Bringing State-of-the-Art GPU-Accelerated Molecular Modeling Tools to the Research Community

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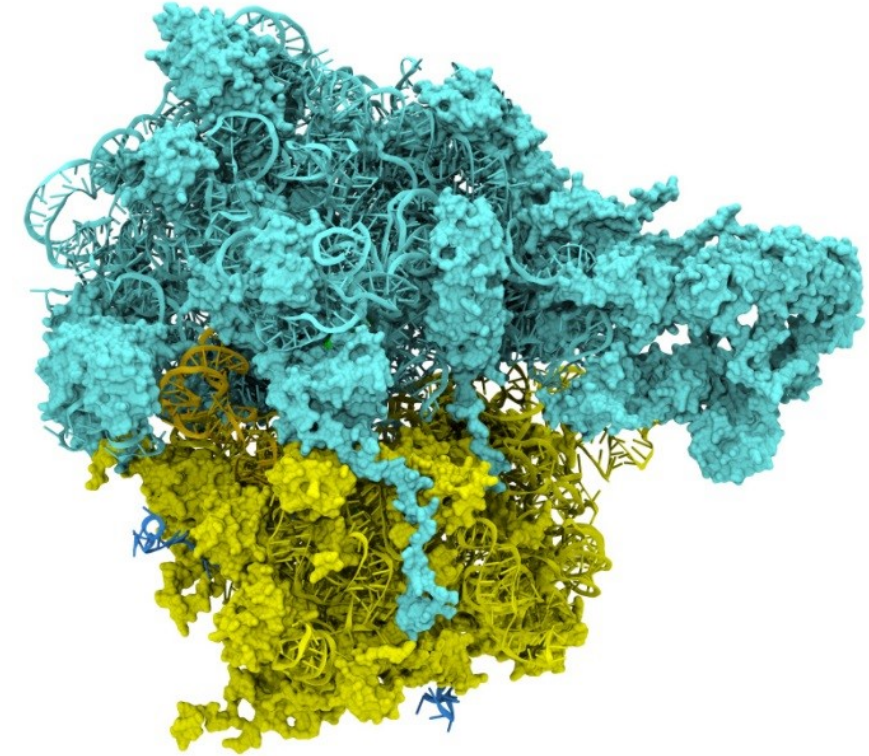
http://www.ks.uiuc.edu/

10:00am-10:50am, San Carlos Room, Hilton Hotel
San Jose, CA, Wednesday, March 20th, 2019

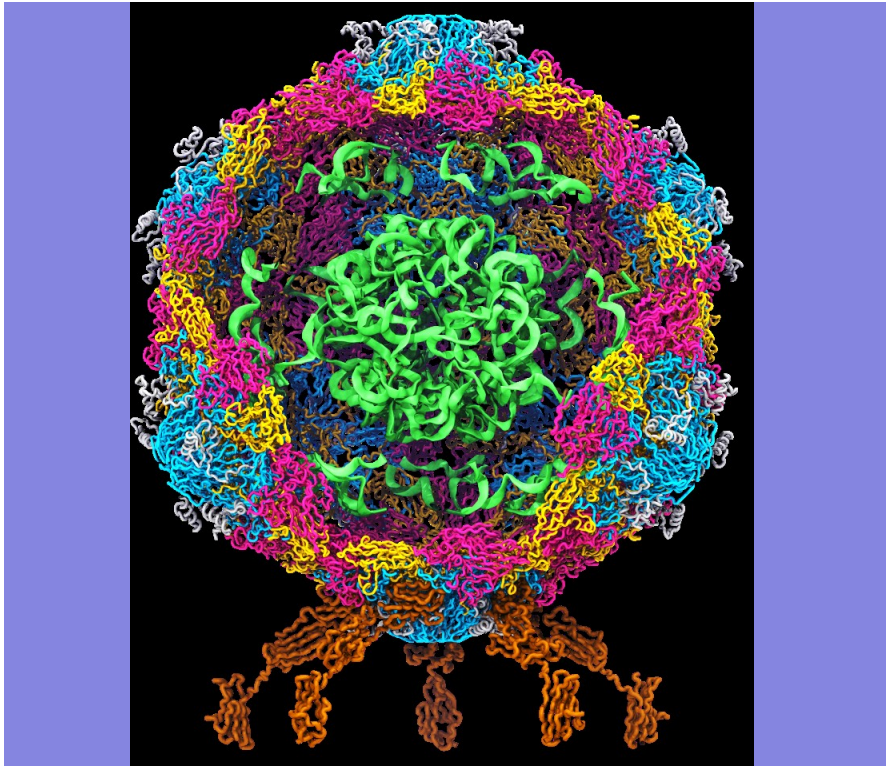
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

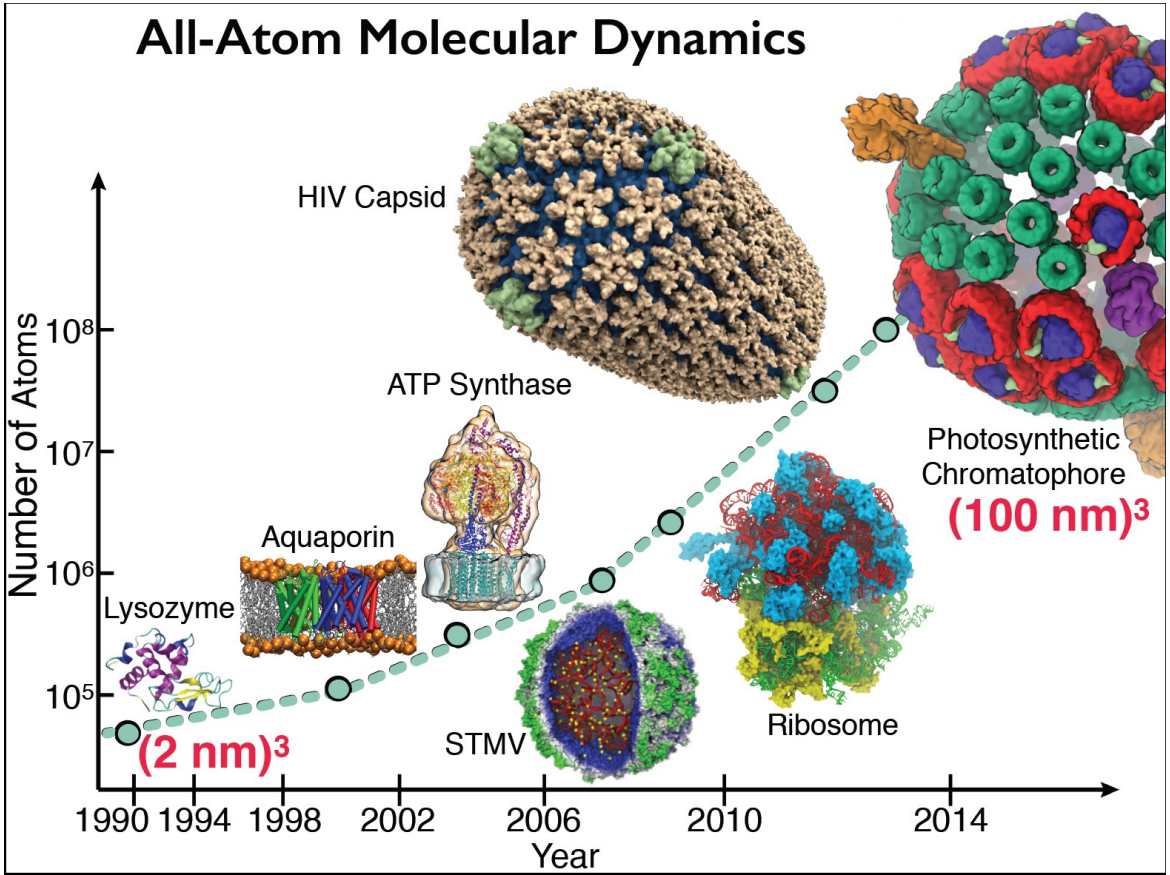


Poliovirus



Goal: A Computational Microscope

Study the molecular machines in living cells

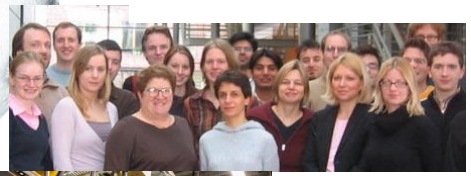


NAMD

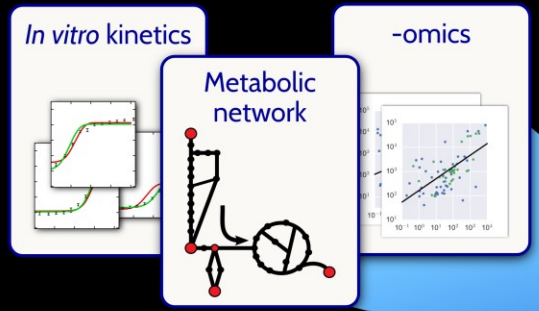
- **Parallel Molecular Dynamics**
- Over 14,000 citations of NAMD
- One program available on all platforms.
  - Desktops and laptops – setup and testing
  - Linux clusters – affordable local workhorses
  - Supercomputers – free allocations on XSEDE
  - Blue Waters – sustained petaflop/s performance
  - **GPUs – from desktop to supercomputers**
- 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

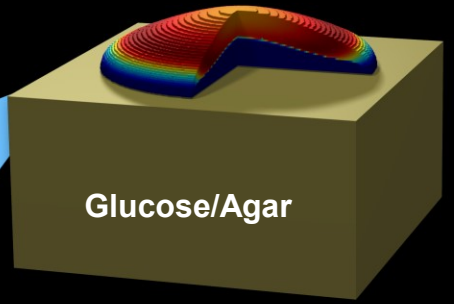


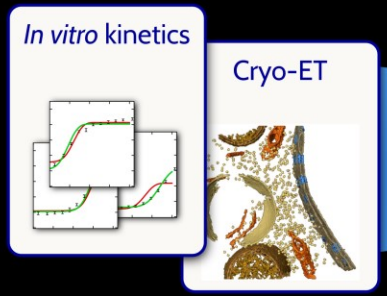
Oak Ridge Summit

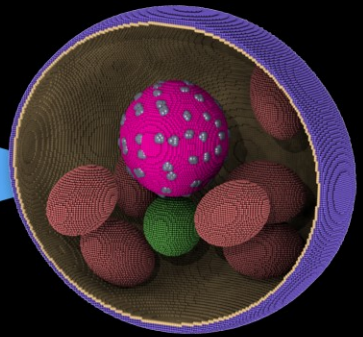


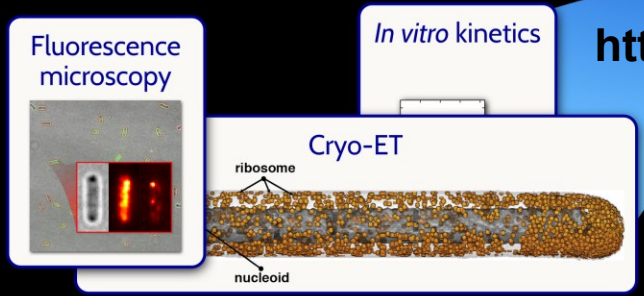
- In
imaging
- Scriptable in Py

ental

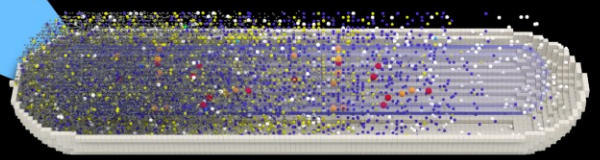






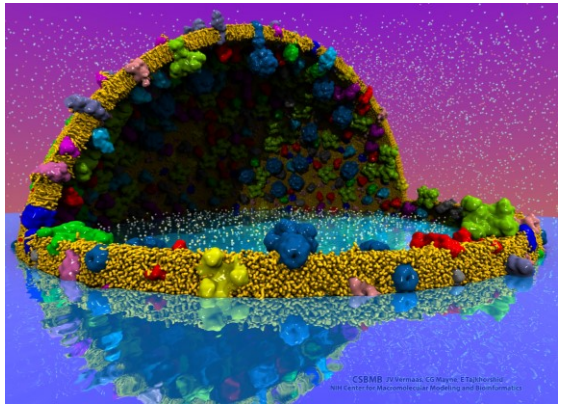


http://ww is.edu/sc

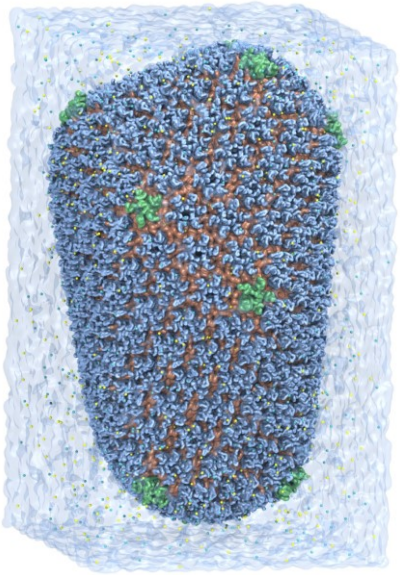


VMD – “Visual Molecular Dynamics”

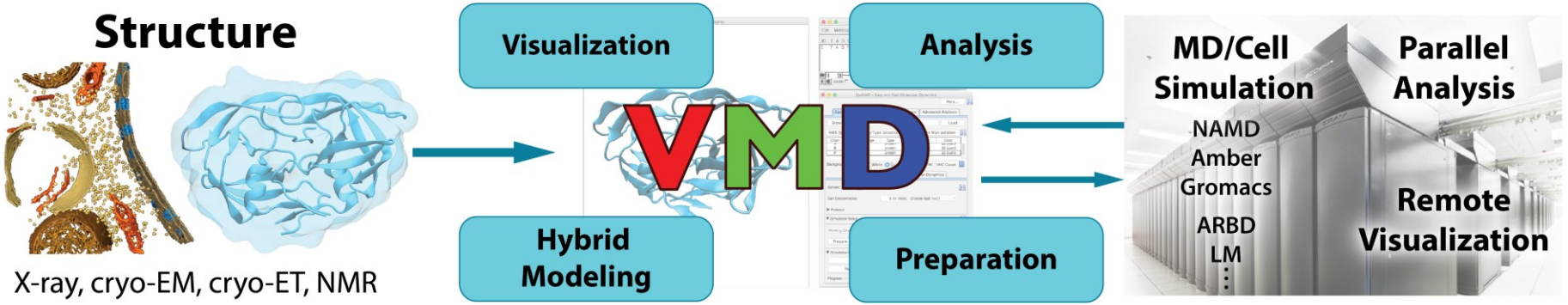
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Sequence information
- User extensible scripting and plugins
- **Over 28,000 citations of VMD**
- http://www.ks.uiuc.edu/Research/vmd/



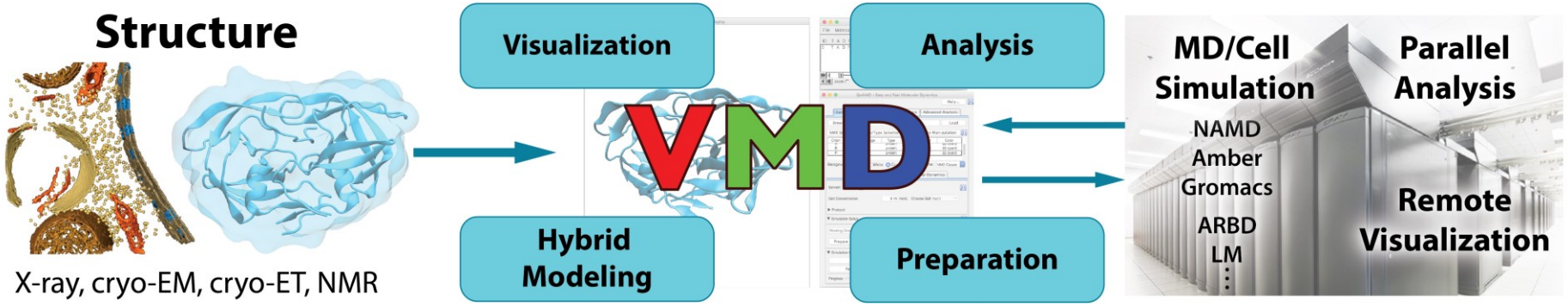
Cell-Scale Modeling



MD Simulation



VMD: Building A Next Generation Modeling Platform



- Provide tools for simulation preparation, visualization, and analysis
  - Reach cell-scale modeling w/ all-atom MD, coarse grained, Lattice Microbes
  - Improved performance, visual fidelity, exploit advanced technologies (GPUs, VR HMDs)
- Enable hybrid modeling and computational electron microscopy
  - Load, filter, process, interpret, visualize multi-modal structural information
- Connect key software tools to enable state-of-the-art simulations
  - Support new data types, file formats, software interfaces
- Openness, extensibility, and interoperability are VMD hallmarks
  - Reusable algorithms made available in NAMD, for other tools

Making Our Research Tools Easily Accessible

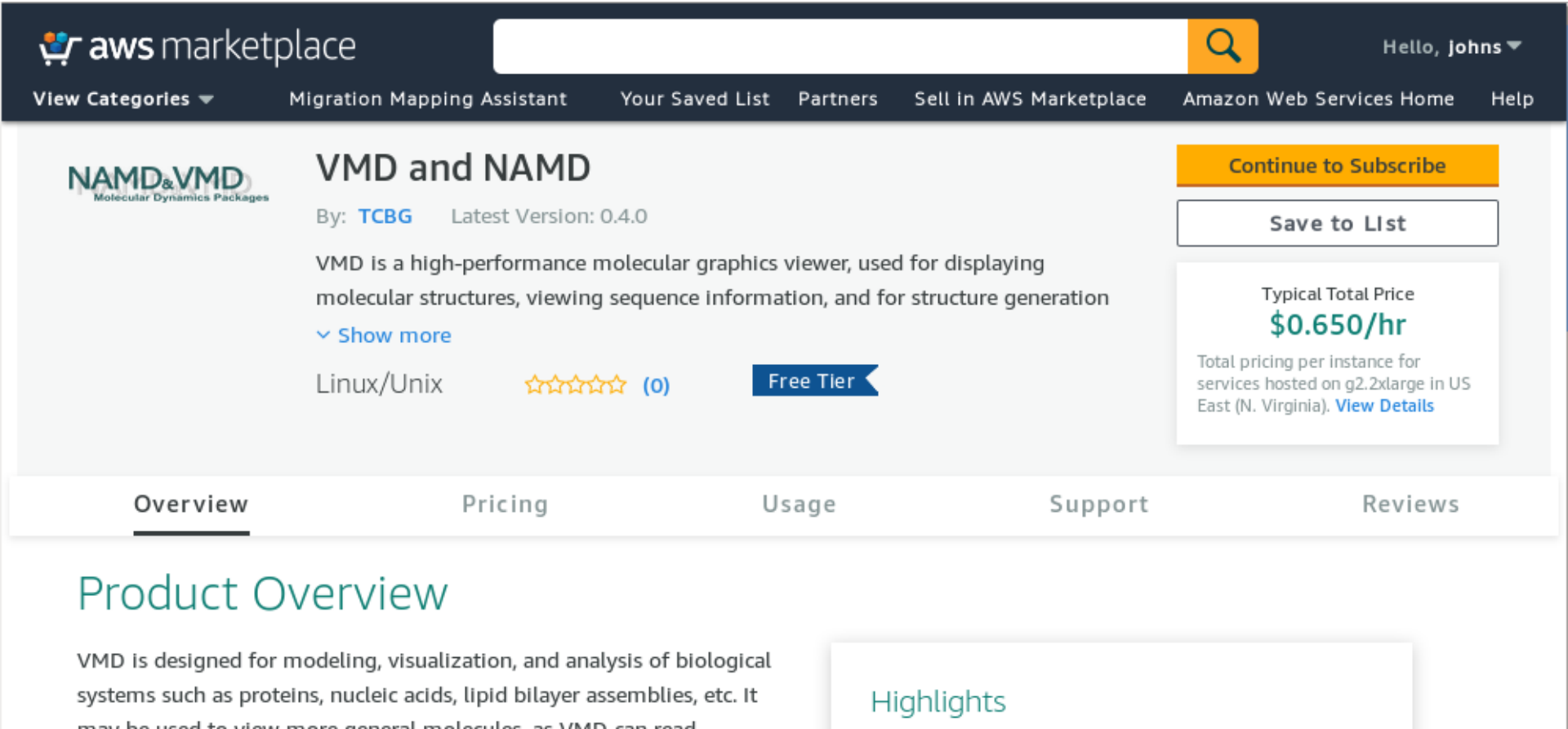
- **Cloud deployment:**
  - Full virtual machines (known as “AMI” in Amazon terminology)
  - Amazon AWS EC2 GPU-accelerated instances: http://www.ks.uiuc.edu/Research/cloud/

- **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**

Our 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



VMD/NAMD NGC Containers, Amazon EC2 AMIs

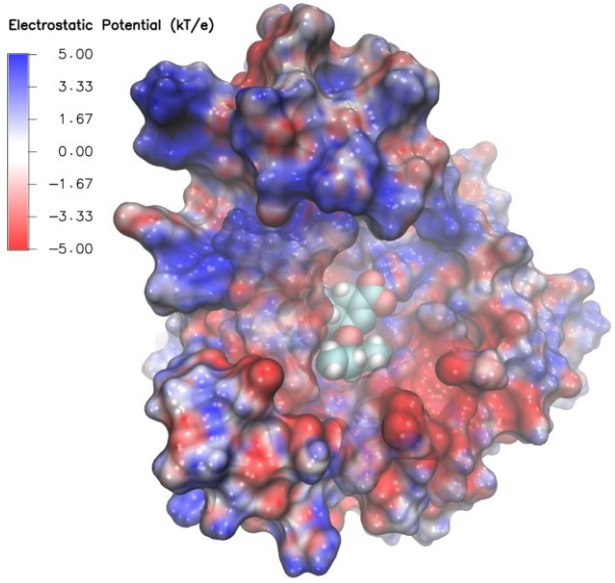
http://www.ks.uiuc.edu/Research/cloud/
https://ngc.nvidia.com/registry/

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.

NAMD+VMD AWS EC2 AMIs

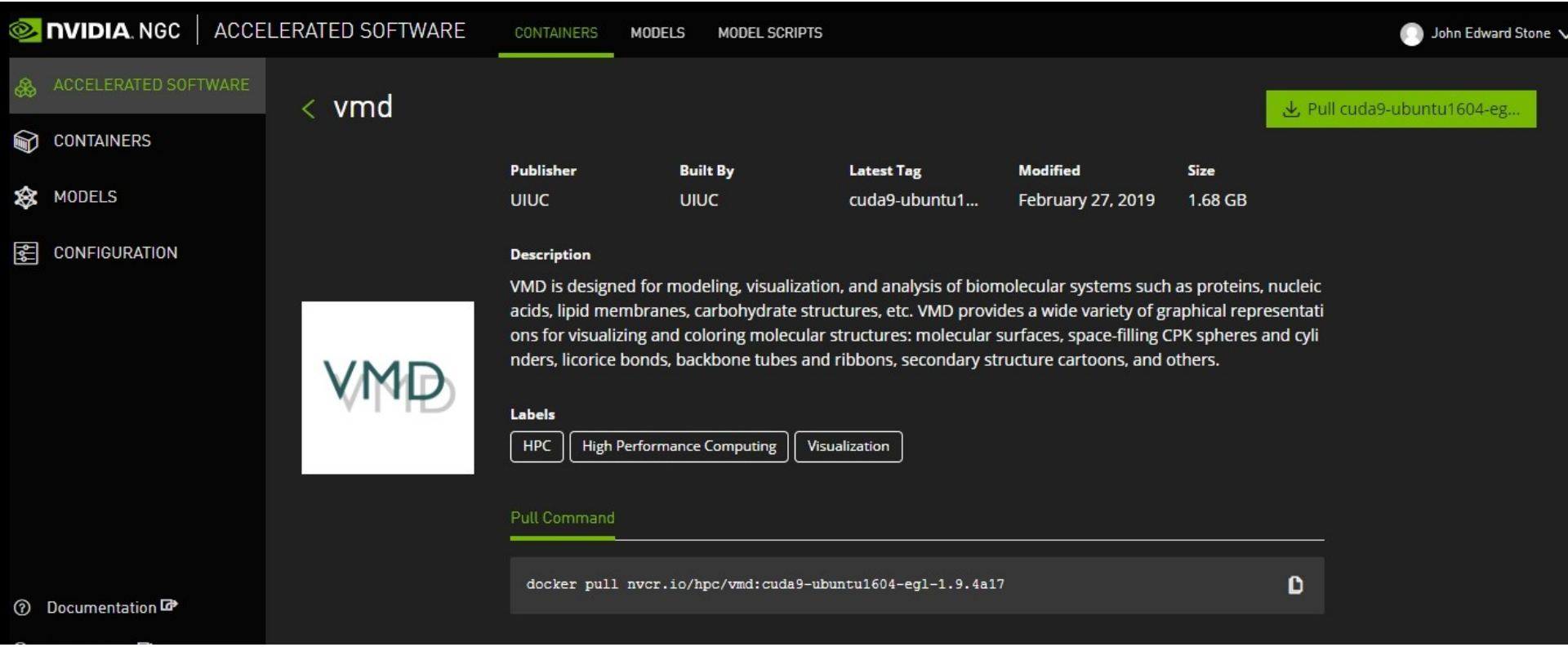
Current Production AMI:

- (ami-064edc9149f8430c8) VMD+NAMD, 64-bit CentOS Linux with DCV remote visualization, created Nov 27, 2018
- This is the current production image using Centos and **DCV** for increased remote visualization performance and smoother interaction. This image will only run on g3 instance types.
- **New AMIs supporting VMD RTX ray tracing coming soon…**

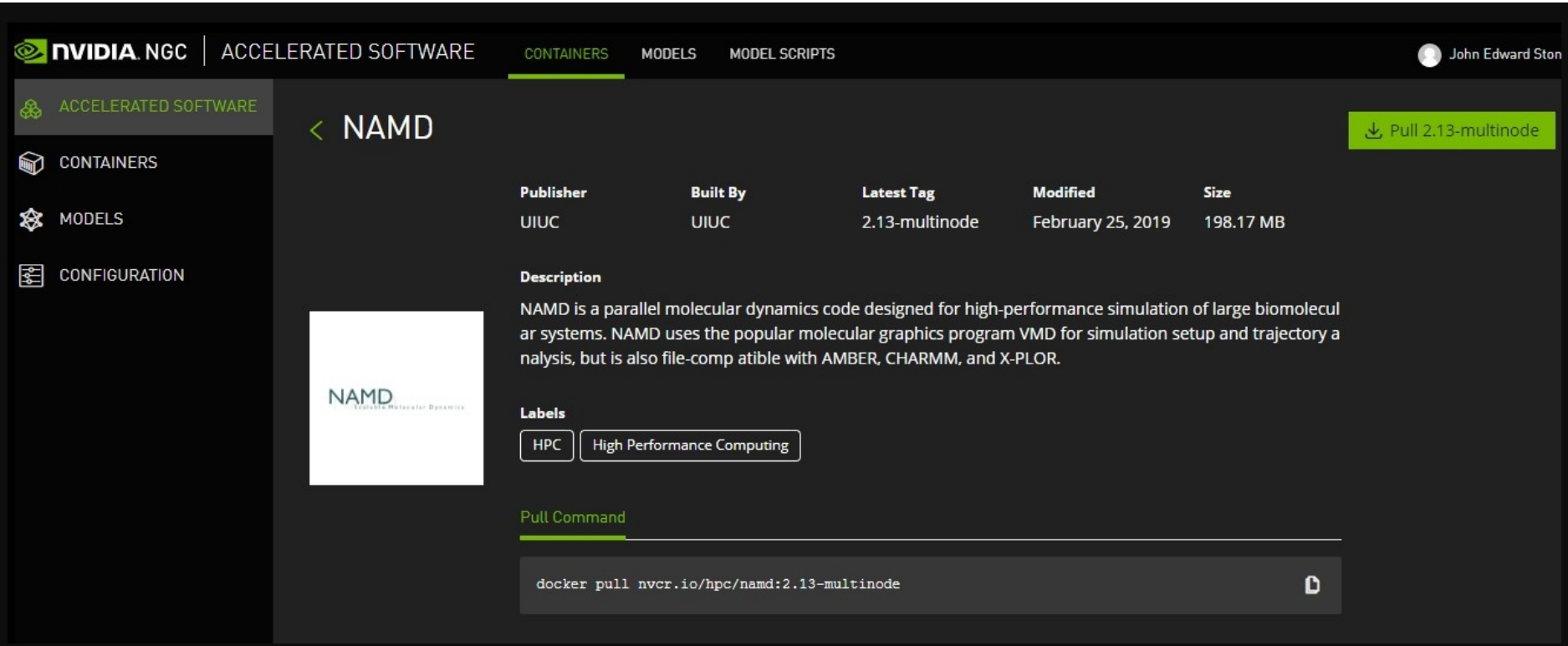
Old Production AMI:

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

VMD, NAMD, LM NGC Containers



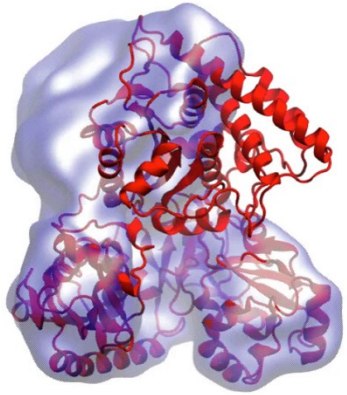
NAMD 2.13 Multi-Node Container



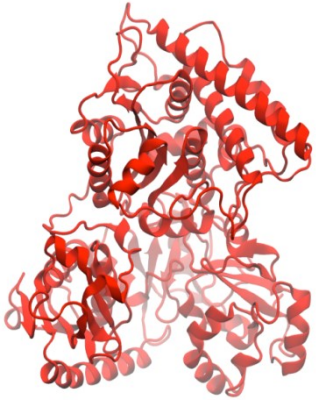
Molecular Dynamics Flexible Fitting (MDFF)

X-ray crystallography → MDFF ← Electron microscopy

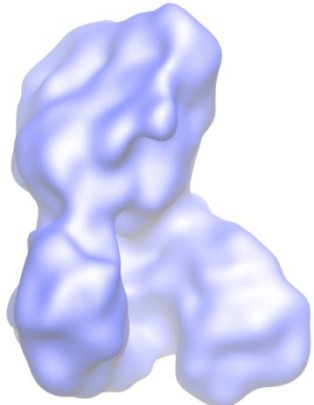
APS at Argonne



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

Molecular Dynamics Flexible Fitting - Theory

Two terms are added to the MD potential

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

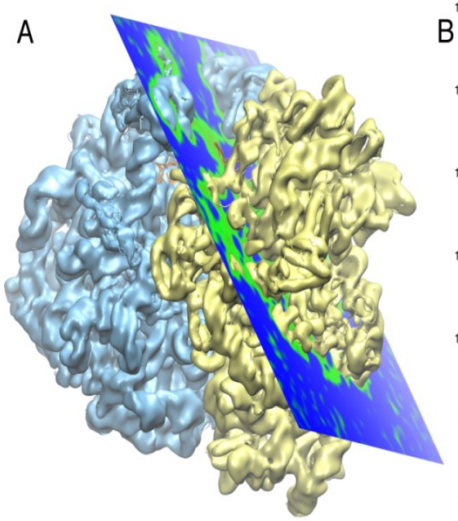
An external potential derived from the EM map is defined on a grid as

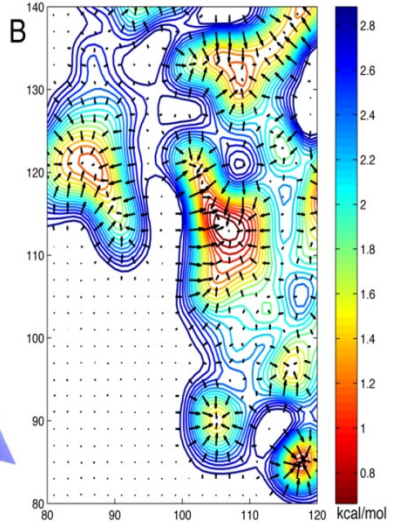
$$U_{EM}(\mathbf{R}) = \sum_j w_j V_{EM}(\mathbf{r}_j)$$

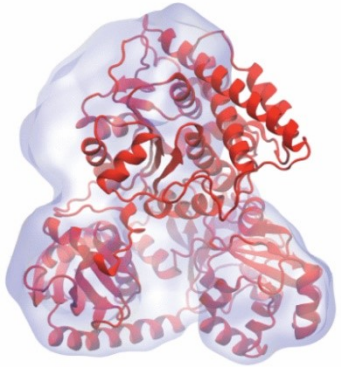
$$V_{EM}(\mathbf{r}) = \begin{cases} \xi \left(1 - \frac{\Phi(\mathbf{r}) - \Phi_{thr}}{\Phi_{max} - \Phi_{thr}}\right) & \text{if } \Phi(\mathbf{r}) \geq \Phi_{thr}, \\ \xi & \text{if } \Phi(\mathbf{r}) < \Phi_{thr}. \end{cases}$$

A mass-weighted force is then applied to each atom

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

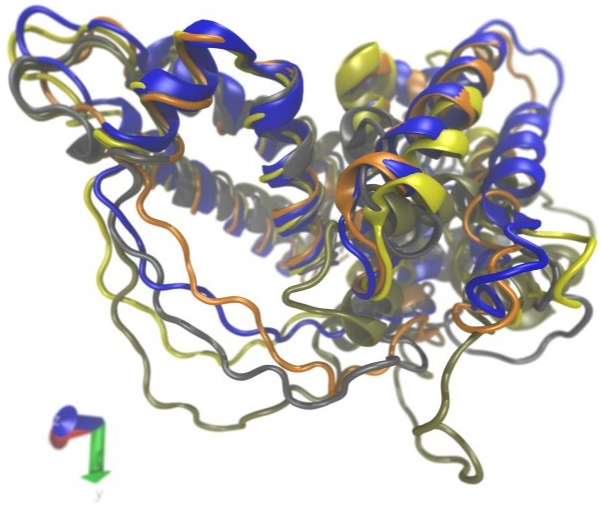






VMD Development Efforts Supporting Integrative Hybrid Modeling

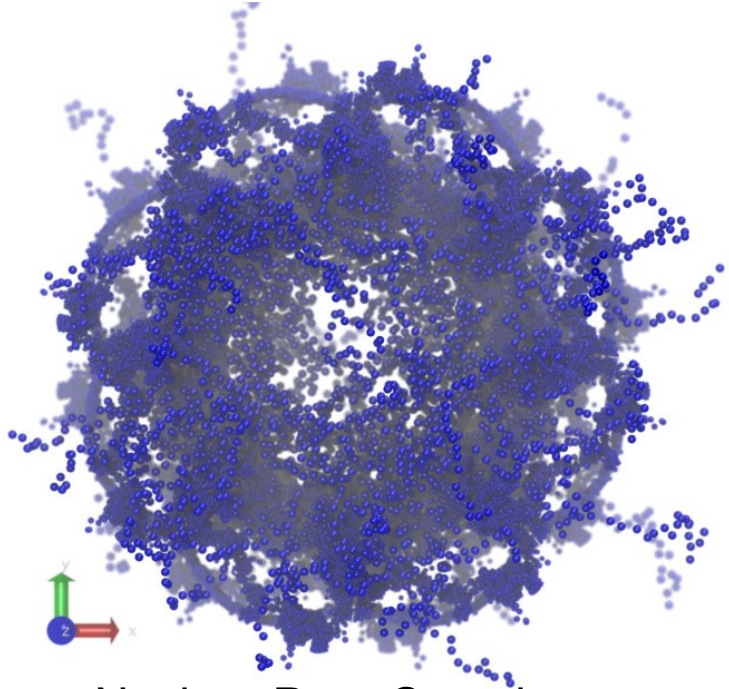
- Extending mmCIF PDBx parser to encompass new IHM-specific records, data types
- Revising VMD “molfile plugin” APIs to communicate IHM data to VMD and represent it natively
- New atom selection keywords that encompass IHM structure data
- New graphical interfaces to query and interact with IHM data both quantitatively and visually



Serum Albumin Domains, PDB-DEV IHM #5

Coarse-Grained IHM Data

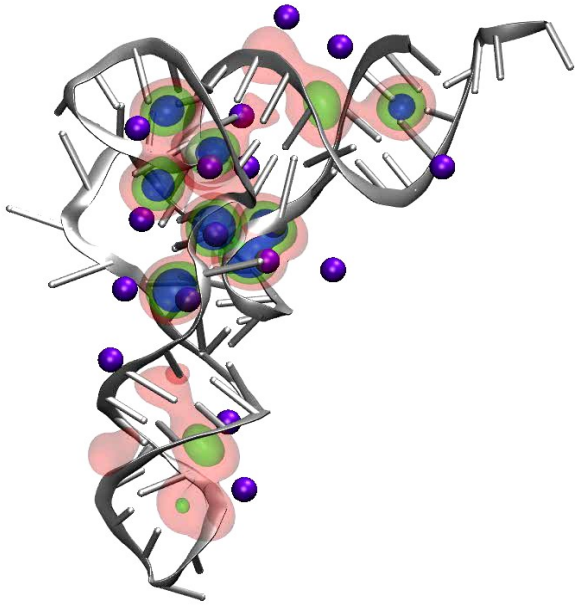
- Coarse grained sphere/bead models
- Restraint information from experiments
- Multi-modal structure alignments, comparisons
- Linkage to underlying experimental images, statistics, etc.



Nuclear Pore Complex,
PDB-DEV IHM #12

Display of Uncertainty, Error in IHM Models

- Query, visualize uncertainty, error, variance, in EM density maps, tomograms, atomic structure
- Requires IHM models to specify these statistics in the files
- Modeling tools, graphical interfaces can use this to guide user modeling tasks, analyses



tRNA magnesium ion occupancy probability density surfaces, VMD volmap plugin

Selected VMD Plugins: Center Developed, and User Developed

Analysis

- APBSRun
- CatDCD
- Contact Map
- GofRGUI
- HeatMapper
- ILSTools
- IRSpecGUI
- MultiSeq
- NAMD Energy
- NAMD Plot
- NetworkView
- NMWiz
- ParseFEP
- PBCTools
- PMEpot
- PropKa GUI
- RamaPlot
- RMSD Tool
- RMSD Trajectory Tool
- RMSD Visualizer Tool
- Salt Bridges
- Sequence Viewer
- Symmetry Tool
- Timeline
- TorsionPlot
- VolMap

Modeling

- AutoIonize
- AutoPSF
- Chirality
- Cionize
- Cispeptide
- CGTools
- Dowser
- ffTK
- Inorganic Builder
- MDFF
- Membrane
- Merge Structs
- Molefacture
- Mutator
- Nanotube
- Psfgen
- RESPTool
- RNAView
- Solvate
- SSRestraints
- Topotools

Visualization

- Clipping Plane Tool
- Clone Rep
- DemoMaster
- Dipole Watcher
- Intersurf
- Navigate
- NavFly
- MultiMolAnim
- Color Scale Bar
- Remote
- Palette Tool
- ViewChangeRender
- ViewMaster
- Virtual DNA Viewer
- VMD Movie Maker

Simulation

- AlaScan
- AutoIMD
- IMDMenu
- NAMD GUI
- NAMD Server
- QMTool

Collaboration

- Remote Control

Data Import and Plotting

- Data Import
- Multiplot
- PDBTool
- MultiText

Externally Hosted Plugins and Extensions

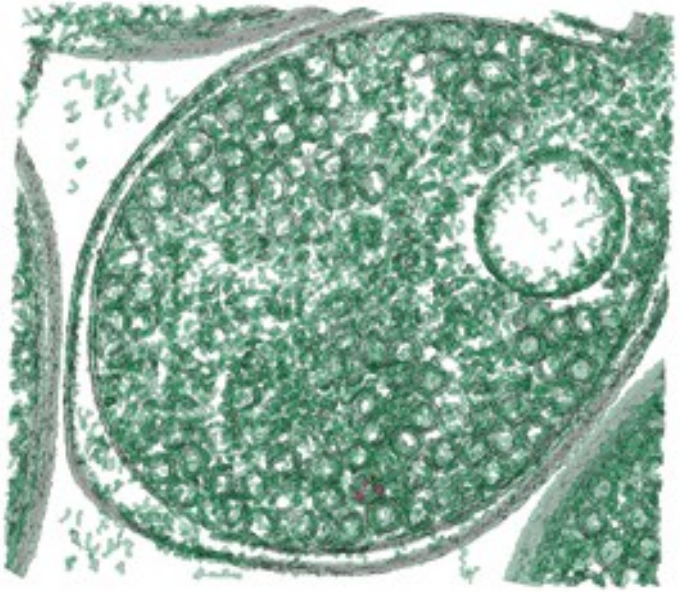
- Check sidechains
- MultiMSMS
- Interactive Essential Dynamics
- Mead Ionize
- Clustering Tool
- iTrajComp
- Swap RMSD
- Intervor
- SurfVol
- vmdICE

75 MolFile I/O Plugins:
structure, trajectory, sequence, and density map

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

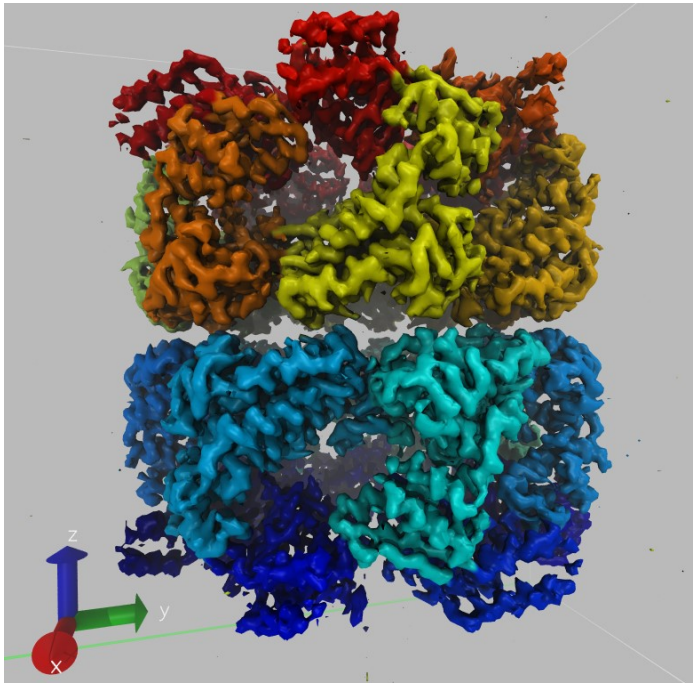
Computing Challenges Posed by Large Hybrid Models

- Techniques like coarse graining allow modeling to reach the cell scale, but data sizes and interactivity remain a tremendous challenge
- Next-generation parallel- and **GPU-accelerated computing** techniques can make powerful analytical and visualization tools **interactive** for the first time:
  - **Clustering analyses** (structure RMSD, quality-of-fit, docking scores, etc)
  - **Image segmentation**, docking, **alignment, fitting**, coarse-graining…

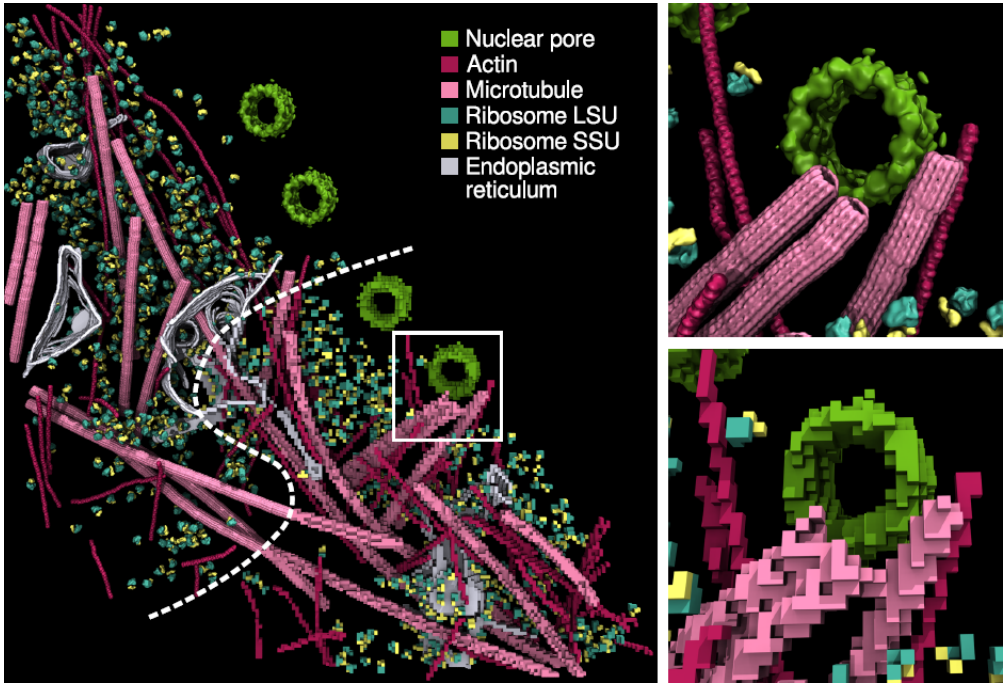


VMD supports analysis and visualization of multi-gigavoxel EM tomograms, density maps

Density Map Segmentation



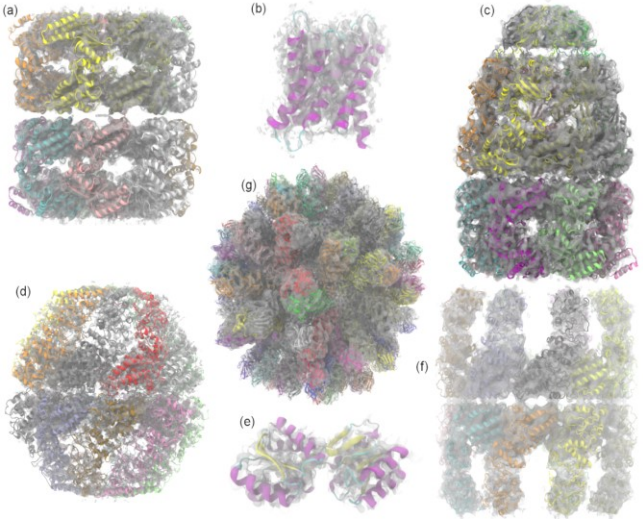
VMD GPU-accelerated density map segmentation of GroEL

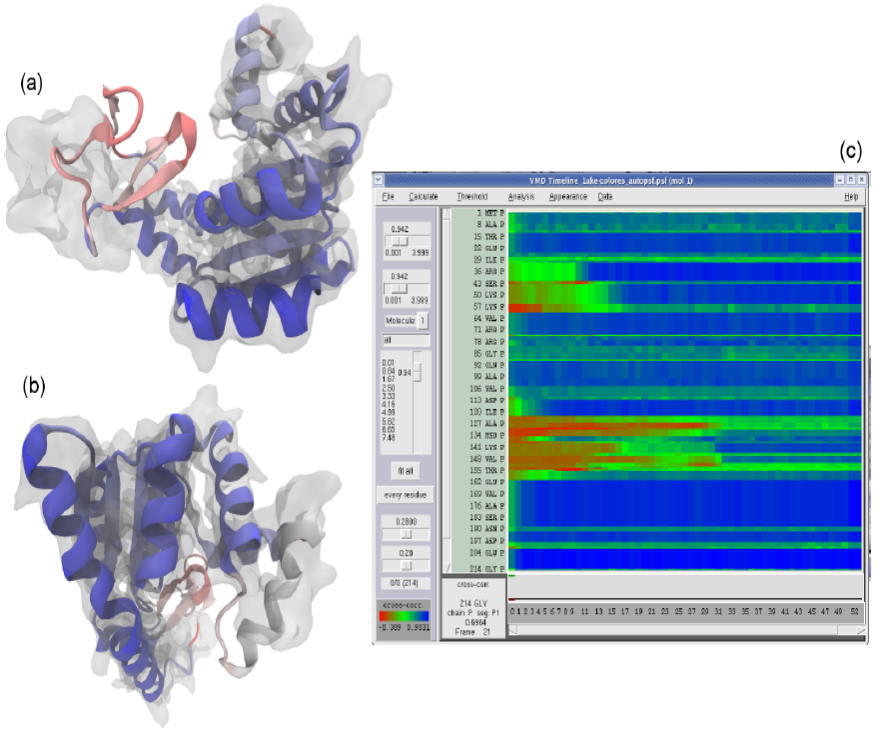


Earnest, et al. J. Physical Chemistry B, 121(15): 3871-3881, 2017.

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

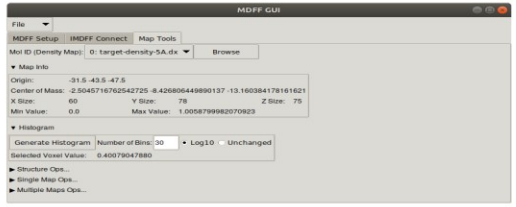
Rabbit Hemorrhagic Disease Virus: 702K atoms, 6.5Å resolution
Volta GPU architecture almost 2x faster than previous gen Pascal:

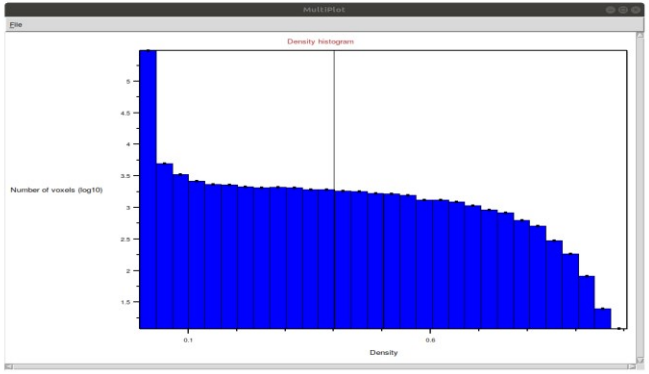
Application and Hardware platform	Runtime, Speedup vs. Chimera,		VMD+GPU
Chimera Xeon E5-2687W (2 socket) [1]	15.860s,	1x	
VMD-CUDA IBM Power8 + 1x Tesla K40 [2]	0.488s,	32x	**0.9x**
VMD-CUDA Intel Xeon E5-2687W + 1x Quadro K6000 [1,2]	0.458s,	35x	**1.0x**
VMD-CUDA Intel Xeon E5-2698v3 + 1x Tesla P100	**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**
VMD-CUDA IBM Power9 "Newell" + 1x Tesla V100	**0.049s,**	**323x**	**9.3x**

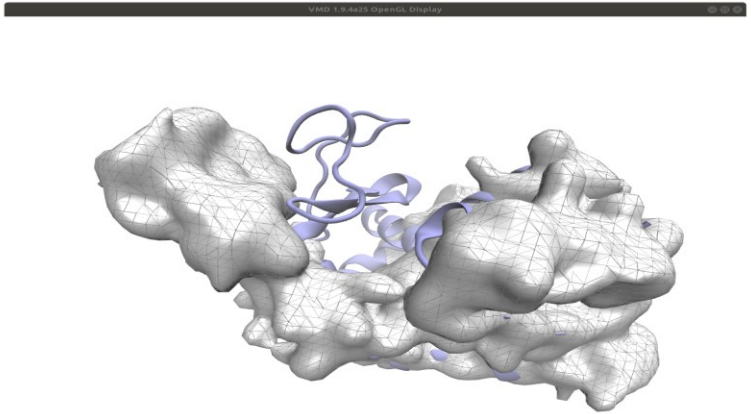
[1] GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting. J. E. Stone, R. McGreevy, B. Isralewitz, and K. Schulten. Faraday Discussions 169:265-283, 2014.
[2] Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software 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.

New VMD MDFF Density Map Tools

- **New** Map Tools tab of MDFF GUI provides wide array of density map manipulation tools including:
  - **New** Rigid Body Fitting
  - **New** Interactive Histogram
  - Trim, Crop, Clamp, Smooth…
  - **Easy Masking routine**
- **New** Density Segmentation
- Add, subtract, multiply maps
- Cross correlation and potential calculations for MDFF



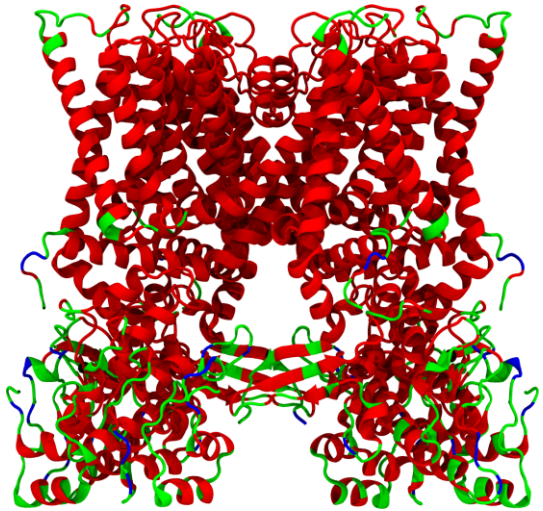




New Density Map Tools - Masking

Easily select and mask density map regions with VMD selection language

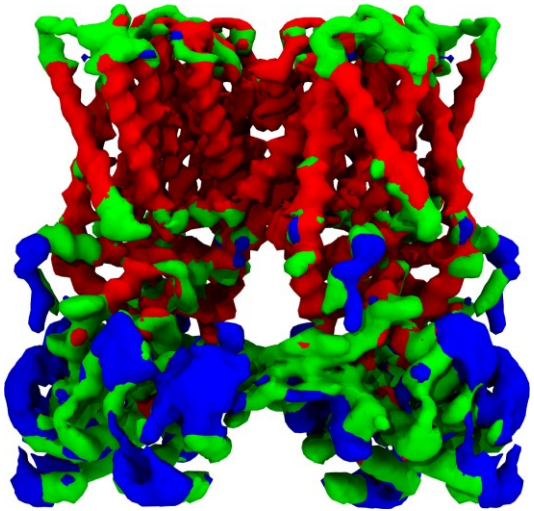
TRPV1 structure (3J5P) and cryo-EM density (emd-5778) colored by local resolution obtained by ResMap



High Res
(~3 Å)

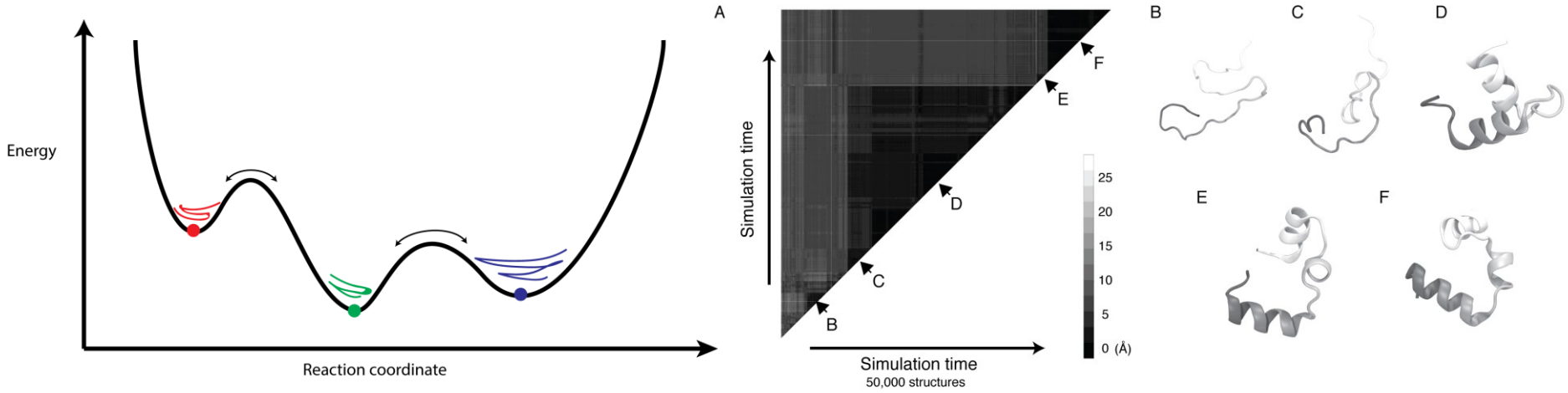
Med Res
(~4 Å)

Low Res
(~5 Å)



A. Kucukelbir, F.J. Sigworth, H.D. Tagare, Quantifying the Local Resolution of Cryo-EM Density Maps, Nature Methods, Volume 11, Issue 1, Pages 63-65, 2014.

Interactive Clustering Analysis of IHM Models, Docking Poses, MD 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.

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

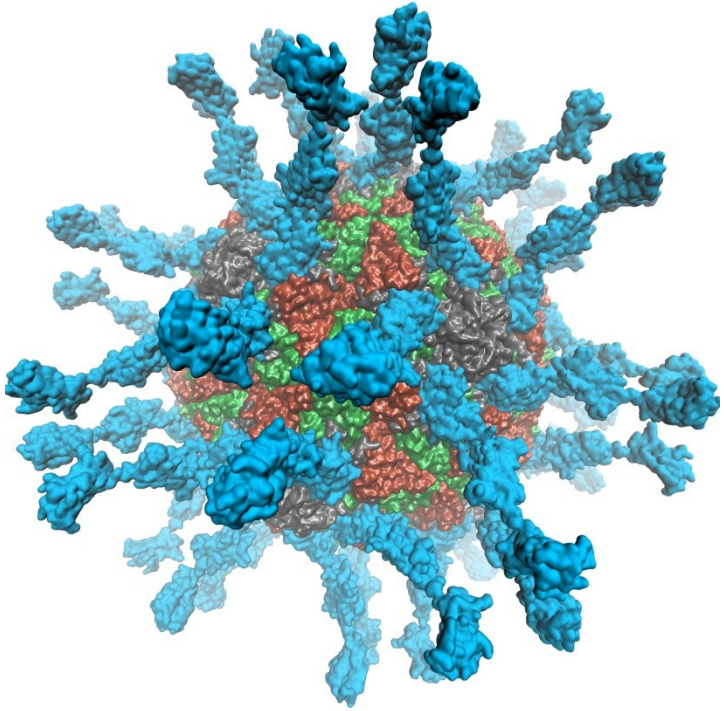
Singharoy, *et al*. eLife 2016

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.

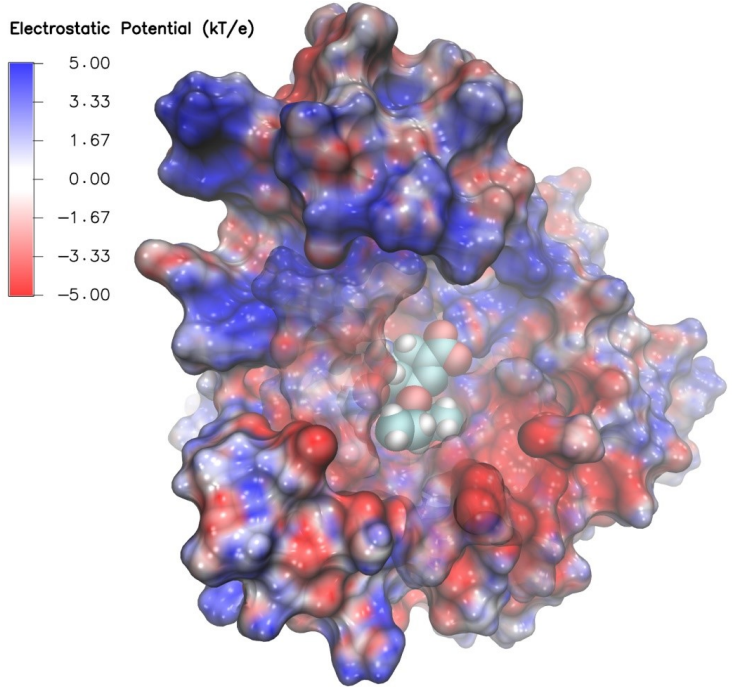
VMD supports EGL for in-situ and parallel rendering on Amazon EC2

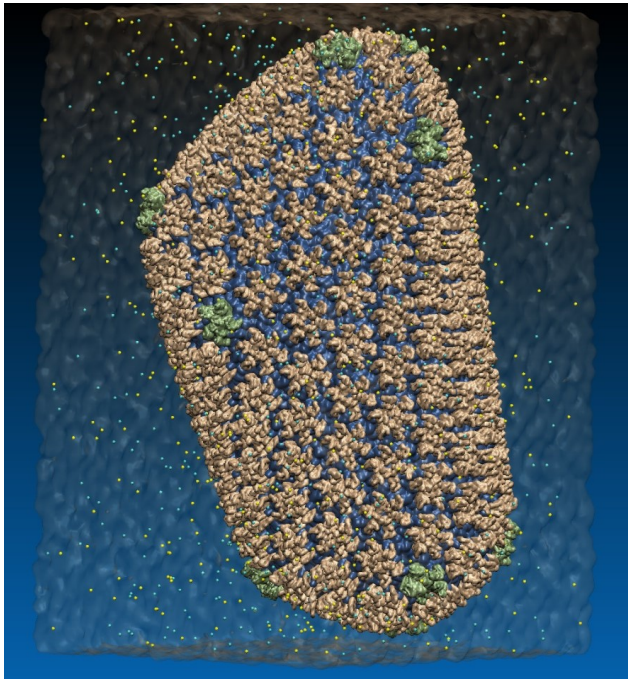
- **No windowing system dependency**
- Easily deploy parallel VMD builds supporting off-screen rendering
- Maintains 100% of VMD OpenGL shaders and rendering features



Poliovirus

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





Swine Flu A/H1N1 neuraminidase bound to Tamiflu

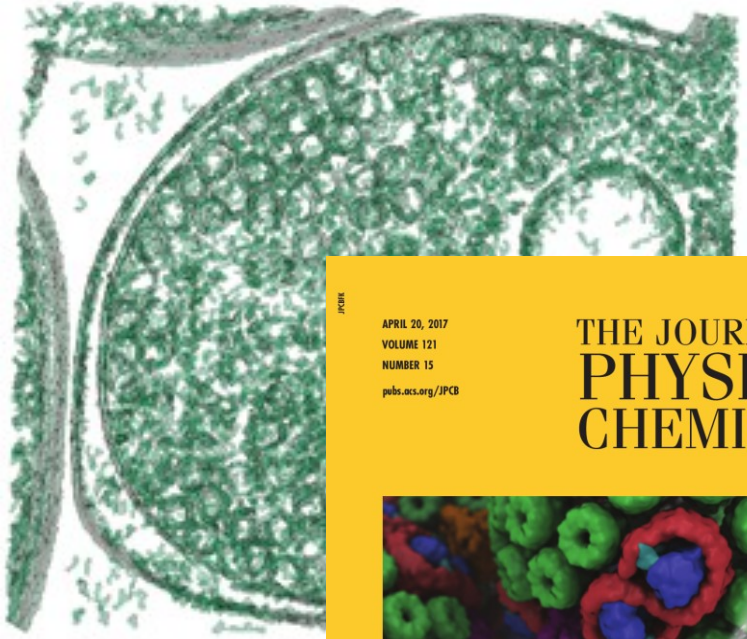
64M atom HIV-1 capsid simulation

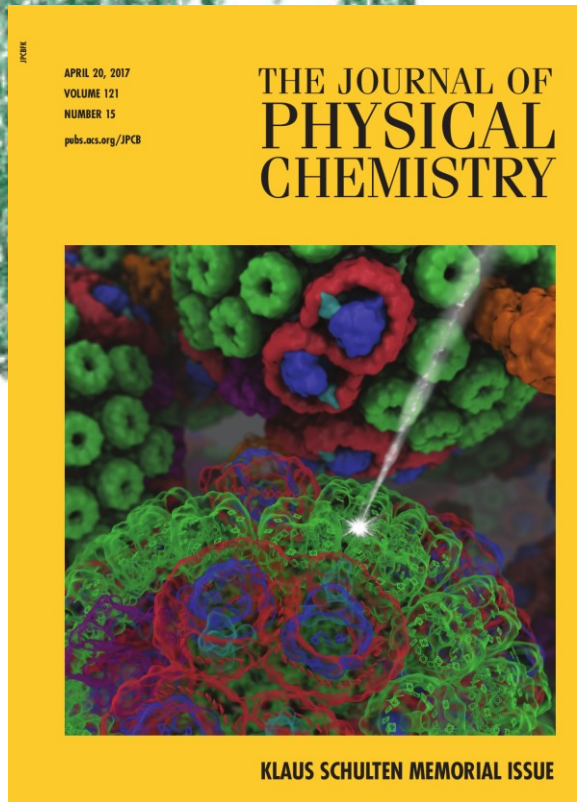
High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL.
J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE IPDPSW, pp. 1014-1023, 2016.

NIH

NEW: Cloud-Based Interactive Remote Visualization

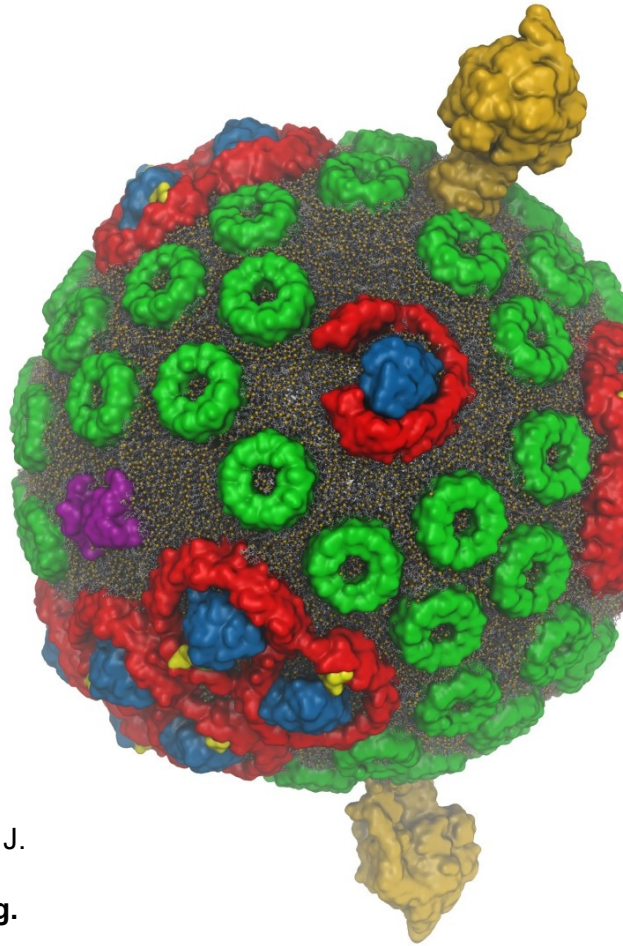
- Built-into VMD itself
- Enable access to massive data sets
- Uses GPU H.264 / HEVC hardware accelerated video encode/decode
- Supports interactive remote visualizations (both rasterization and ray tracing)
- Development ongoing, expected in next major VMD release, in 1H 2019…





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, …



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.

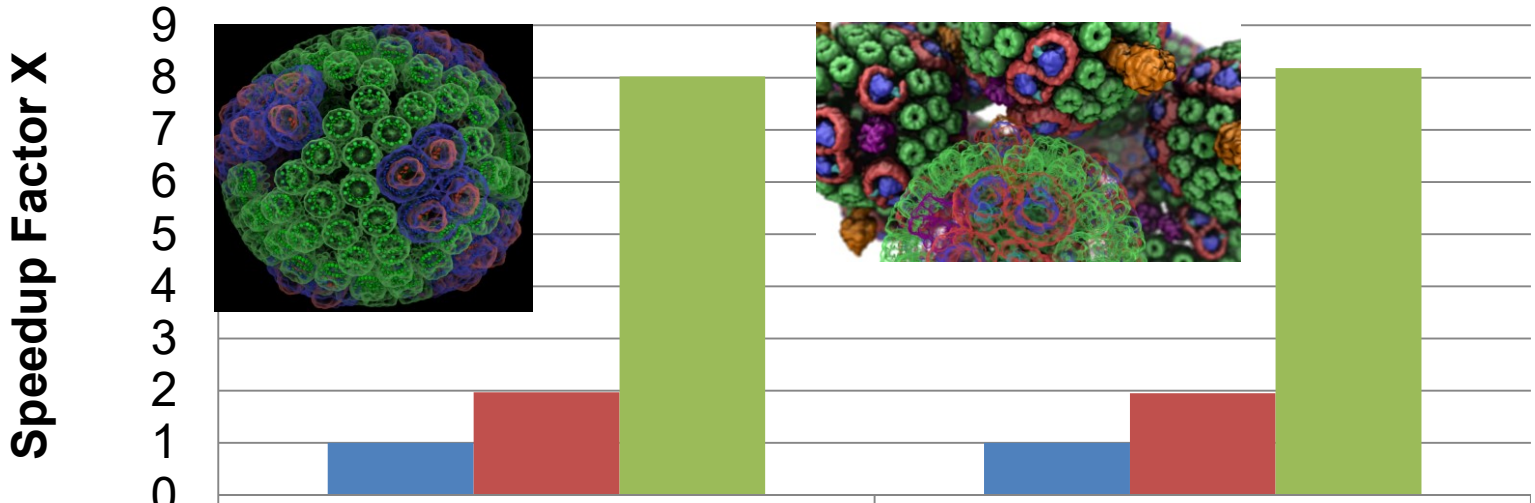
Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail. M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.

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.

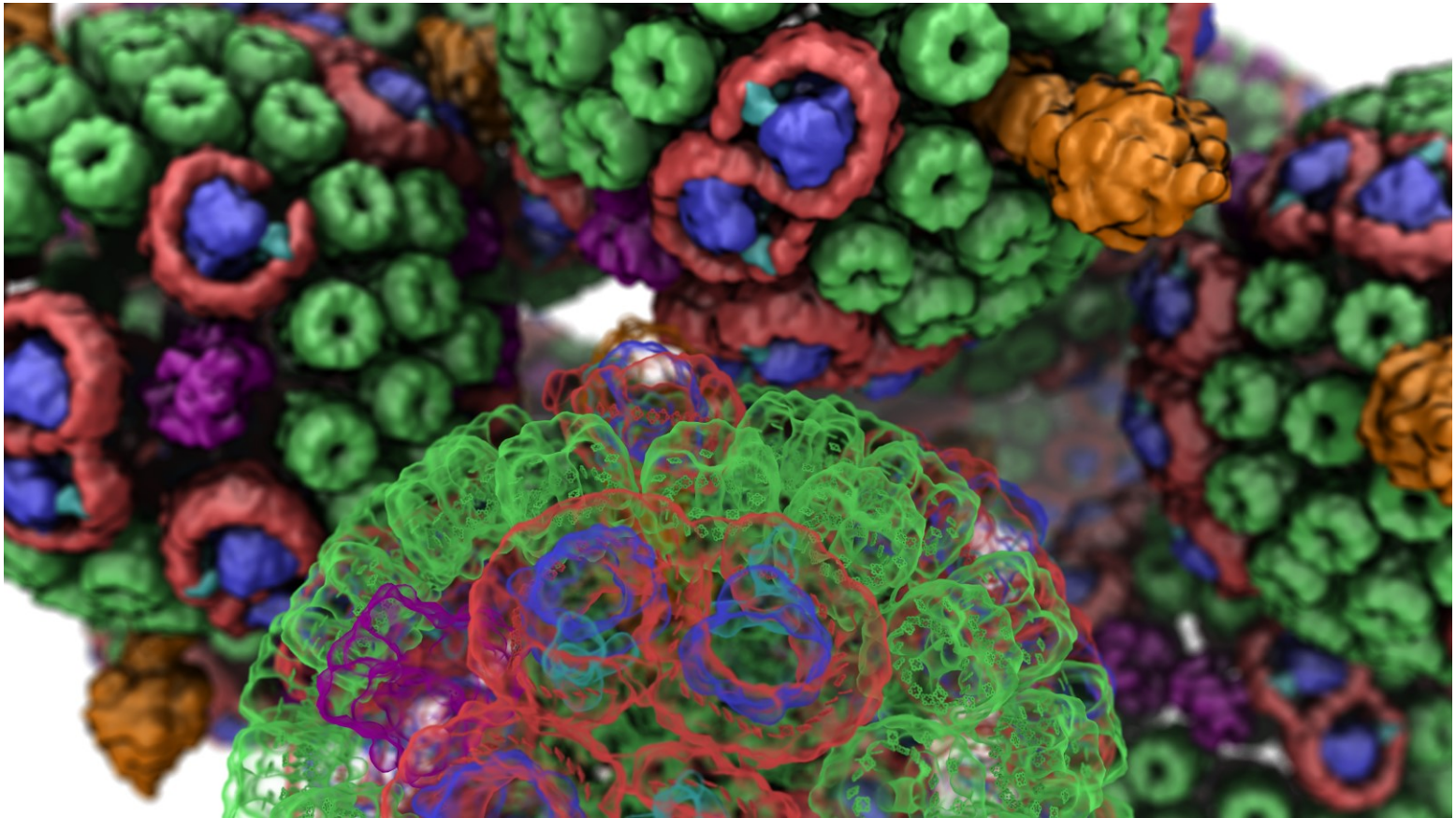
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering J. E. Stone, W. R. Sherman, and K. HPDAV, IPDPSW, pp. 1048-1057, 2016.

VMD OptiX RT performance on Quadro RTX 6000

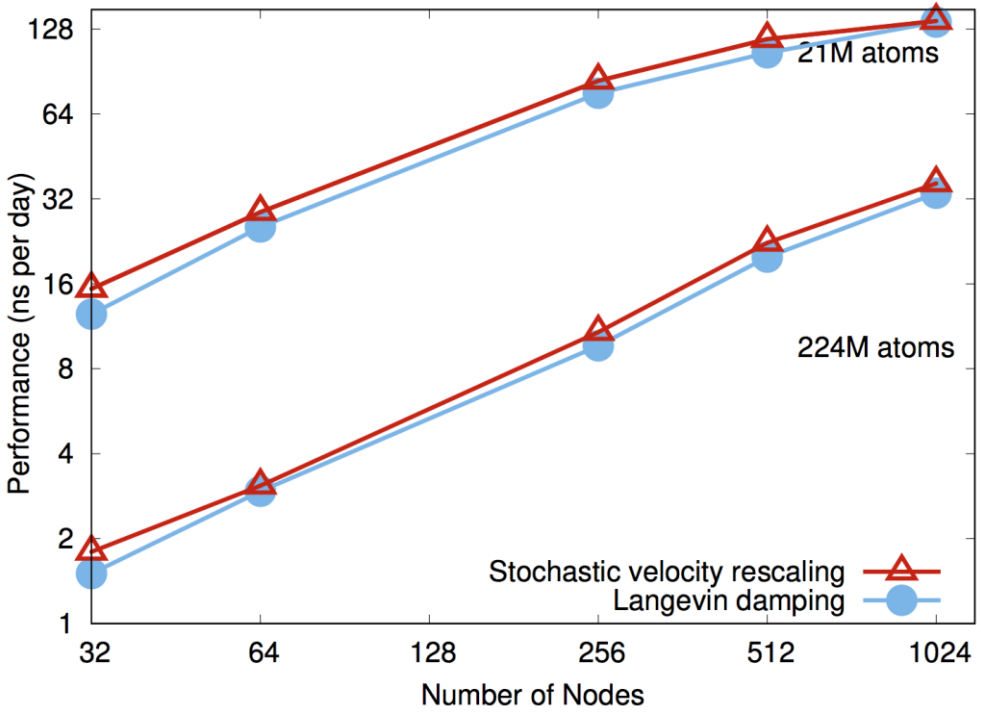


	Chromatophore @ 4Kx4K	Chrom Cell, 512x DoF @ 1080p
Quadro GV100	1	1
2x Quadro GV100	1.97	1.95
Quadro RTX 6000	8.02	8.18

VMD w/ OptiX RTX: High-Fidelity Interactive Ray Tracing of Hybrid Models of Large Complexes, Organelles, Cell-Scale Models



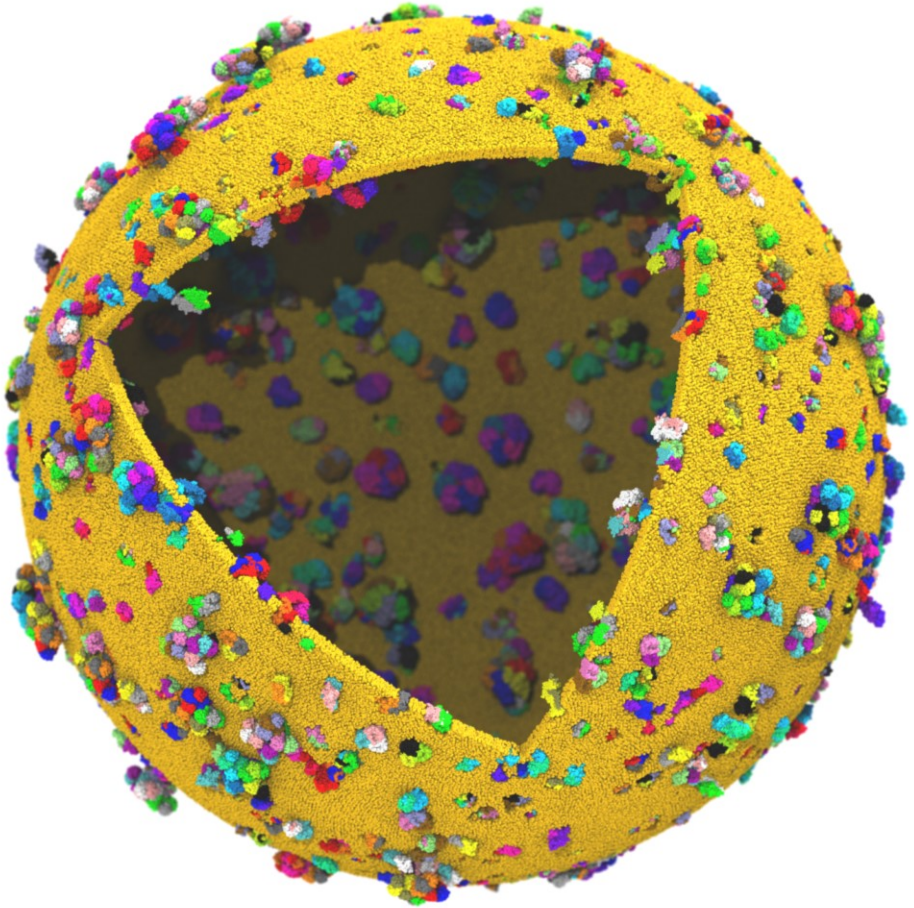
NAMD on Summit, May 2018



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

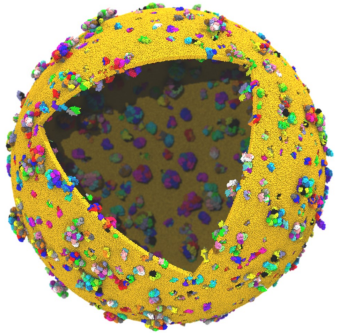
Next Generation: Simulating a Proto-Cell

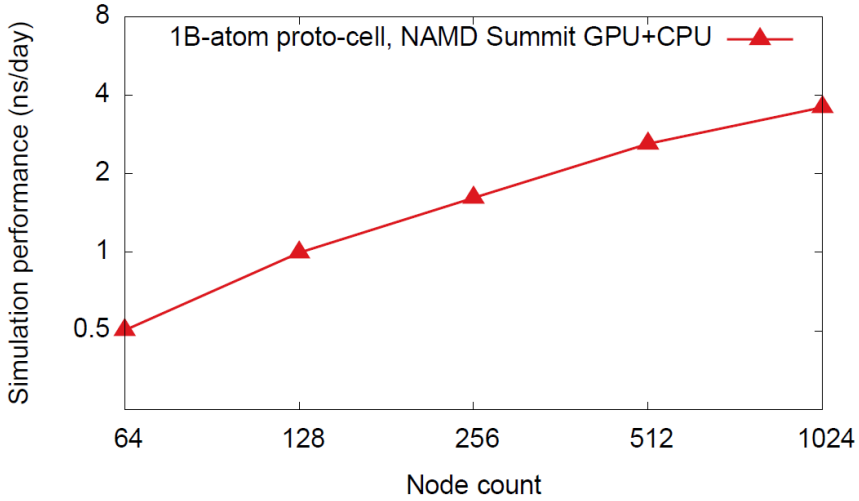
- **ORNL Summit: NVLink-connected Tesla V100 GPUs enable next-gen visualizations**
- 200nm diameter
- ~1 billion atoms w/ solvent
- ~1400 proteins in membrane



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**

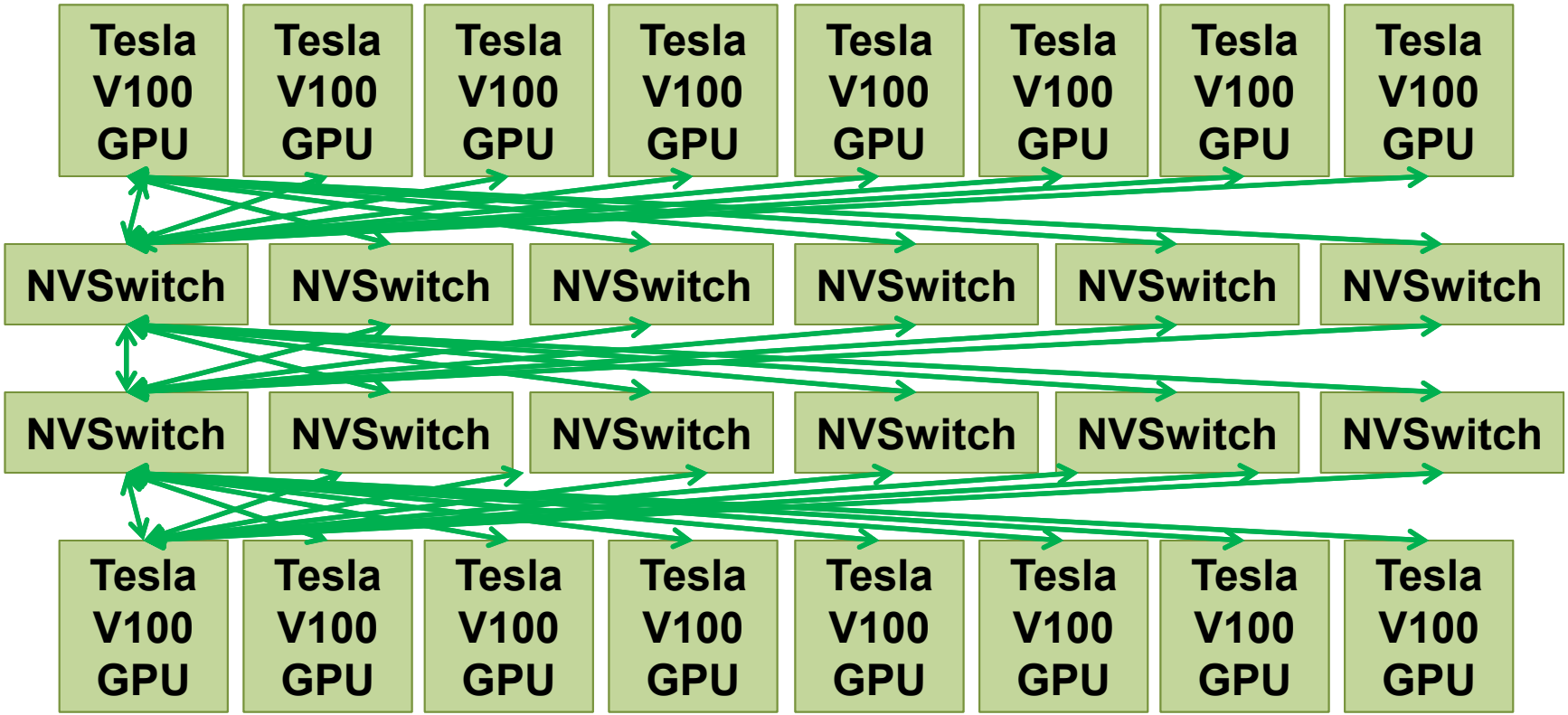




NVIDIA DGX-2

16x 32GB Tesla V100 GPUs w/ 300GB/s NVLink, fully switched

512GB HBM2 RAM w/ **2.4TB/s Bisection Bandwidth, 2 PFLOPS**

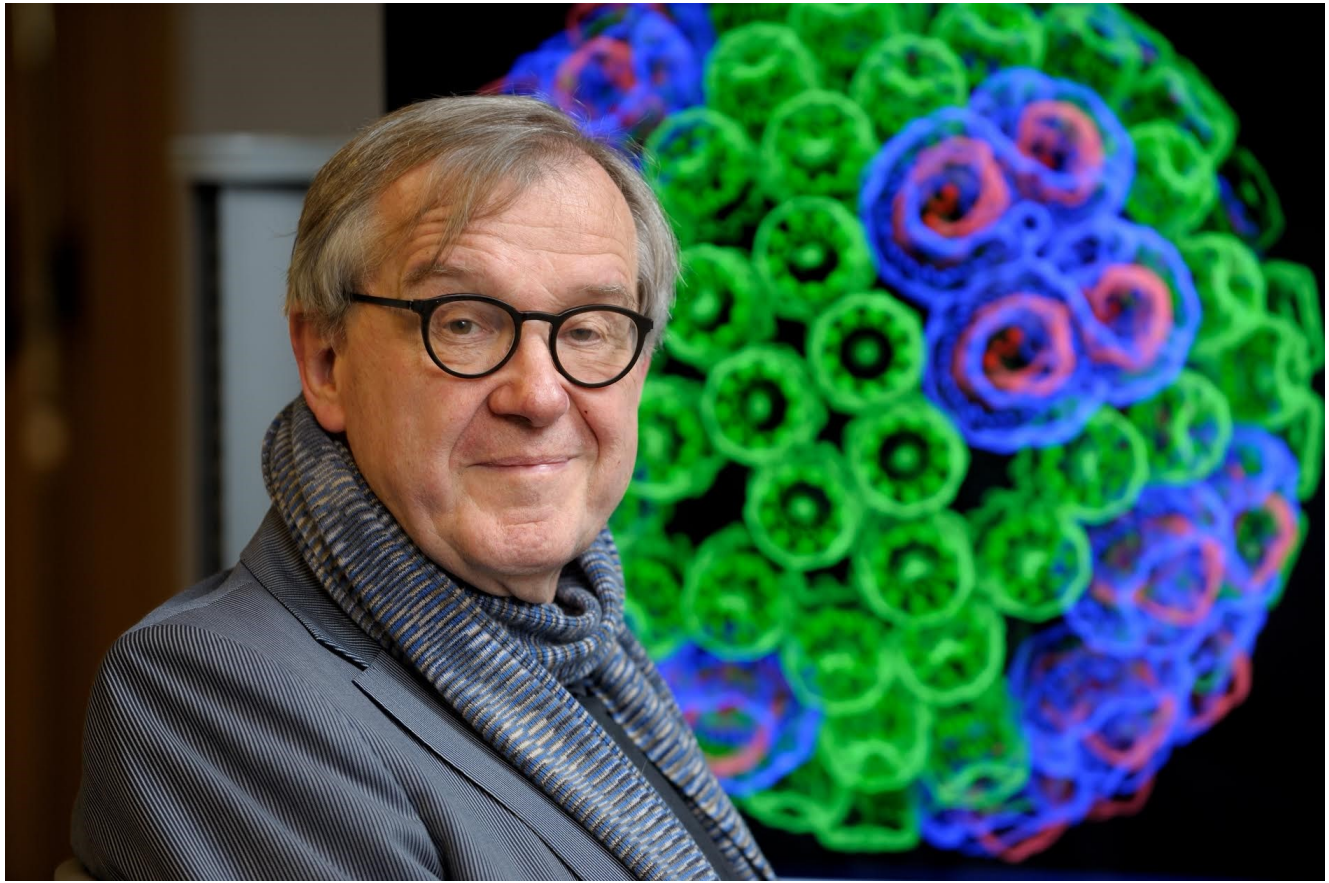


Opportunities and Challenges Posed by Future DGX-2-Like System Designs

- **CPUs "oversubscribed" by GPUs**
- Unfavorable for algorithm designs that perform "siloed" GPU calculations followed by reductions
- GPU algorithms must **dis-involve CPUs to greatest possible extent**
- **Fully-switched NVLink**-connected memory systems permit fine-grained multi-GPU algorithms via direct peer memory load/stores
- Throughput oriented GPU algorithms can hide both local and remote memory latencies gracefully
- **Use atomic operations where needed** during kernel execution rather than bulk-synchronization and reduction ex post facto
- New levels of algorithm sophistication are possible, but not yet well supported by existing high level programming abstractions

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

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- **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.
- **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

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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

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

- **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.

Related Publications

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. E. 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.