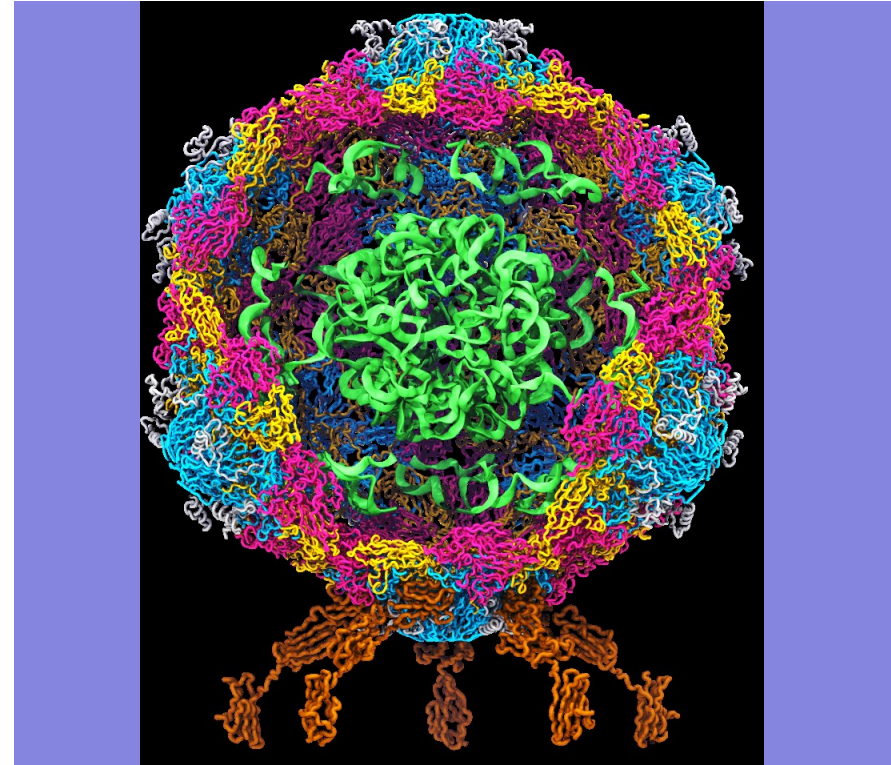
# Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

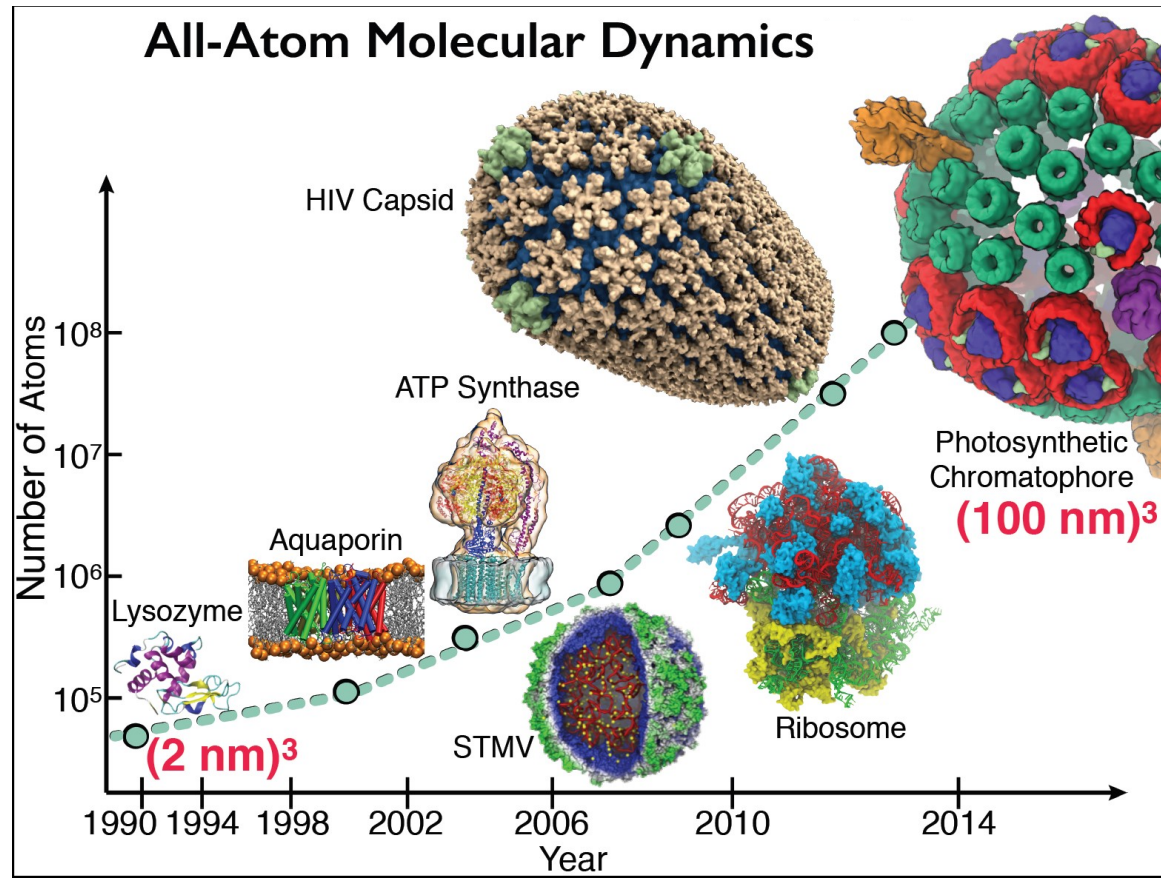


Poliovirus



# Goal: A Computational Microscope

Study the molecular machines in living cells



# NAMD Highlights

- **Parallel Molecular Dynamics**
- Over 12,600 citations of NAMD
- One program available on all platforms.
  - Desktops and laptops – setup and testing
  - Linux clusters – affordable local workhorses
  - Supercomputers – free allocations on XSEDE
  - Blue Waters – sustained petaflop/s performance
  - **GPUs – from desktop to supercomputer**
- User knowledge is preserved across platforms.
  - No change in input or output files.
  - Run any simulation on **any number of cores.**
- Available free of charge to all.

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



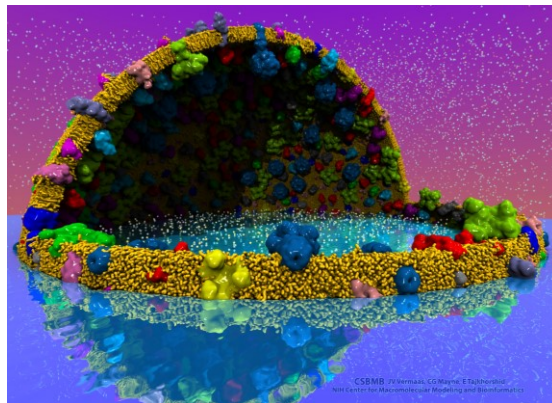
Hands-On Workshops



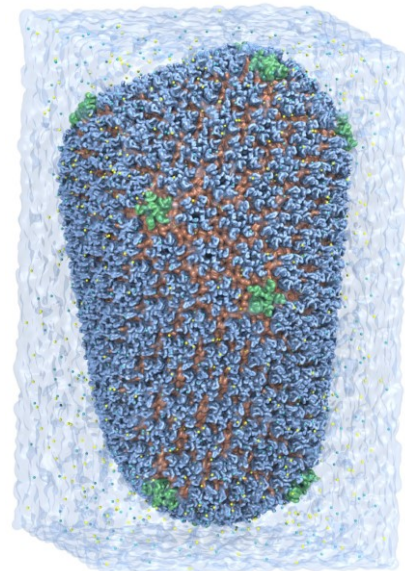
Oak Ridge TITAN

# VMD – “Visual Molecular Dynamics”

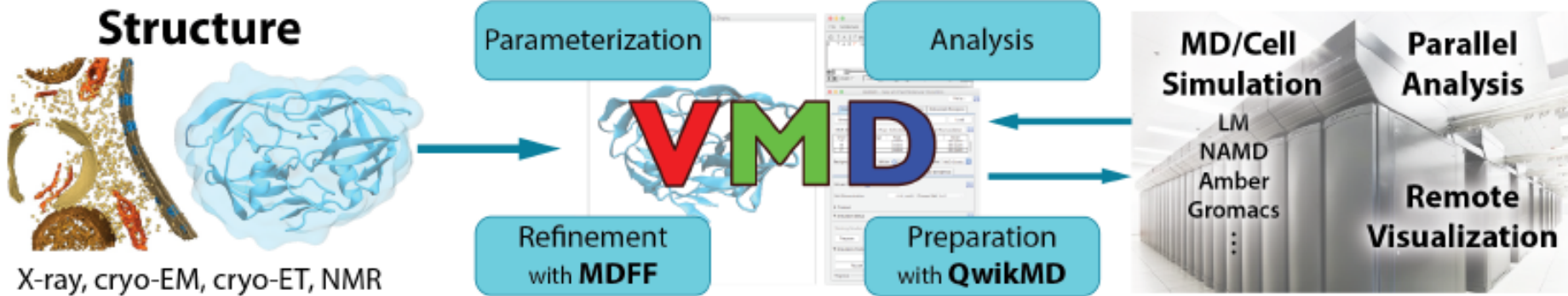
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Sequence information
- User extensible scripting and plugins
- <http://www.ks.uiuc.edu/Research/vmd/>



Cell-Scale Modeling



MD Simulation



# Making Our Research Tools Easily Accessible

- Cloud based deployment
  - Full virtual machines (known as “AMI” in Amazon terminology)
  - Amazon AWS EC2 GPU-accelerated instances:  
<http://www.ks.uiuc.edu/Research/cloud/>
- Docker “container” images available in NVIDIA NGC registry
  - Users obtain Docker images via registry, download and run on the laptop, workstation, cloud, or supercomputer of their choosing
  - <https://ngc.nvidia.com/registry/>
  - <https://ngc.nvidia.com/registry/hpc-vmd>



## Research articles incorporating use of Amazon AWS EC2:

**Molecular dynamics-based refinement and validation for sub-5 Å cryo-electron microscopy maps.** Abhishek Singharoy, Ivan Teo, Ryan McGreevy, John E. Stone, Jianhua Zhao, and Klaus Schulten. *eLife*, 10.7554/eLife.16105, 2016. (66 pages).

**QwikMD-integrative molecular dynamics toolkit for novices and experts.** Joao V. Ribeiro, Rafael C. Bernardi, Till Rudack, John E. Stone, James C. Phillips, Peter L. Freddolino, and Klaus Schulten. *Scientific Reports*, 6:26536, 2016.

**High performance molecular visualization: In-situ and parallel rendering with EGL.** John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014-1023, 2016.

# Easy to Launch: AWS EC2 Marketplace

 aws marketplace



Hello, Johns ▾

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[Migration Mapping Assistant](#)

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[Partners](#)

[Sell in AWS Marketplace](#)

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**NAMD&VMD**  
Molecular Dynamics Packages

## VMD and NAMD

By: [TCBG](#) Latest Version: 0.4.0

VMD is a high-performance molecular graphics viewer, used for displaying molecular structures, viewing sequence information, and for structure generation

▾ [Show more](#)

Linux/Unix



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Typical Total Price  
**\$0.650/hr**

Total pricing per instance for services hosted on g2.2xlarge in US East (N. Virginia). [View Details](#)

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## Product Overview

VMD is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more general molecules, as VMD can read

[Highlights](#)

# NAMD+VMD AWS EC2 AMIs

## Production AMI:

- (ami-a01125df) VMD-NAMD-VNC-R1.9.4.1, 64-bit Ubuntu Linux, EBS storage, HVM, created July 10, 2018

## Pre-release or developmental AMI:

- (ami-ac604ed3) 64-bit Centos 7.5 Linux, EBS storage, HVM
- This is an experimental image using Centos and [DCV](#) for increased remote visualization performance and smoother interaction. This image will only run on g3 instance types.
- Newer DCV-capable AMIs coming soon...



# VMD / NAMD / LM, NGC Containers

## Registry

[Get API Key](#)



### Documentation

How to use NGC containers on supported platforms >

### Repositories

**nvidia** ^

**hpc** v

- candle
- gamess
- gromacs
- lammps
- lattice-microbes
- namd
- relion
- vmd

**nvidia-hpcvis** v

- index
- paraview-holodeck
- paraview-index
- paraview-optim

### hpc/vmd

```
docker pull nvcr.io/hpc/vmd:cuda9-ubuntu1604-egl-1.9.4a17
```

## VMD

VMD is designed for modeling, visualization, and analysis of biomolecular systems such as proteins, nucleic acids, lipid membranes, carbohydrate structures, etc. VMD provides a wide variety of graphical representations for visualizing and coloring molecular structures: molecular surfaces, space-filling CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, secondary structure cartoons, and others.

VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VMD can act as a graphical front end for an external MD program by

# Molecular Dynamics Flexible Fitting (MDFF)

X-ray crystallography



APS at Argonne

MDFF

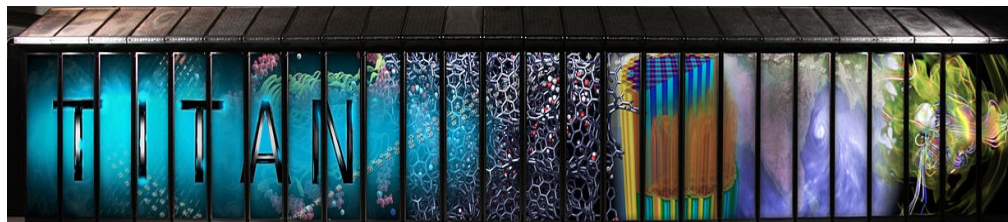
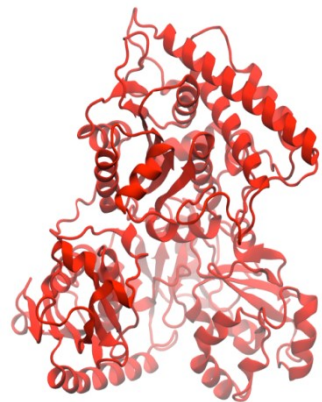


Electron microscopy

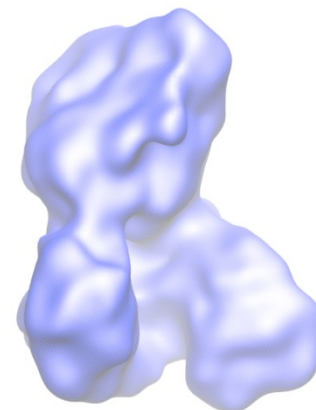


FEI microscope

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



# Molecular Dynamics Flexible Fitting - Theory

Two terms are added to the MD potential

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

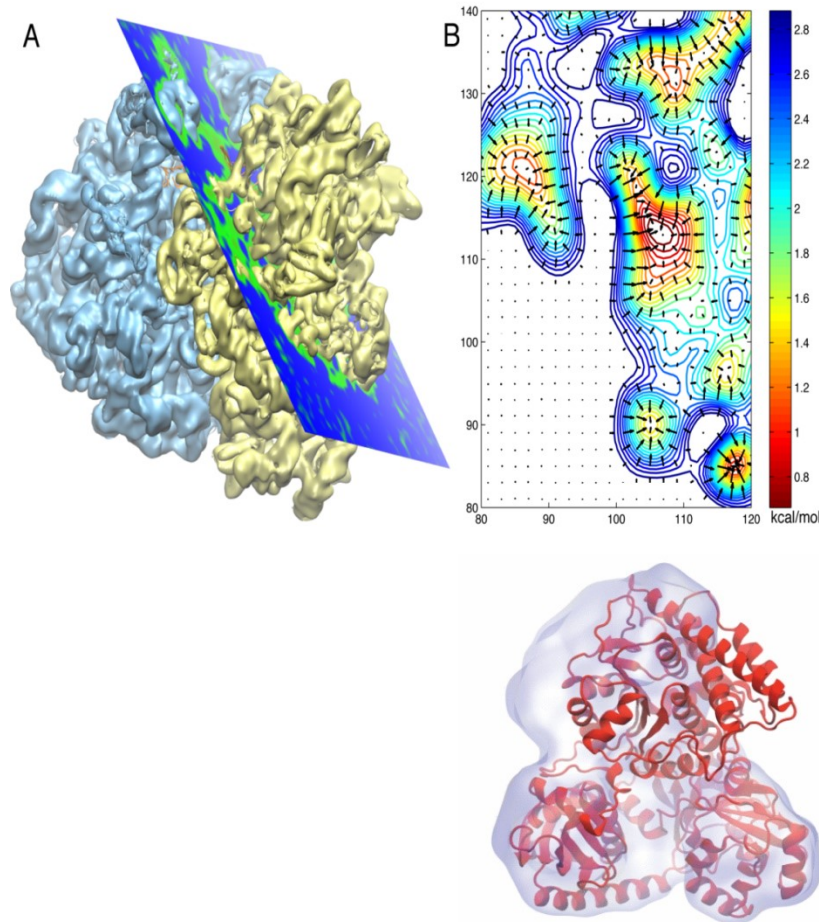
An external potential derived from the EM map is defined on a grid as

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

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

A mass-weighted force is then applied to each atom

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



# MDFF on the Cloud Costs Less than a Cup of Coffee

ReMDFF (Resolution Exchange) requires many cores but little compute time, making it a good candidate for cloud computing

Singharoy, *et al.* eLife 2016

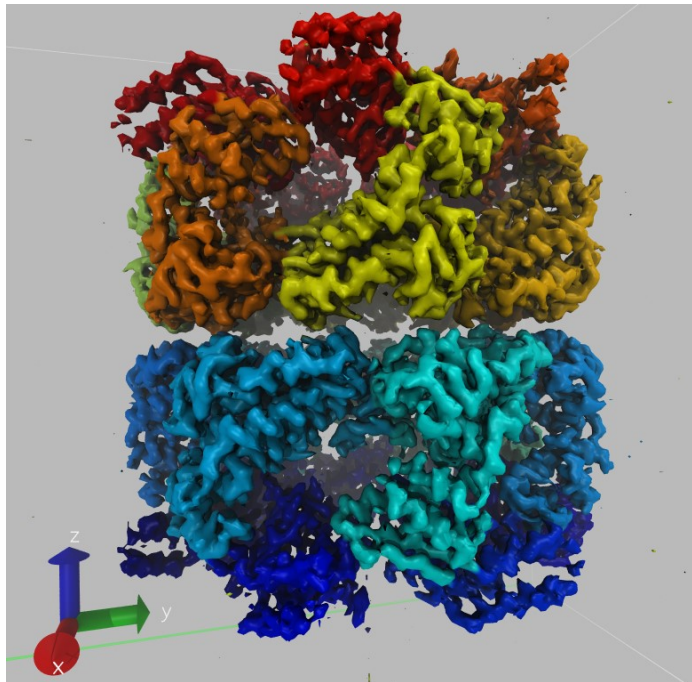
Molecule	Instance	Performance (ns/day)	Time (hours)	Simulation Cost / ns (\$)
Adenylate Kinase	p3.2xlarge	112	0.2	0.67
Acetyl-CoA Synthase	p3.2xlarge	82	0.3	0.89
J1 Nitrilase	p3.2xlarge	5	4.8	14.6



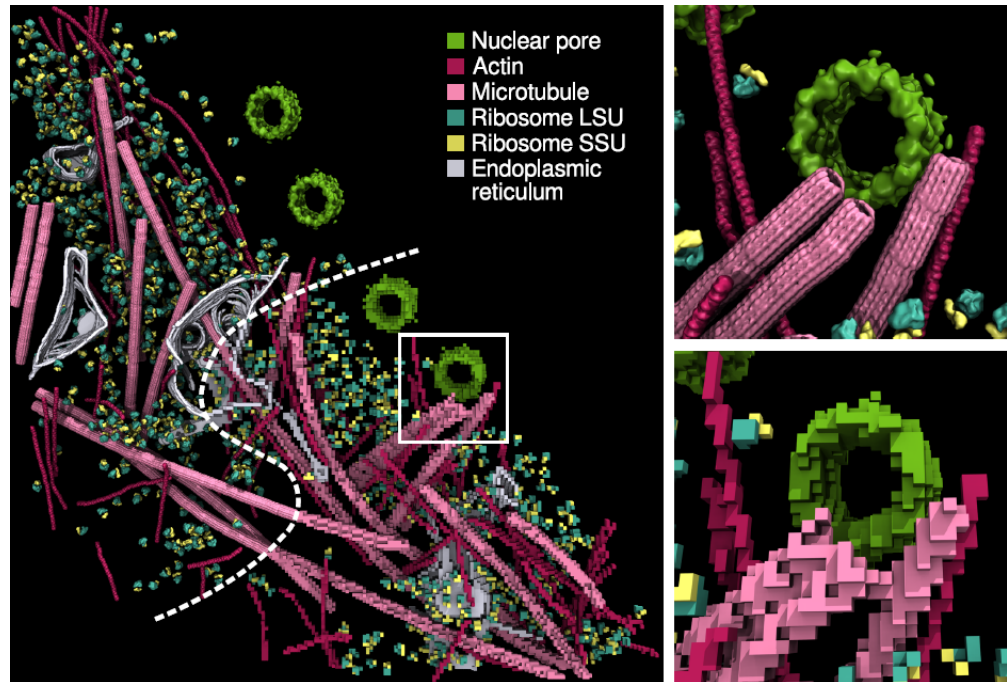
Cloud computing allows researchers to focus on the scientific challenges of their project without having to worry about local availability and administration of suitable computer hardware and installing or compiling software.



# Density Map Segmentation



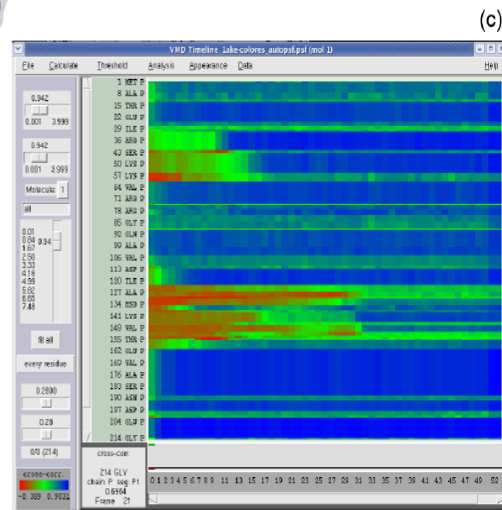
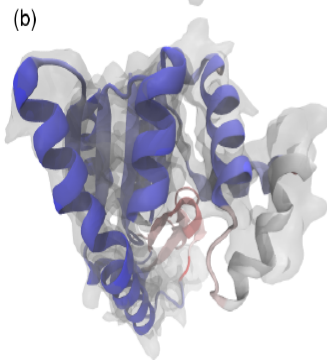
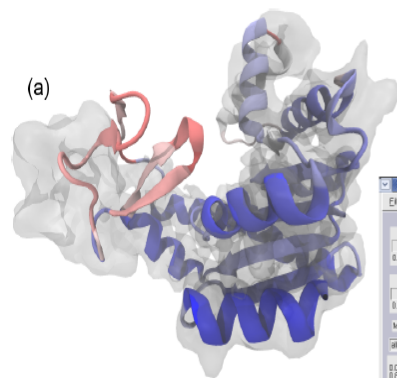
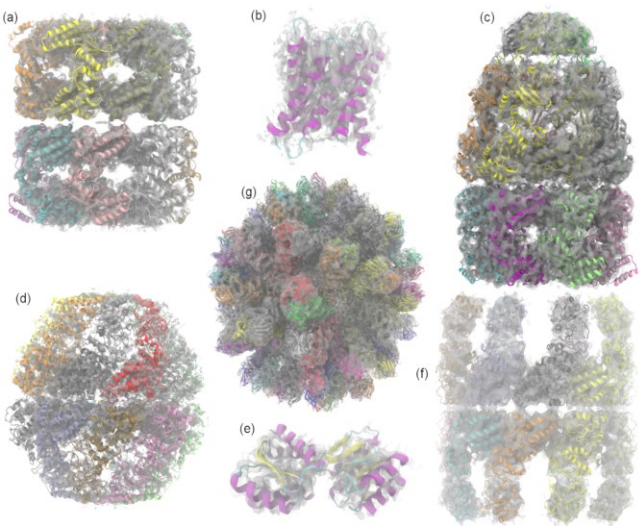
VMD GPU-accelerated density map segmentation of GroEL



Earnest, et al. *J. Physical Chemistry B*, 121(15): 3871-3881, 2017.

# 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** from an **all-atom structure**.



**MDFF Cross Correlation Timeline**  
**Regions with poor fit**      **Regions with good fit**

# VMD Tesla V100 Cross Correlation Performance

Rabbit Hemorrhagic Disease Virus: 702K atoms, 6.5Å resolution  
Volta GPU architecture almost 2x faster than previous gen Pascal:

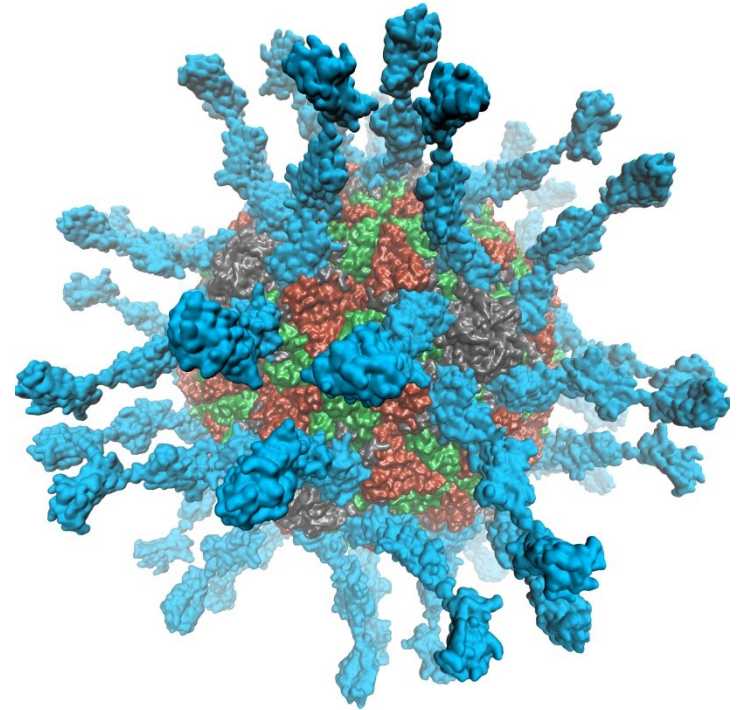
Application and Hardware platform	Runtime, Speedup vs. Chimera, VMD+GPU
Chimera Xeon E5-2687W (2 socket) [1]	15.860s, 1x
VMD-CUDA IBM Power8 + 1x Tesla K40 [2]	0.488s, 32x <b>0.9x</b>
VMD-CUDA Intel Xeon E5-2687W + 1x Quadro K6000 [1,2]	0.458s, 35x <b>1.0x</b>
<b>VMD-CUDA Intel Xeon E5-2698v3 + 1x Tesla P100</b>	<b>0.090s,</b> 176x <b>5.1x</b>
<b>VMD-CUDA IBM Power8 “Minsky” + 1x Tesla P100</b>	<b>0.080s,</b> 198x <b>5.7x</b>
<b>VMD-CUDA Intel Xeon E5-2697Av4 + 1x Tesla V100</b>	<b>0.050s,</b> 317x <b>9.2x</b>
<b>VMD-CUDA IBM Power9 “Newell” + 1x Tesla V100</b>	<b>0.049s,</b> 323x <b>9.3x</b>

[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.

# VMD supports EGL for in-situ and parallel rendering on Amazon EC2

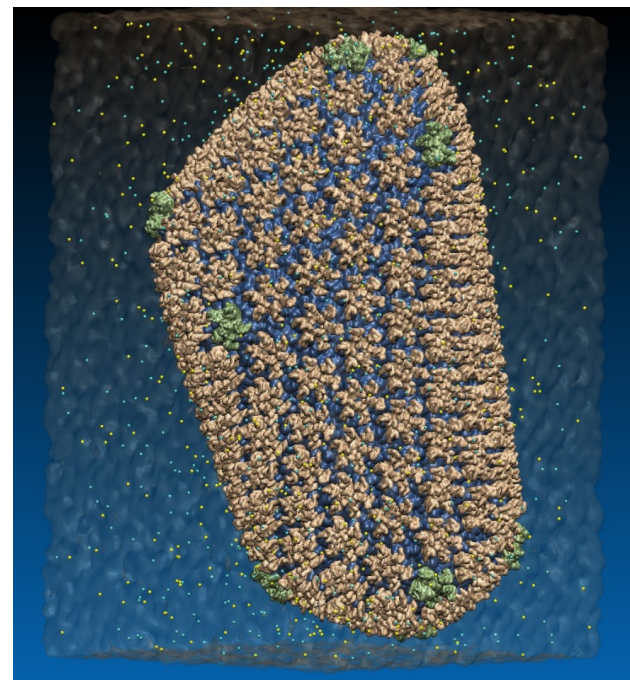
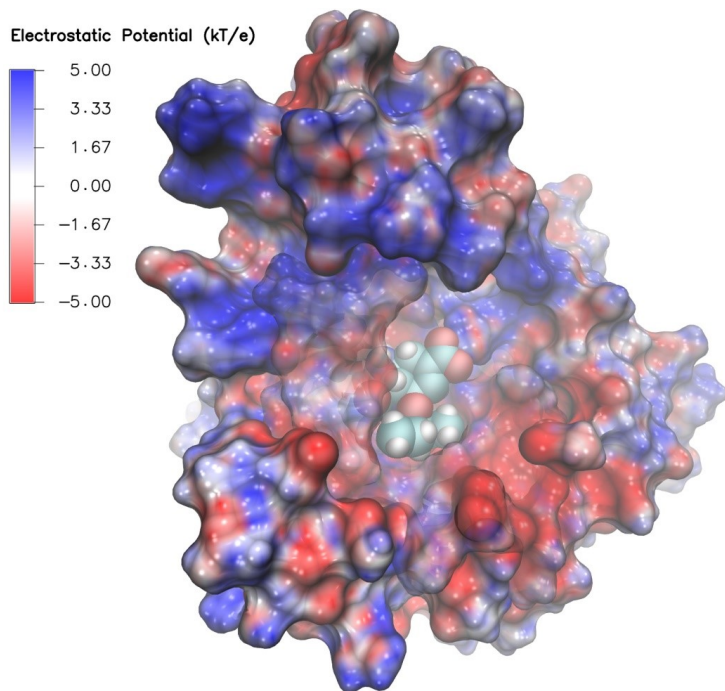
- **No windowing system dependency**
- Easily deploy parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features



**Poliovirus**



# VMD EGL Rendering: Supports full VMD GLSL shading features Vulkan support coming soon...



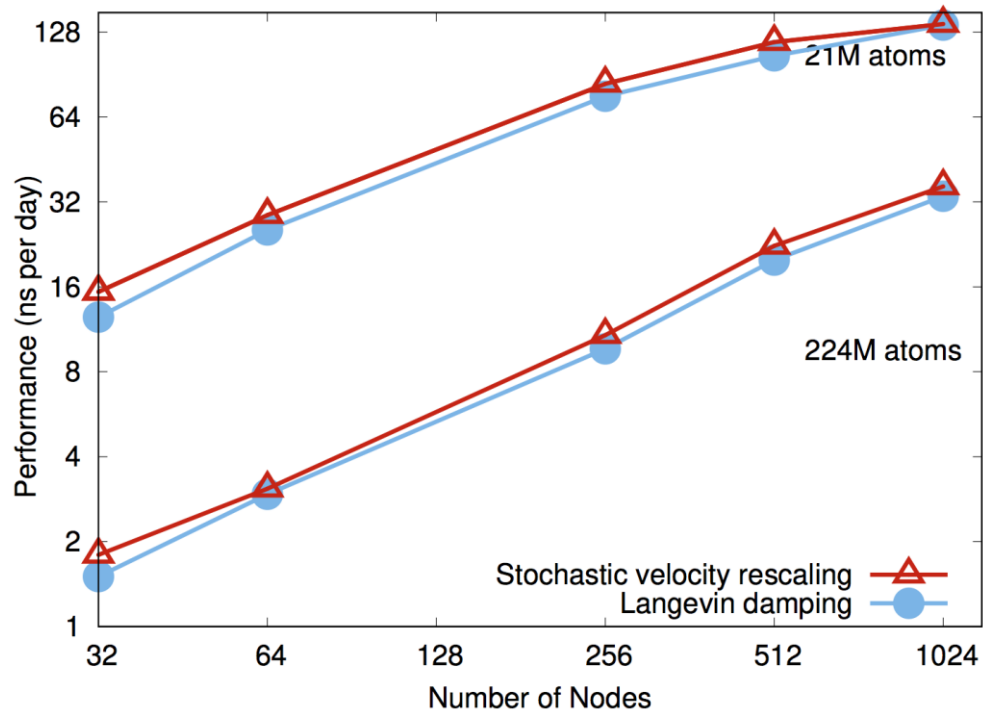
**Swine Flu A/H1N1 neuraminidase bound to Tamiflu**

**64M atom HIV-1 capsid simulation**

**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.

# NAMD on Summit, May 2018



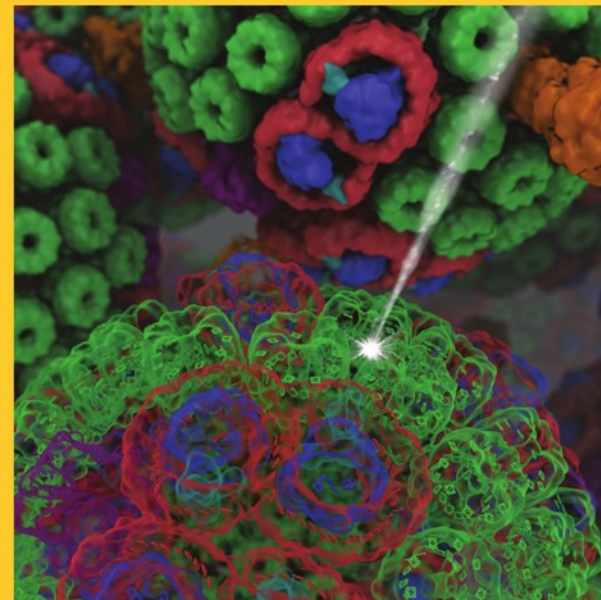
**NAMD simulations can generate up to 10TB of output per day on 20% of Summit**

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THE JOURNAL OF  
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CHEMISTRY**

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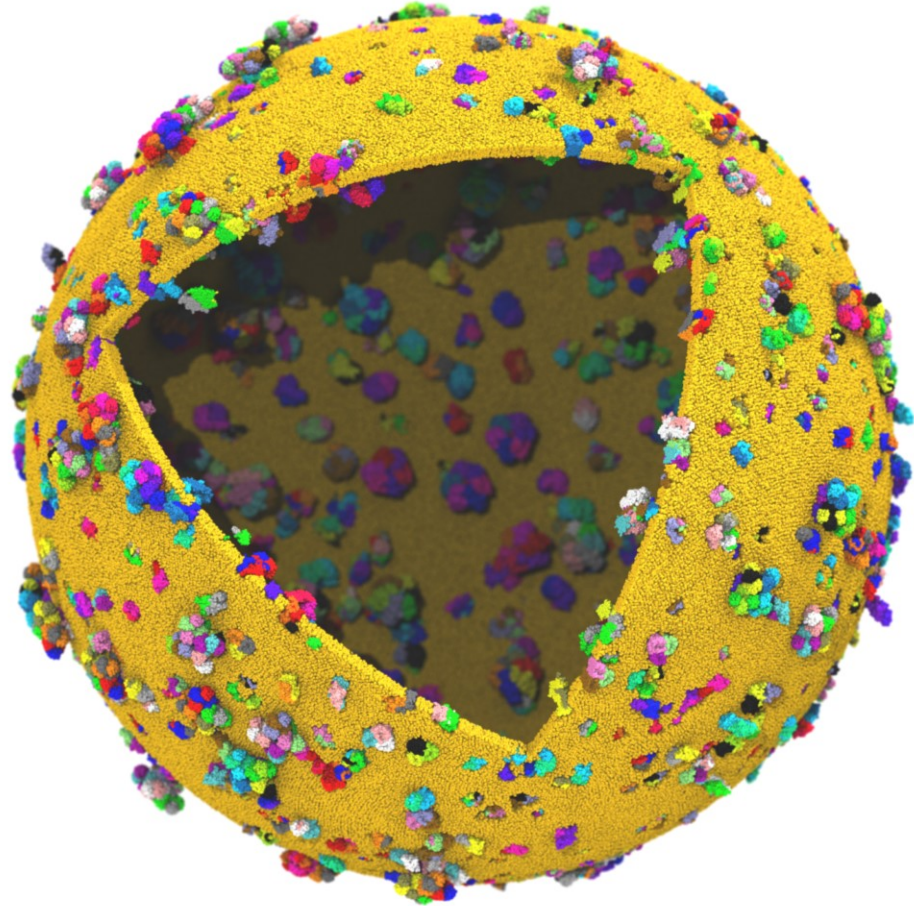
KLAUS SCHULTEN MEMORIAL ISSUE

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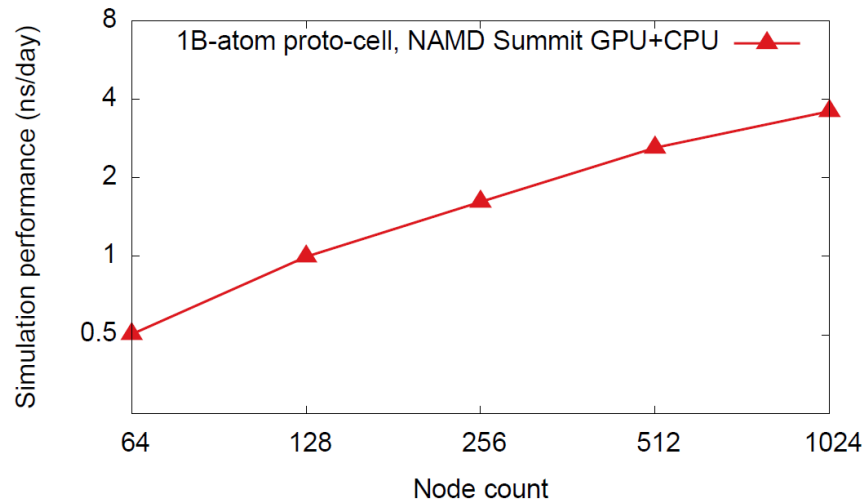
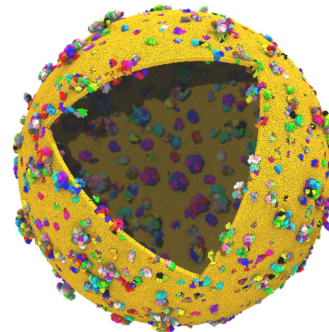
# Next Generation: Simulating a Proto-Cell

- **ORNL Summit:  
NVLink-connected Tesla V100  
GPUs enable next-gen  
visualizations**
- 200nm diameter
- ~1 billion atoms w/ solvent
- ~1400 proteins in membrane



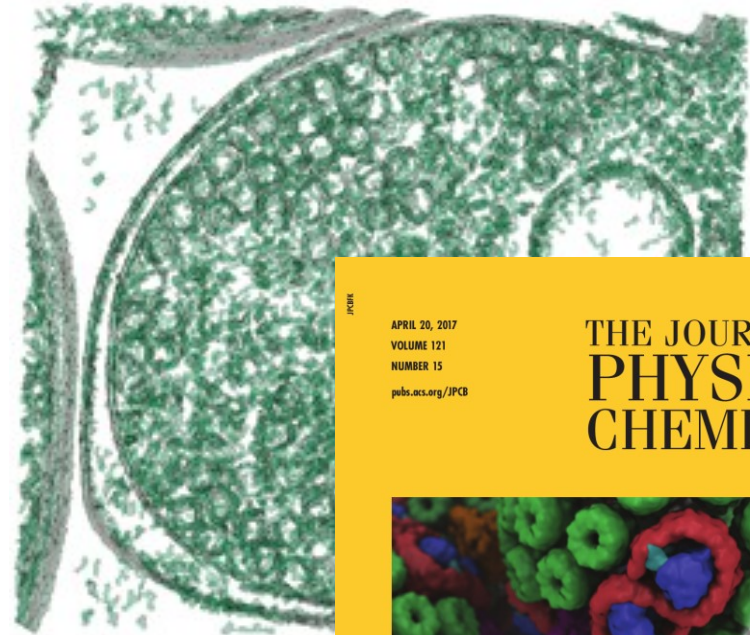
# Proto-Cell Data Challenges

- **1B-atom proto-cell requires nodes with more than TB RAM to build complete model...**
- **1B-atom proto-cell binary structure file: 63GB**
- **Trajectory frame atomic coordinates: 12GB, 1.2TB/ns of simulation (1 frame per 10ps)**
- **Routine modeling and visualization tasks are a big challenge at this scale**
  - **Models contain thousands of atomic-detail components** that must work together in harmony
  - **Exploit persistent memory technologies** to enable “instant on” operation on massive cell-scale models – eliminate several minutes of startup during analysis/visualization of known structure
  - **Sparse output of results at multiple timescales** will help ameliorate visualization and analysis I/O
- **Need for in-situ and remote visualization**



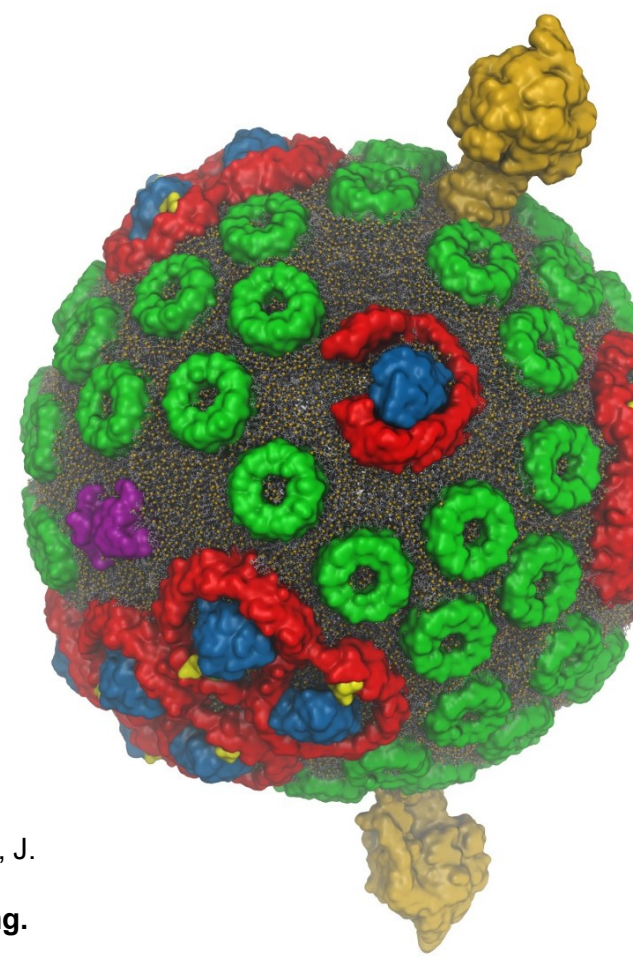
# NEW: Cloud-Based Interactive Remote Visualization

- Built-into VMD itself
- Enable access to massive data sets
- Uses GPU H.264 / HEVC hardware accelerated video encode/decode
- Supports interactive remote visualizations (both rasterization and ray tracing)
- Development ongoing, expected in next major VMD release, in 1H 2019...



# VMD Interactive Ray Tracing

- **Exploit computational power to improve rendering of the structural details of biomolecular complexes**
- **Remote visualization tasks on very large macromolecular complexes**
- High fidelity shading, shadows, AO lighting, depth of field, ...



**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.

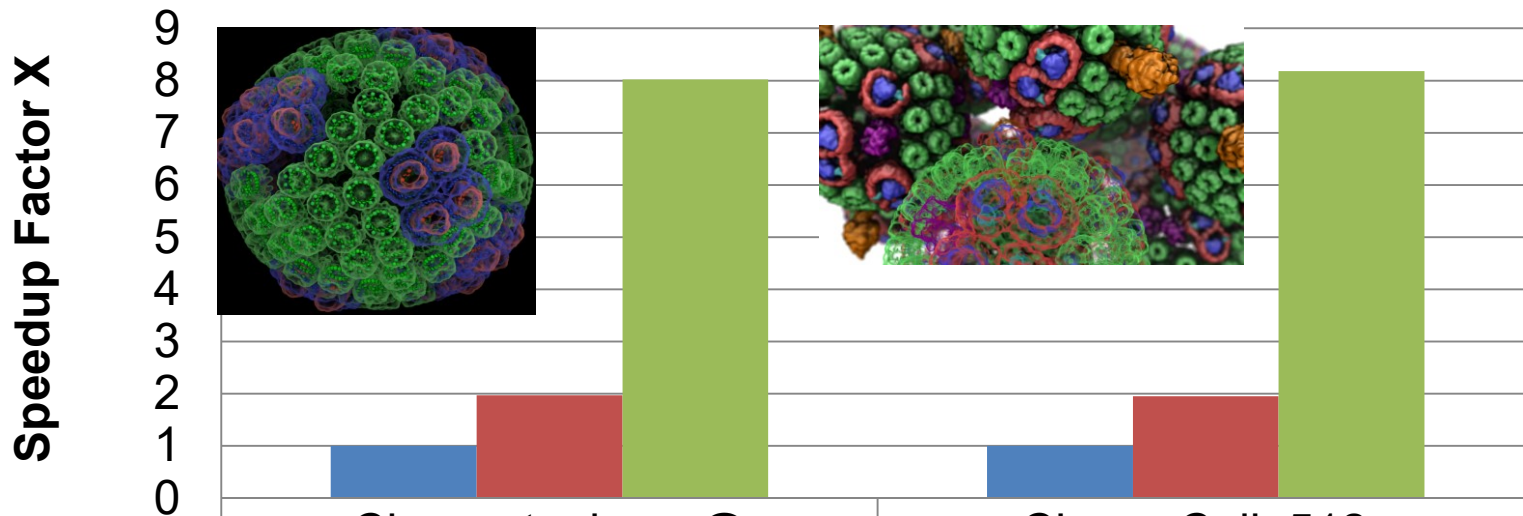
**Chemical Visualization of Human Pathogens: the Retroviral Capsids.** J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.

**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.

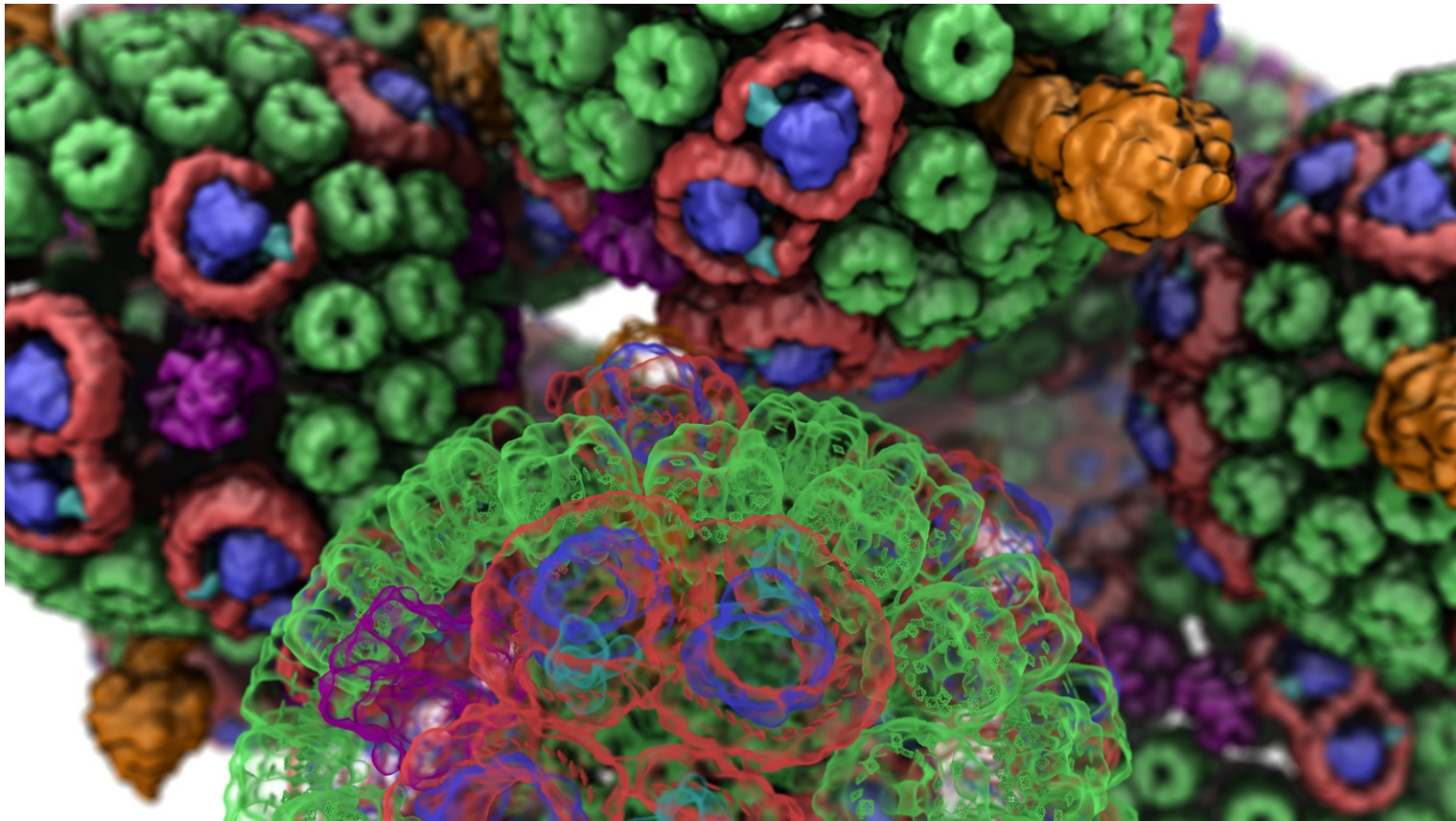
**VMD/OptiX GPU Ray Tracing of all-atom Chromatophore w/ lipids.**

# VMD OptiX RT performance on Quadro RTX 6000



	Chromatophore @ 4Kx4K	Chrom Cell, 512x DoF @ 1080p
■ Quadro GV100	1	1
■ 2x Quadro GV100	1.97	1.95
■ Quadro RTX 6000	8.02	8.18

# VMD/OpiX RTX Acceleration





# VMD/NAMD NGC Containers, Amazon EC2 AMIs

<http://www.ks.uiuc.edu/Research/cloud/>

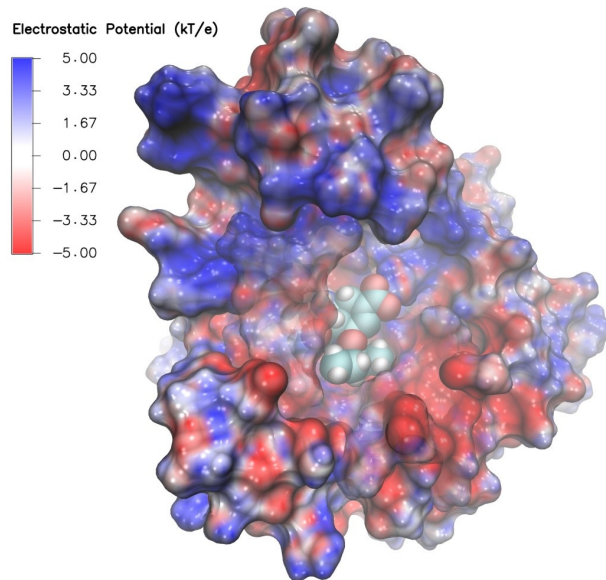
<https://ngc.nvidia.com/registry/>

NAMD

- **CUDA-accelerated simulation**

VMD:

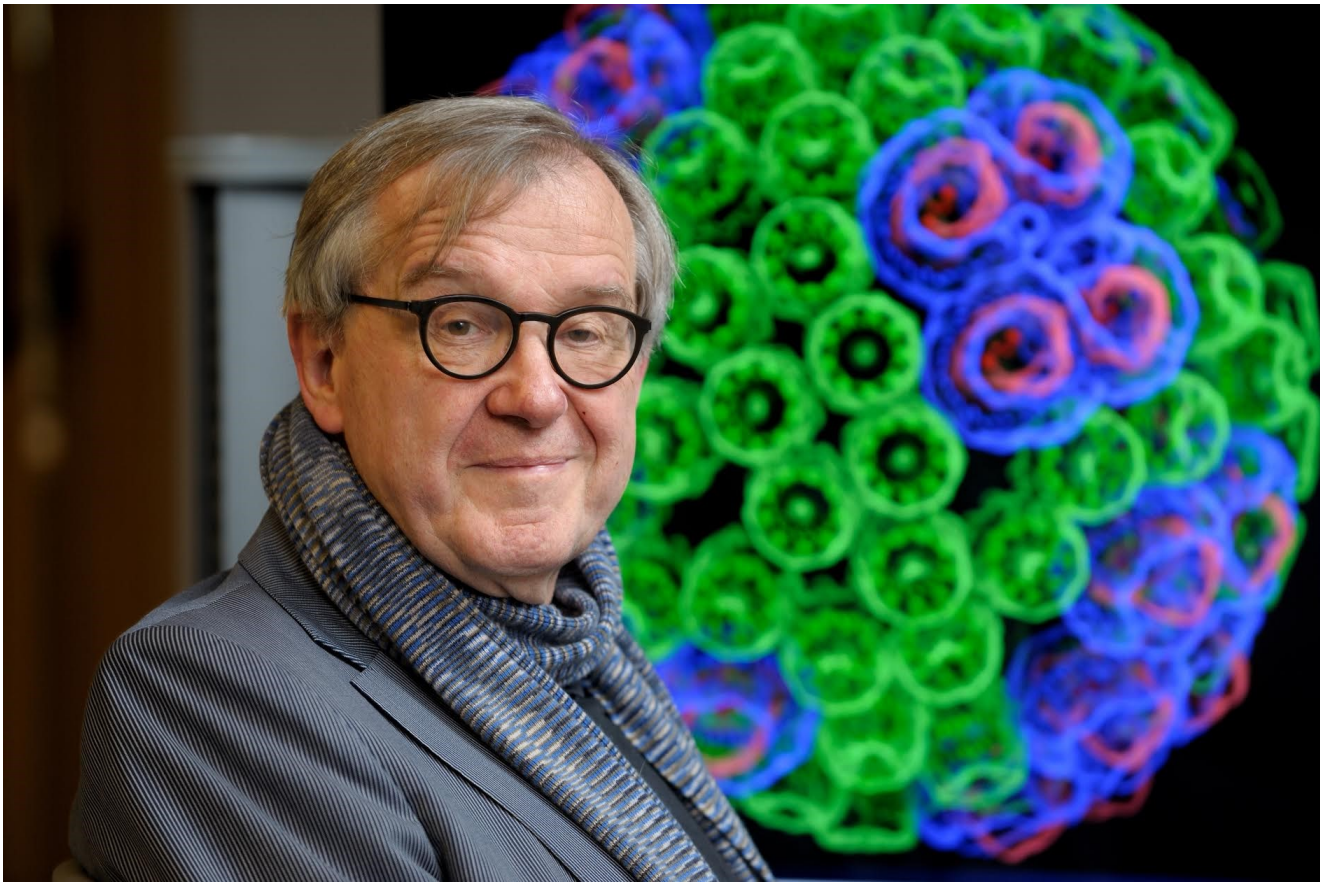
- CUDA-accelerated analysis
- EGL off-screen rendering – no windowing system needed
- OptiX high-fidelity GPU ray tracing engine built in
- **NEW: Remote Visualization Streaming**
- All dependencies included
- **Easy to deploy on diverse GPU accelerated platforms**



**High performance molecular visualization: In-situ and parallel rendering with EGL.** J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014-1023, 2016.

# 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*

# Related Publications

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

- **Scalable Molecular Dynamics with NAMD on the Summit System.** B. Acun, D. J. Hardy, L. V. Kale, K. Li, J. C. Phillips, and J. E. Stone. (In press)
- **NAMD goes quantum: An integrative suite for hybrid simulations.** Melo, M. C. R.; Bernardi, R. C.; Rudack T.; Scheurer, M.; Riplinger, C.; Phillips, J. C.; Maia, J. D. C.; Rocha, G. D.; Ribeiro, J. V.; Stone, J. E.; Neese, F.; Schulten, K.; Luthey-Schulten, Z.; Nature Methods 15:351-354, 2018.
- **Challenges of Integrating Stochastic Dynamics and Cryo-electron Tomograms in Whole-cell Simulations.** T. M. Earnest, R. Watanabe, J. E. Stone, J. Mahamid, W. Baumeister, E. Villa, and Z. Luthey-Schulten. J. Physical Chemistry B, 121(15): 3871-3881, 2017.
- **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, and K. Schulten. International Workshop on OpenPOWER for HPC (IWOPH'16), LNCS 9945, pp. 188-206, 2016.
- **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 Distributed Processing Symposium Workshop (IPDPSW), pp. 1048-1057, 2016.
- **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 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.** J. E. Stone, M. J. Hallock, J. C. Phillips, J. R. Peterson, Z. Luthey-Schulten, and K. Schulten. 25th International Heterogeneity in Computing Workshop, IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW), pp. 89-100, 2016.

# Related Publications

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

- **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.
- **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*, 26(5):1405-1418, 2015.
- **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.
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