Fighting HIV with GPU-Accelerated Petascale Computing

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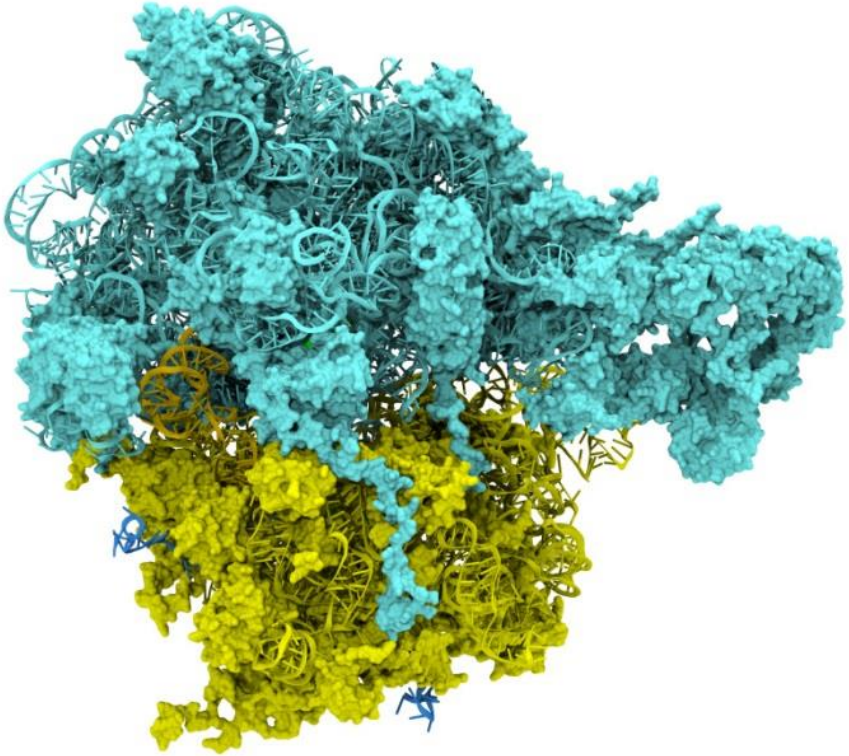
Supercomputing 2013 Exhibition

Denver, CO, November 19, 2013

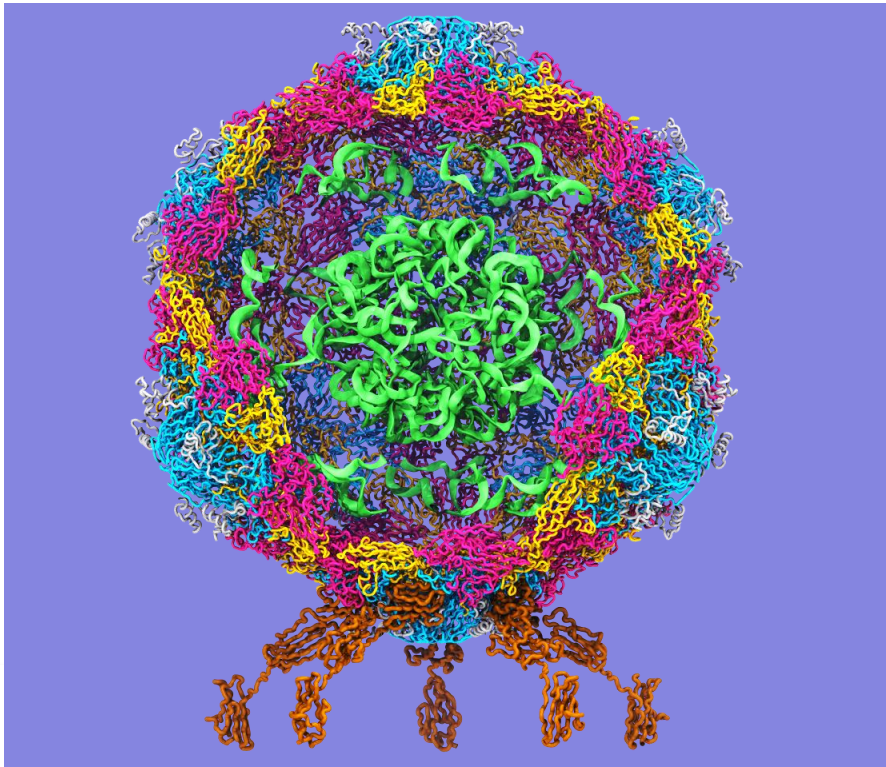
Goal: A Computational Microscope

Study the molecular machines in living cells

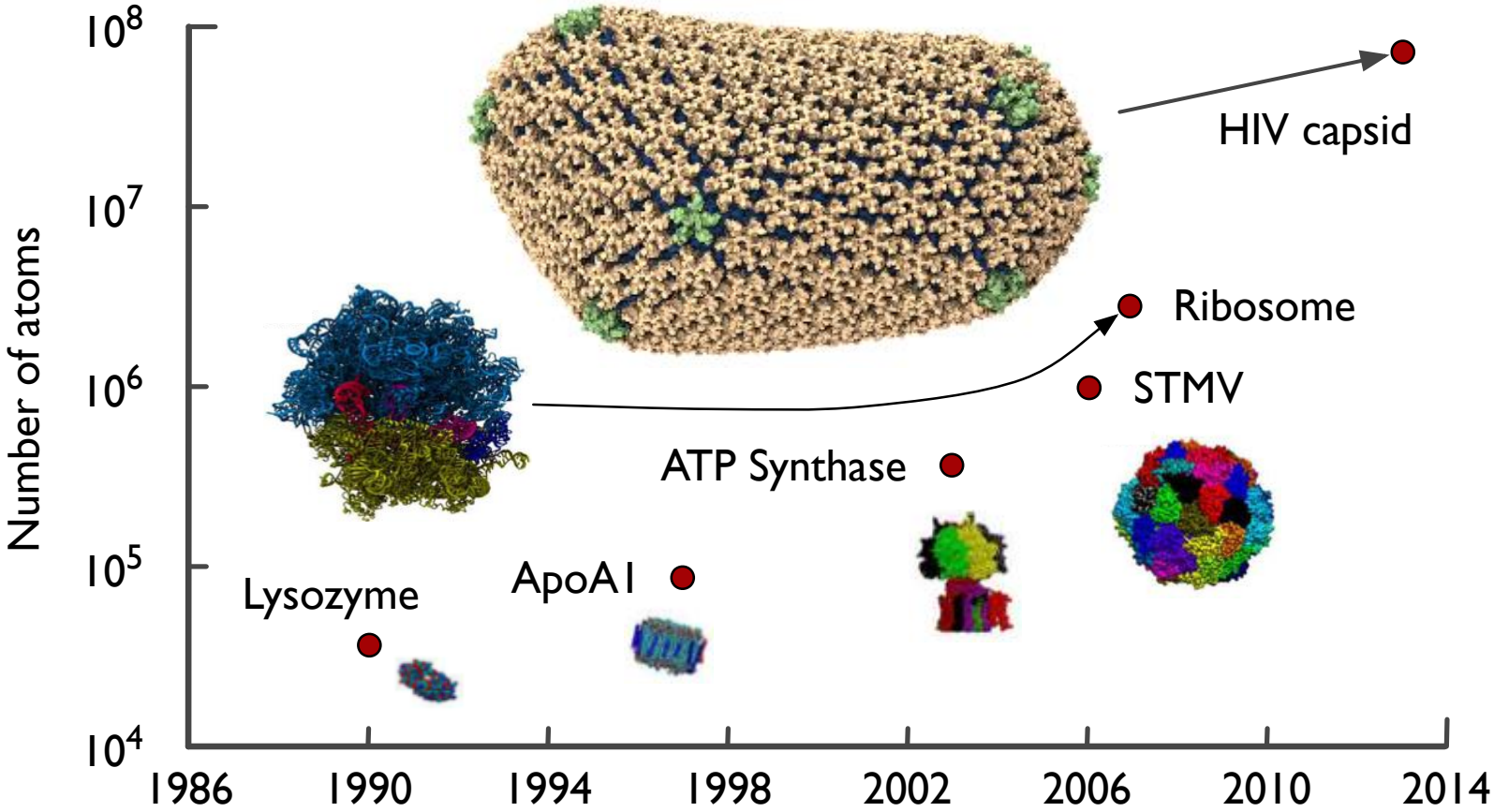
Ribosome: target for antibiotics



Poliovirus

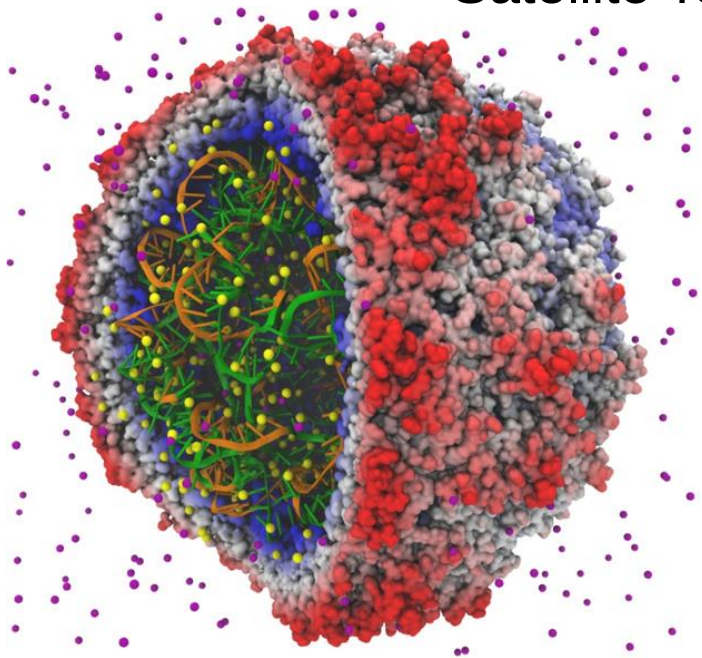


NAMD and VMD Use GPUs & Petascale Computing to Meet Computational Biology's Insatiable Demand for Processing Power



First Simulation of a Virus Capsid (2006)

Satellite Tobacco Mosaic Virus (STMV)



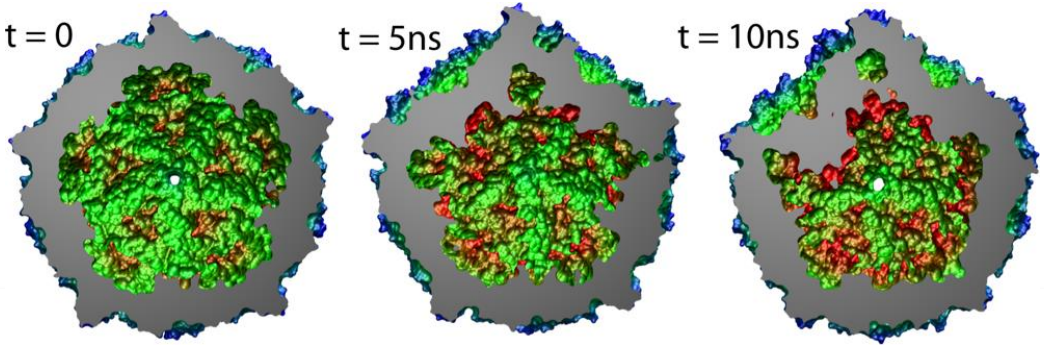
1 million atoms
A huge system for 2006

First MD simulation of a complete virus capsid

STMV smallest available capsid structure

STMV simulation, visualization, and analysis pushed us toward GPU computing!

MD showed that STMV capsid collapses without its RNA core



Freddolino et al., ***Structure***, **14**:437 (2006)

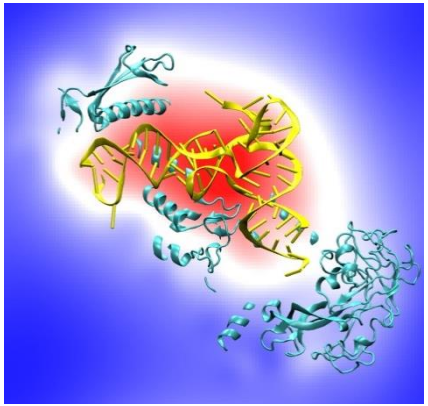
Taking STMV From a “Hero” Simulation to a “Routine” Simulation with GPUs

- The STMV project was a turning point
  - Preparing STMV models and placing ions tremendously demanding computational task
  - Existing approaches to visualizing and analyzing the simulation began to break down
- It was already clear in 2006 that the study of viruses relevant to human health would require a long-term investment in **better parallel algorithms and extensive use of acceleration technologies in NAMD and VMD**
- **These difficulties led us to accelerate key modeling tasks with GPUs**

VMD Electrostatics: Our First Use of CUDA

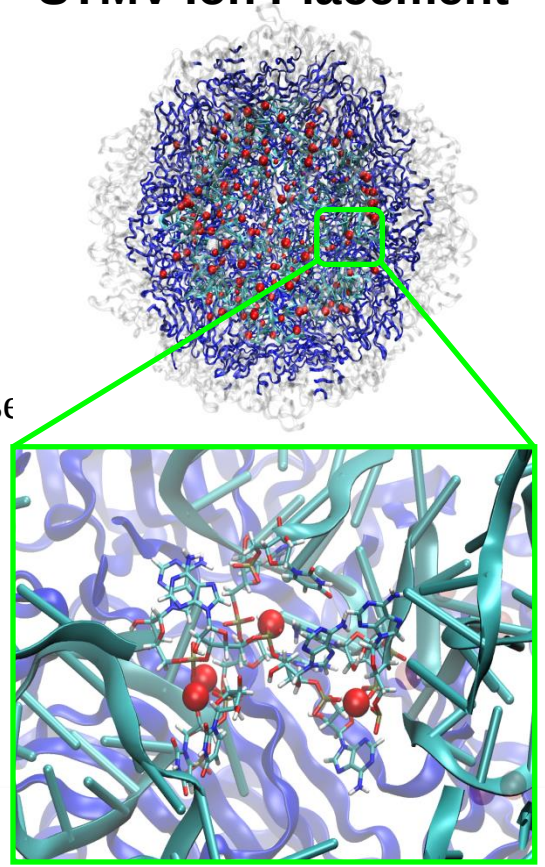
- **CUDA 0.7: Spring 2007**
- Electrostatic potential maps evaluated on 3-D lattice:

$$V_i = \sum_j \frac{q_j}{4\pi\epsilon_0 |\mathbf{r}_j - \mathbf{r}_i|}$$



Isoleucine tRNA synthetase

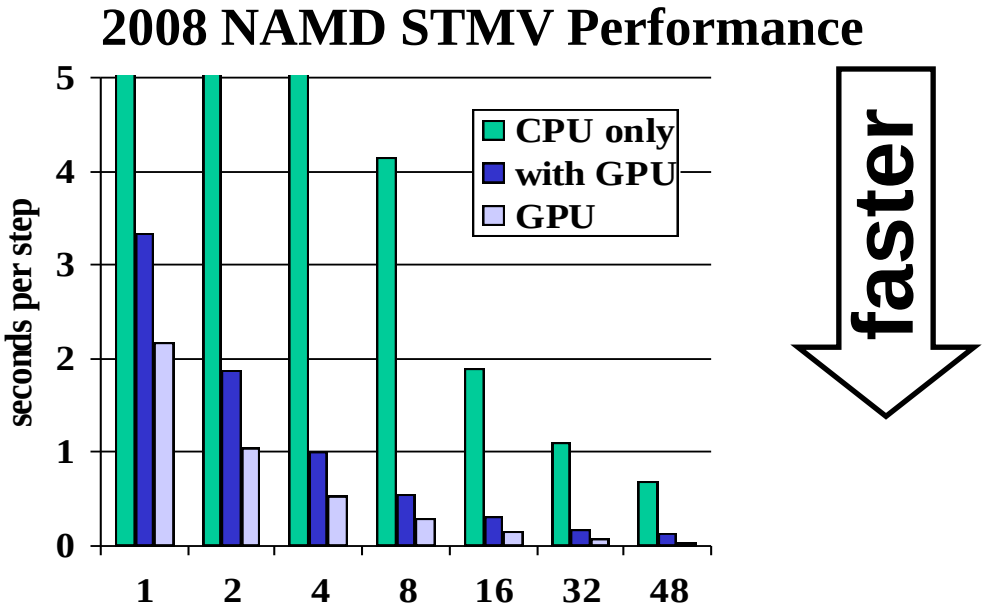
STMV Ion Placement



- Applications include:
  - Ion placement for structure building
  - Visualization and analysis

Accelerating Molecular Modeling Applications with Graphics Processors.
Stone et al., J. Computational Chemistry, 28:2618-2640, 2007.

Bringing NAMD to GPU Clusters



2.4 GHz Opteron + Quadro FX 5600

2008 NCSA “QP” GPU Cluster

Adapting a message-driven parallel application to GPU-accelerated clusters.
Phillips et al. In SC '08: Proceedings of the 2008 ACM/IEEE Conference on Supercomputing, 2008.

Getting Past the “Chicken and the Egg”

- GPU clusters still rare circa 2009-2011, most were not quite big enough to be used for large scale production science yet … but the potential was definitely there
- Performance and power efficiency benefits were seen for NAMD, VMD, others, on ever larger node counts
- Larger GPU accelerated systems were on the horizon

GPU Clusters for High Performance Computing. Kindratenko et al., IEEE Cluster’09, pp. 1-8, 2009.

Probing biomolecular machines with graphics processors. Phillips et al. CACM, 52:34-41, 2009.

GPU-accelerated molecular modeling coming of age. Stone et al., J. Mol. Graphics and Modelling, 29:116-125, 2010.

Quantifying the impact of GPUs on performance and energy efficiency in HPC clusters. Enos et al., International Conference on Green Computing, pp. 317-324, 2010.

Fast analysis of molecular dynamics trajectories with graphics processing units-radial distribution function histogramming. Levine et al., J. Computational Physics, 230:3556-3569, 2011.

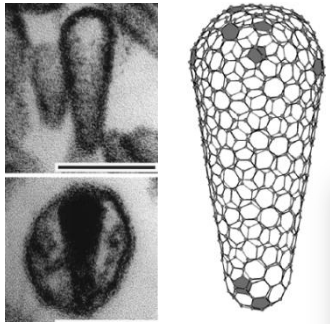
Blue Waters and the HIV Capsid

All-atom HIV-1 capsid structure solved

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

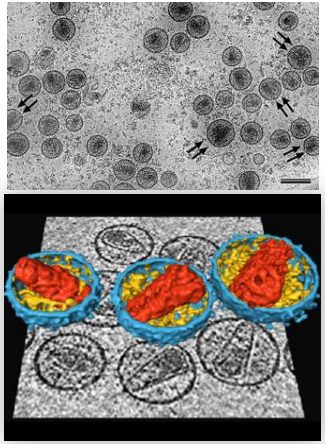
Structural Route to the HIV-1 Capsid

1st TEM (1999)

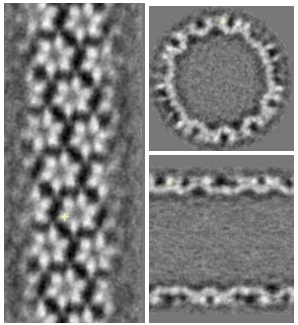


Ganser et al. *Science*, 1999
Briggs et al. *EMBO J*, 2003
Briggs et al. *Structure*, 2006

1st tomography (2003)

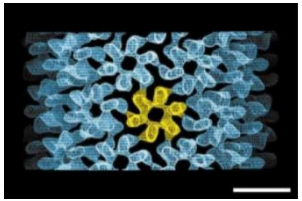


cryo-ET (2006)



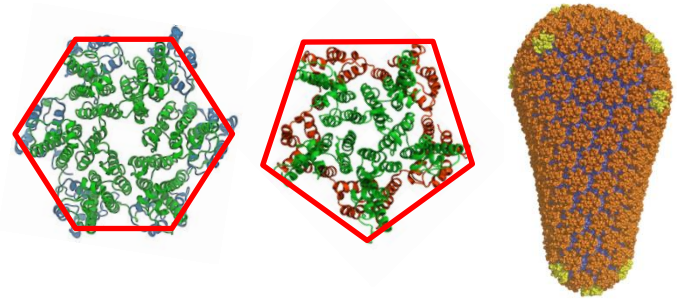
Byeon et al., *Cell* 2009

hexameric tubules



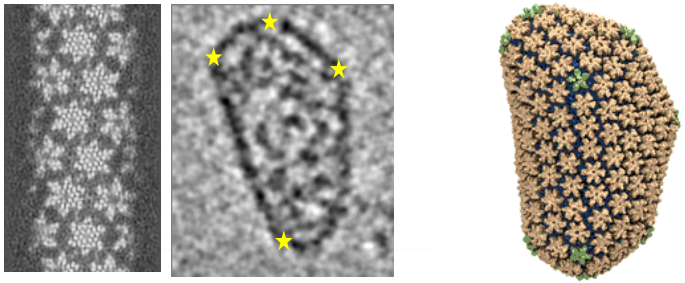
Li et al., *Nature*, 2000

Crystal structures of separated hexamer and pentamer



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

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

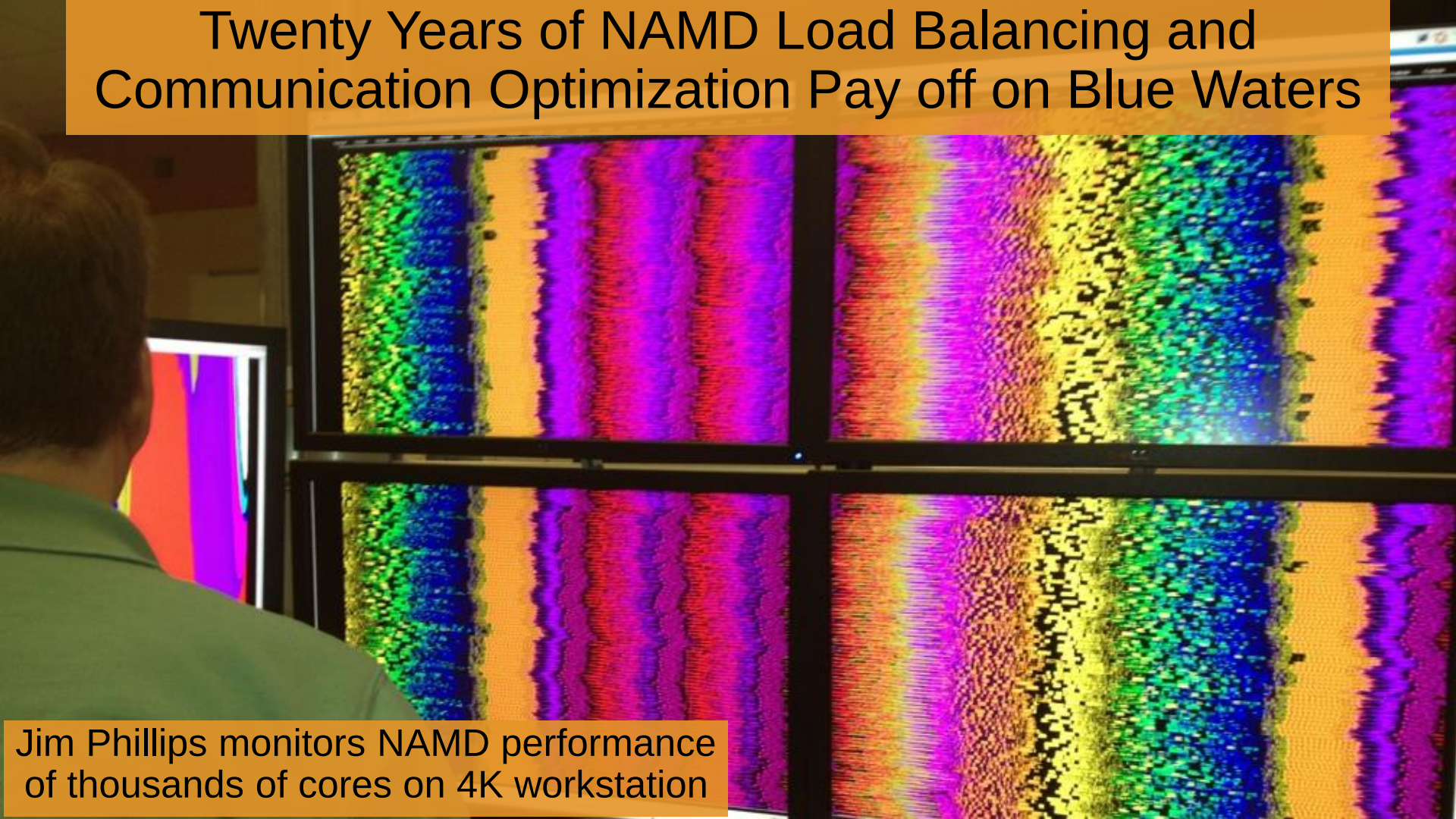


Zhao et al. , *Nature* 497: 643-646 (2013)

Blue Waters Posed Many Challenges

- Scale NAMD to 100M atoms
  - Read new .js file format
  - Distribute or compress static molecular structure data
  - Parallel atomic data input
  - Use shared memory in a node
  - Parallel load balancing
  - Parallel, asynchronous trajectory and restart file output
  - 2D decomposition of 3D FFT
  - Limit steering force messages
  - Fix minimizer stability issues
- Also build benchmarks…
- Scale NAMD to 300K cores
  - Charm++ shared memory tuning
  - IBM Power7 network layer
  - IBM BlueGene/Q network layer
  - Cray Gemini network layer
  - Cray torus topology information
  - Charm++ replica layers
  - Optimize for physical nodes
  - Adapt trees to avoid throttling
  - Optimize for torus topology
  - Optimize for parallel filesystem
- **Optimize for new GPUs…**

Twenty Years of NAMD Load Balancing and Communication Optimization Pay off on Blue Waters

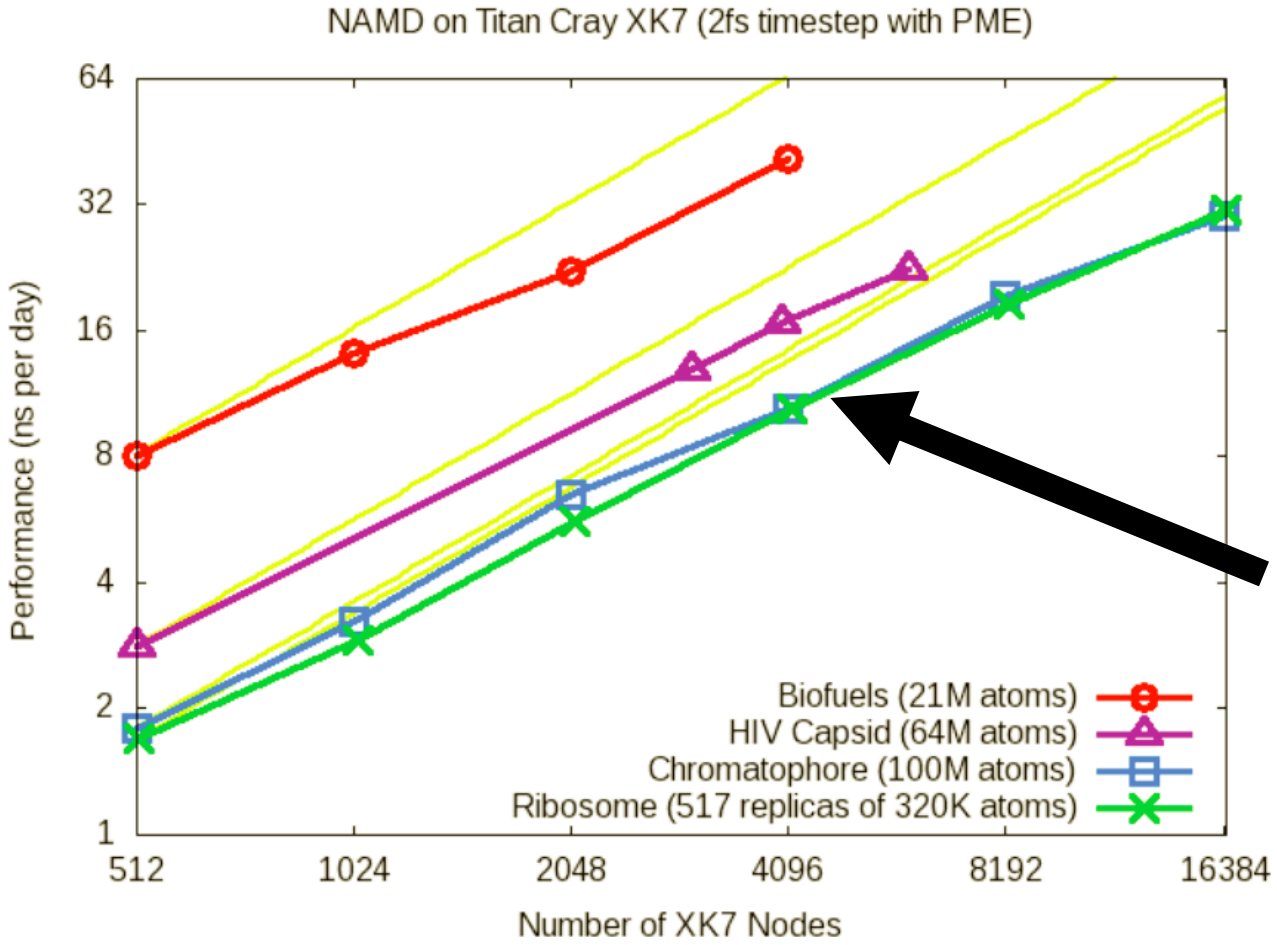


Jim Phillips monitors NAMD performance of thousands of cores on 4K workstation

New NAMD+GPUs Will Make Petascale Routine

- 100M-atom simulations need to be commonly available
  - Commodity clusters to the rescue (again)
- GPUs are the future of supercomputing
  - GPU performance growing exponentially
  - GPUs communicate directly via InfiniBand etc.
- **Future NAMD will be GPU-centric**
  - Enabled by Charm++ MPI-interoperability
  - Focus on enabling ~10-100M-atom simulations
  - Benefits extend to smaller simulations
- Rack of 160 GPUs can match 5% of Blue Waters today
  - Dedicated 24/7 to a single simulation

NAMD Cray XK7 Performance August 2013

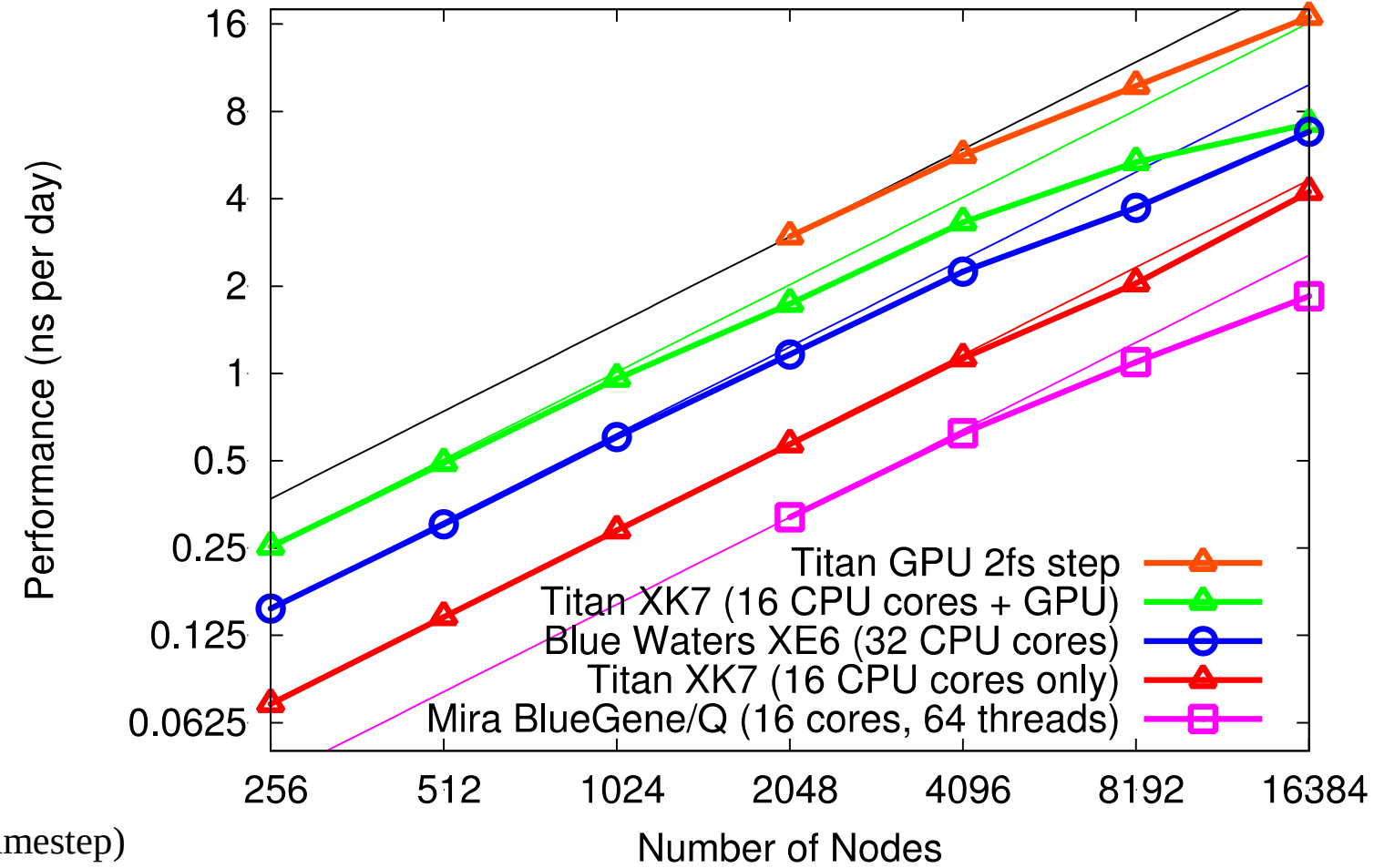


NAMD XK7 vs. XE6

Speedup: 3x-4x

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

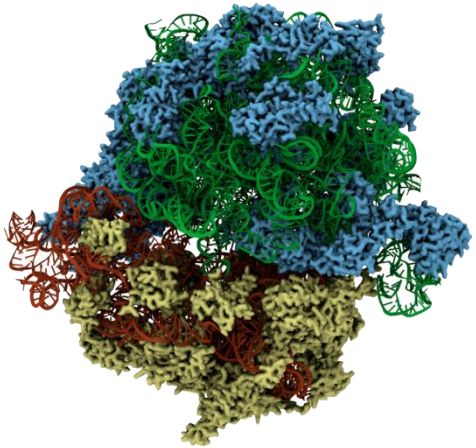
240M atom Influenza Virus Scales to Entire Petascale Machines



(1fs timestep)

Other Projects Using Petascale Computing

From cellular machines to the pharmacy...



ribosome

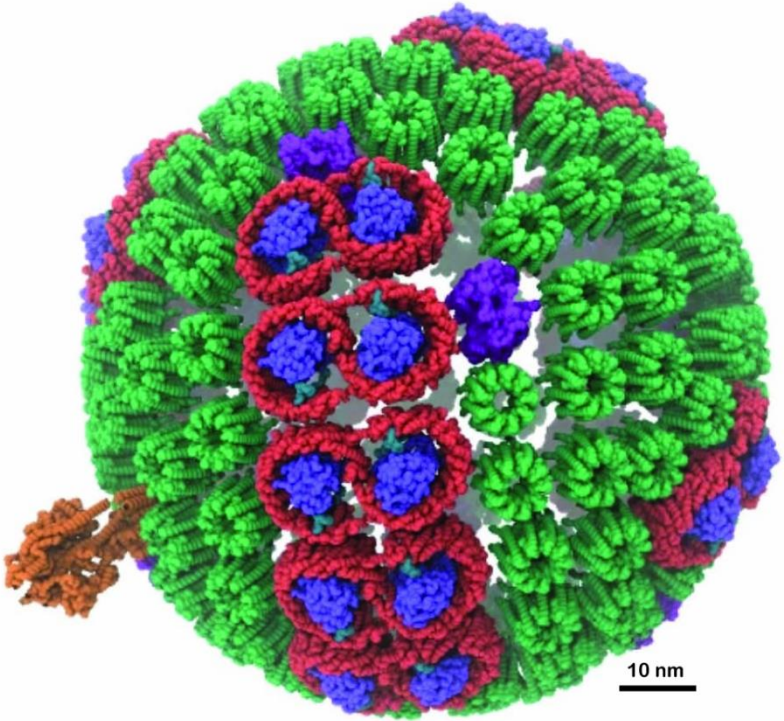
3 M atoms, multiple replicas

From woodchips to gasoline...

second-generation biofuels

> 10 M atoms

From solar energy to cellular fuel...

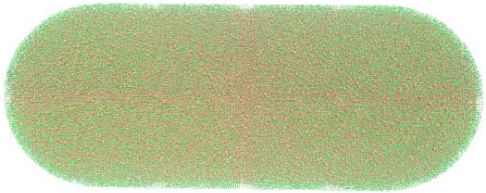


photosynthetic chromatophore

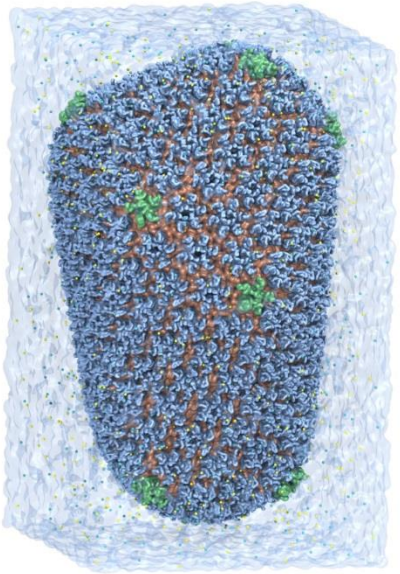
100 M atoms

VMD – “Visual Molecular Dynamics”

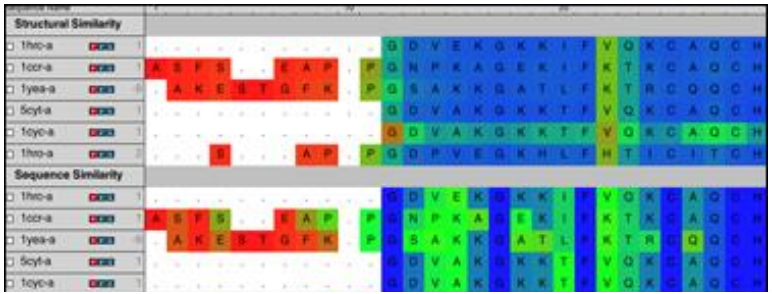
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



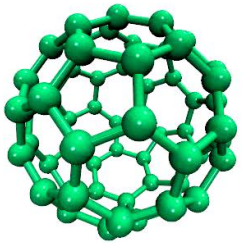
Whole Cell Simulation



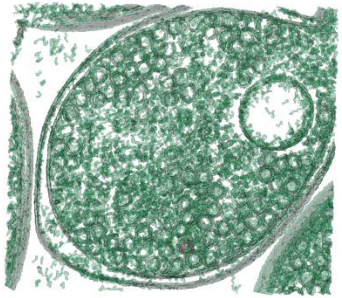
MD Simulations



Sequence Data



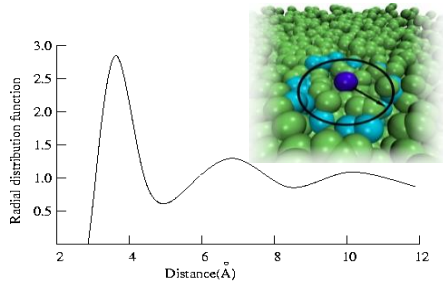
Quantum Chemistry

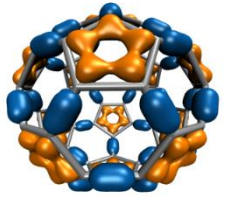


CryoEM, Cellular Tomography

CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

VMD GPU-Accelerated Feature or Kernel	Exemplary speedup vs. multi-core CPU (e.g. 4-core CPU)
Molecular orbital display	**30x**
Radial distribution function	**23x**
Molecular surface display	**15x**
Electrostatic field calculation	**11x**
Ray tracing w/ shadows, AO lighting	**8x**
Ion placement	6x
MDFF density map synthesis	6x
Implicit ligand sampling	6x
Root mean squared fluctuation	6x
Radius of gyration	5x
Close contact determination	5x
Dipole moment calculation	4x





VMD Supports Petascale Biology

- **Where to put the data?**
  - Trajectories too large to download
  - **Analyze 231 TB trajectory set in 15 min**, parallel I/O @ **275 GB/sec** on 8,192 nodes
- **Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis tasks**
  - GPU electrostatics, RDF, density quality-of-fit
  - OpenGL Pbuffer off-screen rendering support
  - GPU ray tracing w/ ambient occlusion lighting
- VMD analysis calculations and movie renderings use dynamic load balancing, tested with up to 262,144 CPU cores
- Available on: NCSA Blue Waters, ORNL Titan, Indiana Big Red II

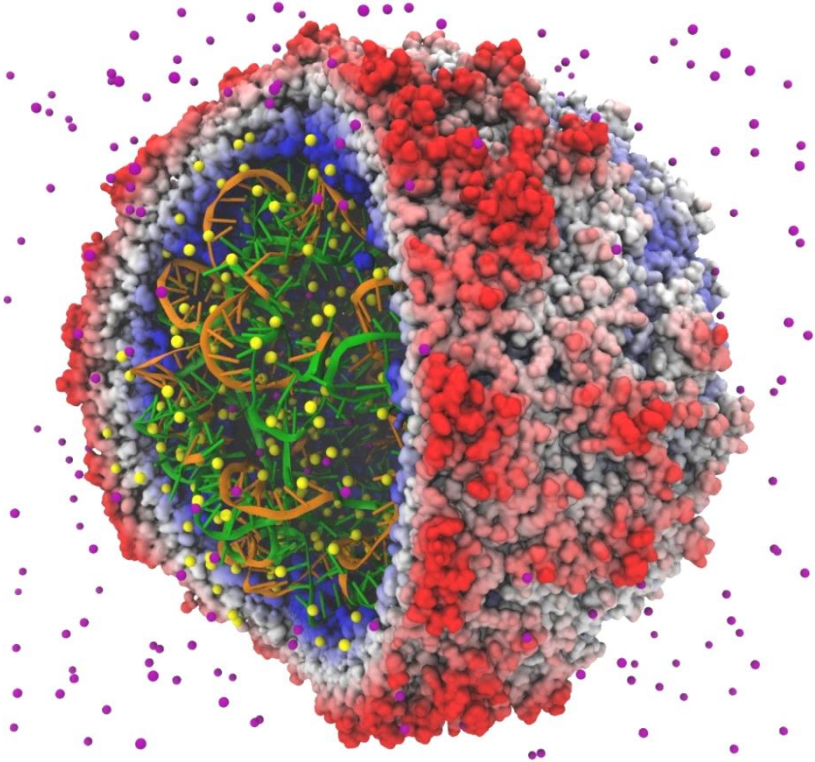
NCSA Blue Waters
Cray XE6 / XK7 Supercomputer

22,640 XE6 CPU nodes

4,224 XK7 nodes w/ GPUs enable fast VMD analysis and visualization

VMD “QuickSurf” Representation

- Displays continuum of structural detail:
  - All-atom, coarse-grained, cellular models
  - Smoothly variable detail controls
- Linear-time algorithm, scales to millions of particles, as **limited by memory capacity**
- Uses multi-core CPUs and GPU acceleration to enable **smooth interactive animation** of molecular dynamics trajectories w/ up to ~1-2 million atoms
- **GPU acceleration yields 10x-15x speedup vs. multi-core CPUs**



Satellite Tobacco Mosaic Virus

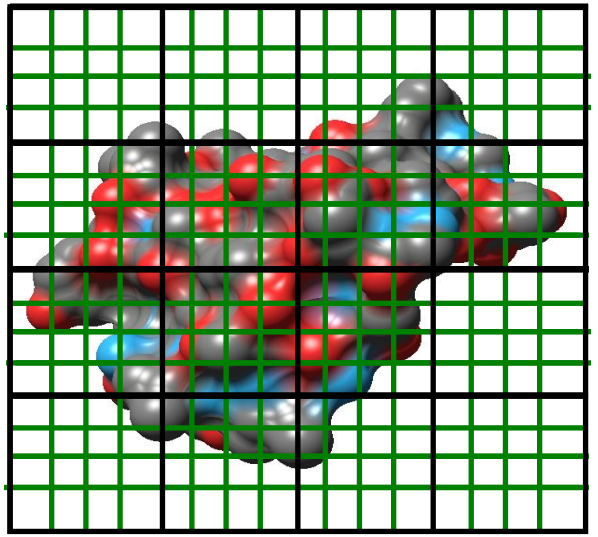
Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.
M. Krone, J. E. Stone, T. Ertl, K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012

QuickSurf Algorithm Improvements

- **50%-66% memory use, 1.5x-2x speedup**
- Build spatial acceleration data structures, optimize data for GPU
- Compute 3-D density map, 3-D color texture map with **data-parallel *"gather"* algorithm**:

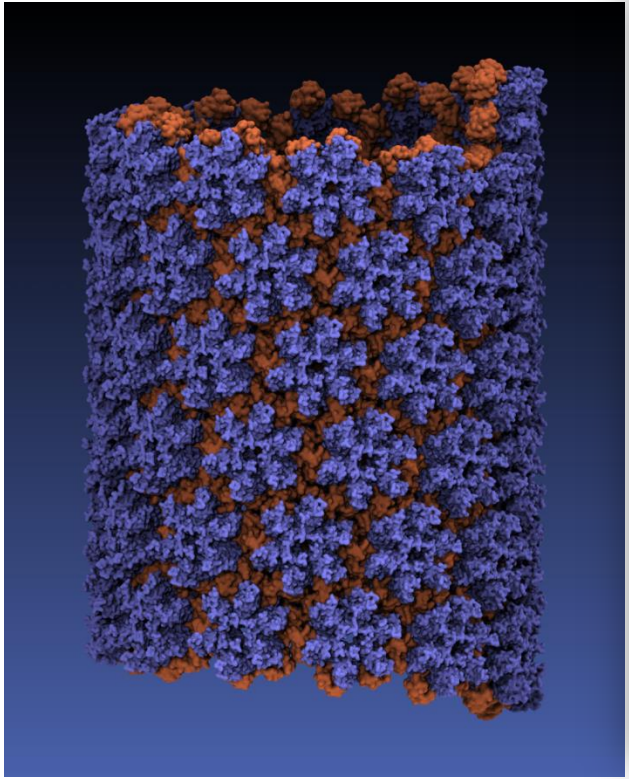
$$\rho(\vec{r}; \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{i=1}^{N} e^{\frac{-|\vec{r}-\vec{r}_i|^2}{2\alpha^2}}$$

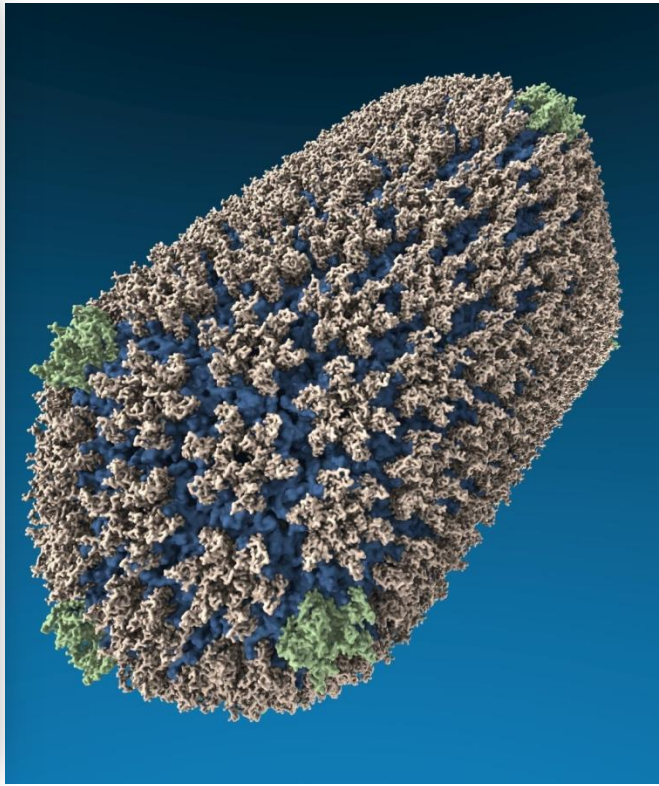
- Normalize, quantize, and compress density, color, surface normal data **while in registers**, before writing out to GPU global memory
- Extract isosurface, maintaining quantized/compressed data representation



3-D density map lattice, spatial acceleration grid, and extracted surface

VMD “QuickSurf” Representation, Ray Tracing

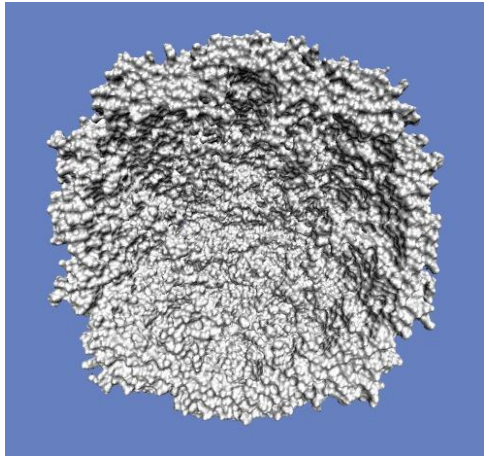




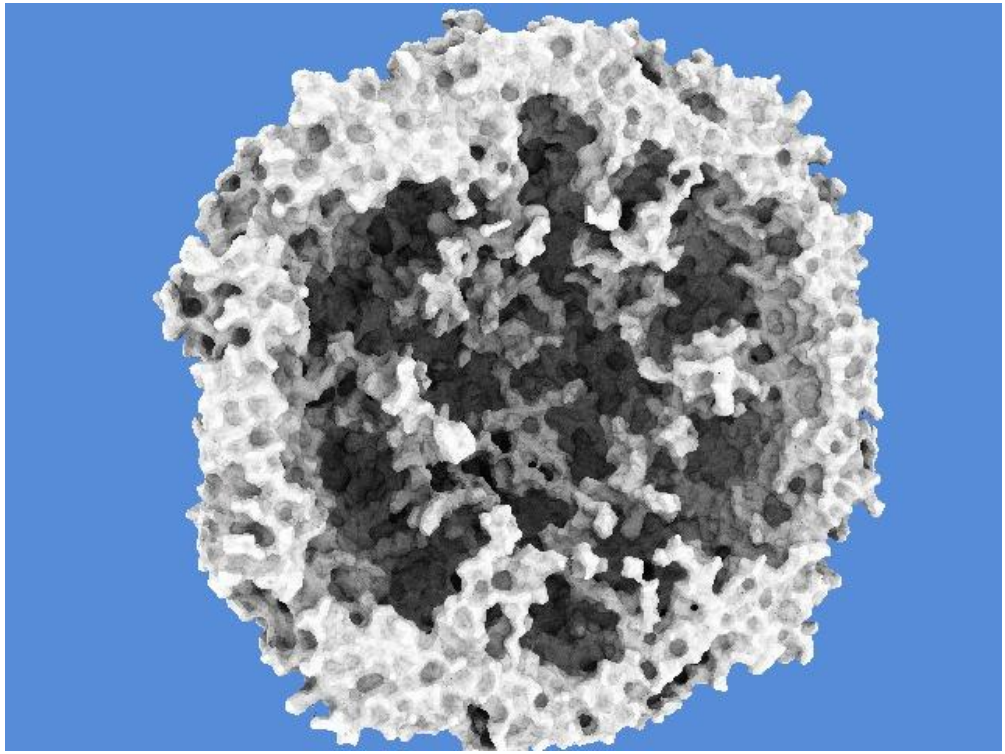
All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

Ray Tracing of VMD Molecular Graphics

- **STMV virus capsid on a laptop GeForce GTX 560M**
- **Ambient occlusion lighting**, shadows, reflections, transparency, and much more…



Standard OpenGL rasterization



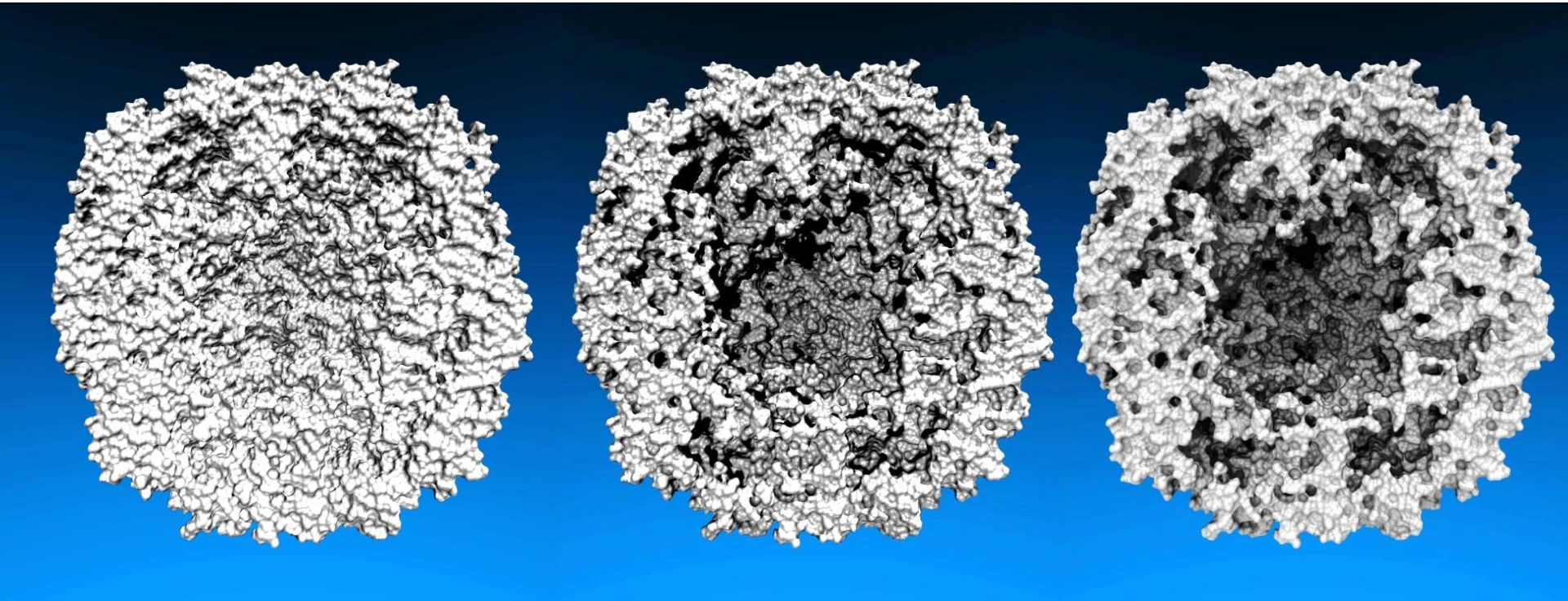
VMD w/ new GPU ray tracing engine based on CUDA + OptiX

Lighting Comparison

Two lights, no shadows

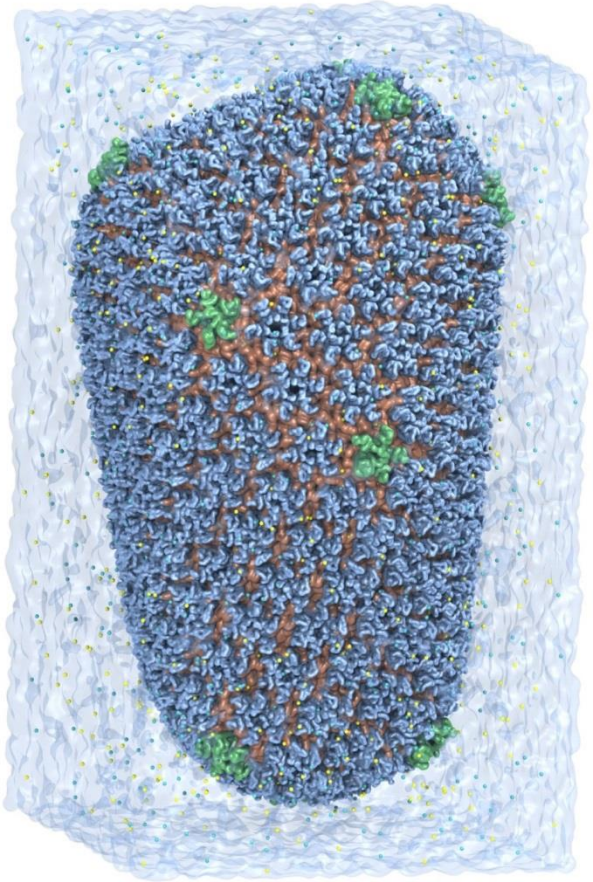
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit

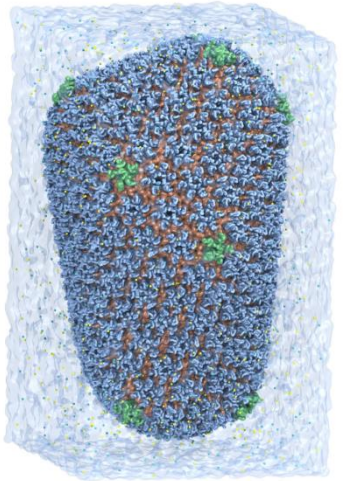


GPU Ray Tracing of HIV-1 on Blue Waters

- 64M atom simulation, 1079 movie frames
- **Ambient occlusion lightin**g, shadows, transparency, antialiasing, depth cueing, **144 rays/pixel minimum**
- GPU memory capacity hurdles:
  - Regen BVH every simulation timestep, when graphical representations change
  - Surface calc. and ray tracing each use **over 75% of K20X 6GB on-board GPU memory,** even with quantized/compressed colors, surface normals, …
  - Evict non-RT GPU data to host prior to ray tracing



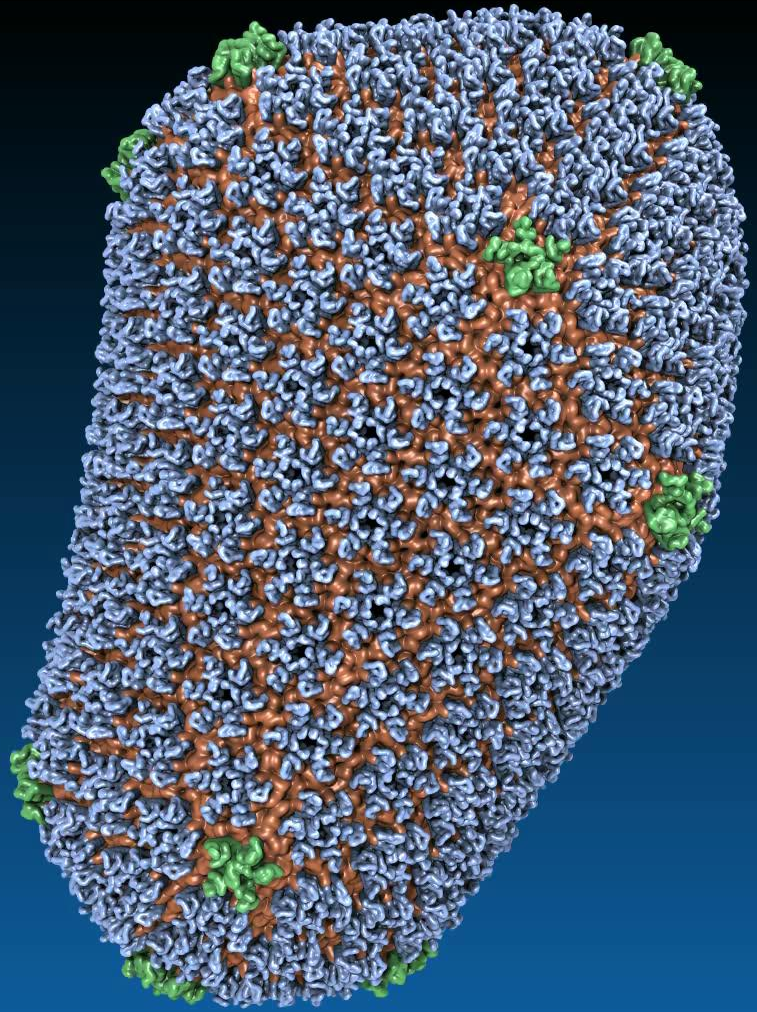
HIV-1 Parallel HD Movie Rendering on Blue Waters Cray XE6/XK7



New “TachyonL-OptiX” on XK7 vs. Tachyon on XE6:
K20X GPUs yield **up to eight times** geom+ray tracing speedup

Node Type and Count	Script Load Time	State Load Time	Geometry + Ray Tracing	Total Time
256 XE6 CPUs	7 s	160 s	**1,374 s**	**1,541 s**
512 XE6 CPUs	13 s	211 s	808 s	1,032 s
64 XK7 Tesla K20X GPUs	2 s	38 s	655 s	695 s
128 XK7 Tesla K20X GPUs	4 s	74 s	331 s	410 s
256 XK7 Tesla K20X GPUs	7 s	110 s	**171 s**	**288 s**

GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
Stone et al. In UltraVis'13: Eighth Workshop on Ultrascale Visualization Proceedings, 2013.



Center Facilities Enable Petascale Biology

External Resources, 90% of our Computer Power

Over the past five years our Center has assembled all necessary hardware and infrastructure to prepare and analyze petascale molecular dynamics simulations, and ***makes these facilities available to visiting researchers***.

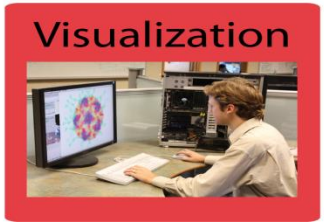
Simulation Output

10 Gigabit Network

Petascale Gateway Facility

High-End Workstations

Immediate On-Demand Computation



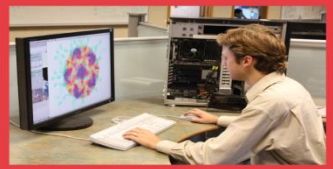
Virtual Facilities to Enable Petascale ***Anywhere***

High-end visualization and analysis workstations currently available only in-person in labs like ours must be ***virtualized and embedded at supercomputer centers***.

Storage

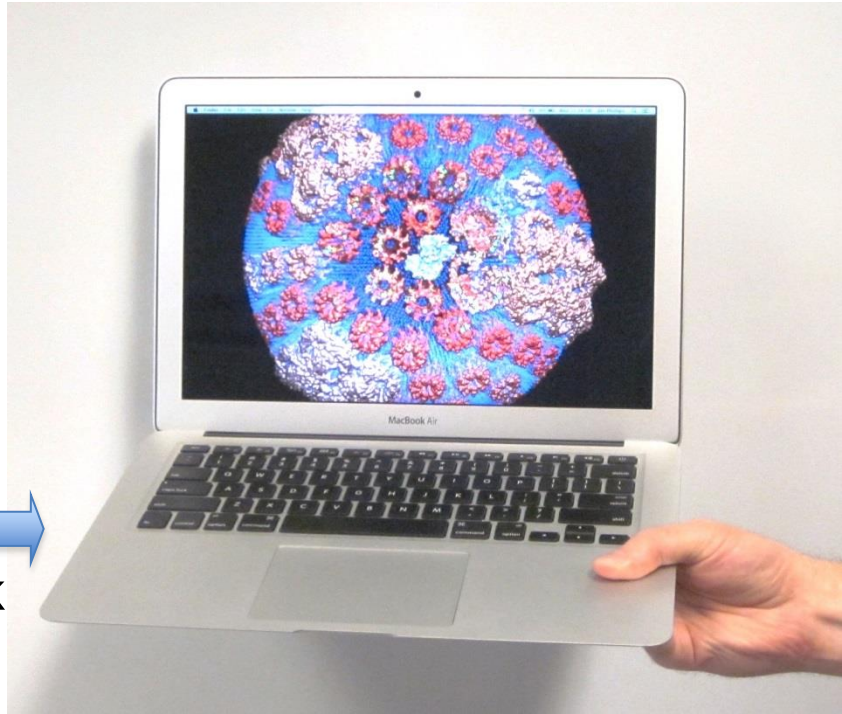
Compute

Visualization



Compressed Video

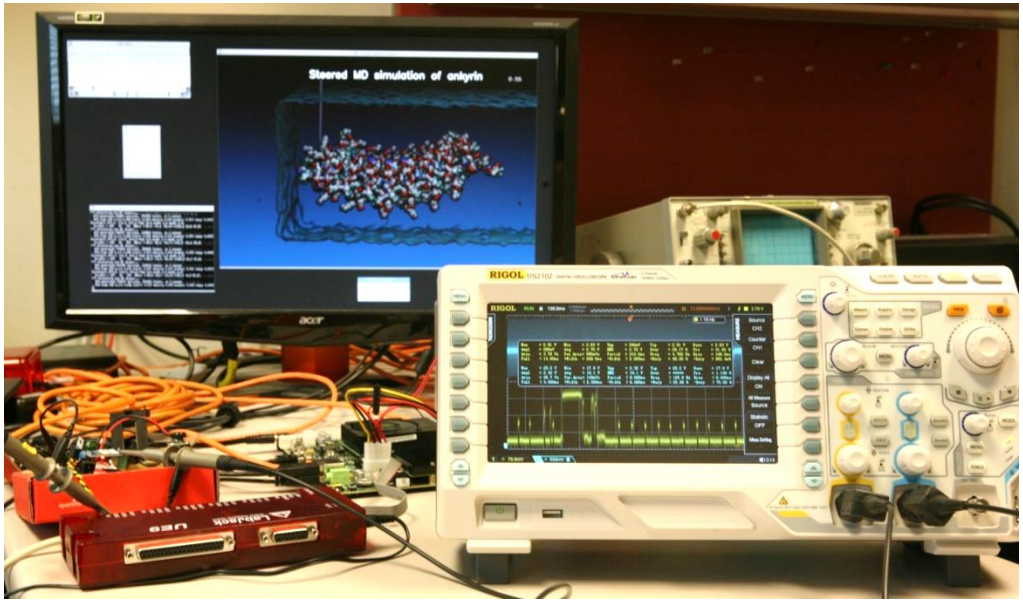
~1 Gigabit Network



Optimizing GPU Algorithms for Power Consumption

NVIDIA “Carma” and “Kayla” Tegra ARM processors, single board computers with CUDA-enabled GPUs

Platform	Normalized performance/watt (higher is better)
Intel Core i7-3960X	1.00x
NVIDIA Kayla w/ GeForce 680	1.03x
NVIDIA Kayla w/ GeForce Titan	1.22x
NVIDIA Kayla w/ Quadro K4000	1.76x
NVIDIA Kayla w/ Quadro K2000	2.02x
NVIDIA Kayla w/ GTX 640	**2.51x**



Tegra+GPU energy efficiency measurement testbed

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  - NIH support: 9P41GM104601, 5R01GM098243-02
  - DOE INCITE


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Urbana-Champaign

GPU Computing Publications

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

- **GPU-accelerated molecular visualization on petascale supercomputing platforms.** J. E. Stone, K. L. Vandivort, and Klaus Schulten. In UltraVis'13: Eighth Workshop on Ultrascale Visualization Proceedings, pp. 6:1-6:8, 2013.
- **Early Experiences Scaling VMD Molecular Visualization and Analysis Jobs on Blue Waters.** J. E. 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. E. 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. E. 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. Vandivort, and K. Schulten. G. Bebis et al. (Eds.): *7th International Symposium on Visual Computing (ISVC 2011)*, LNCS 6939, pp. 1-12, 2011.

GPU Computing Publications

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

- **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.
- **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.

GPU Computing 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. 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.

GPU Computing 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.