# GPU-Accelerated Visualization and Analysis of Petascale Molecular Dynamics Simulations

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

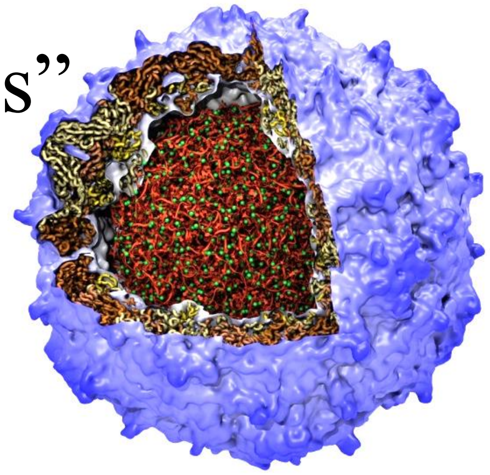
**http://www.ks.uiuc.edu/Research/gpu/**

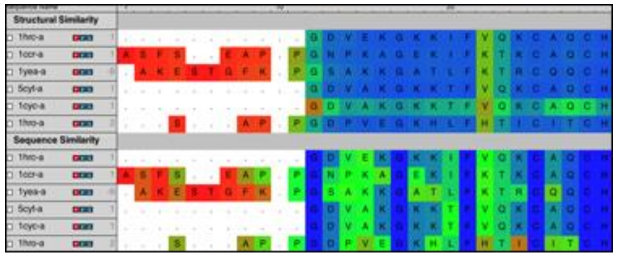
Missouri S&T, Research and Technology Day,

September 16, 2014

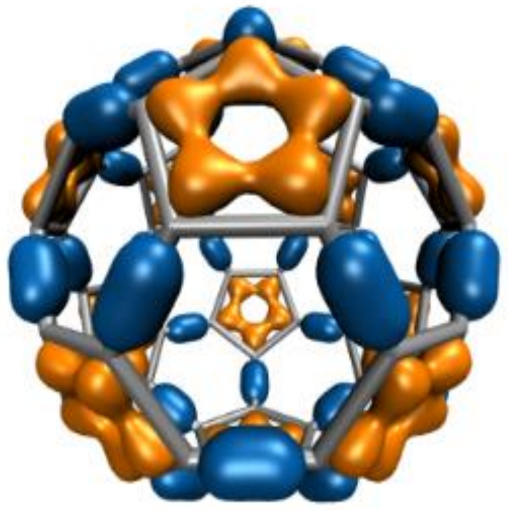
## VMD – “Visual Molecular Dynamics”

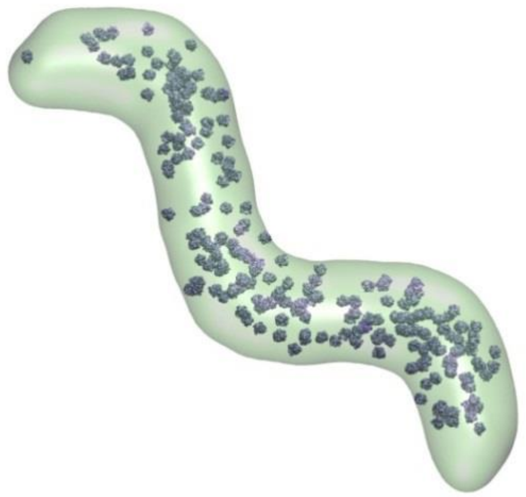
- Visualization and analysis of:
  - molecular dynamics simulations
  - quantum chemistry calculations
  - particle systems and whole cells
  - sequence data
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/

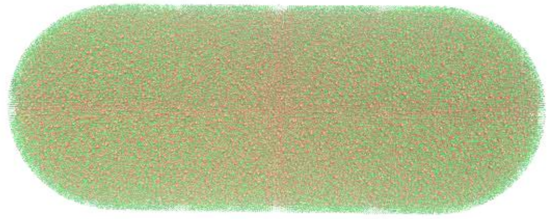

Poliovirus



Ribosome Sequences


Electrons in
Vibrating Buckyball

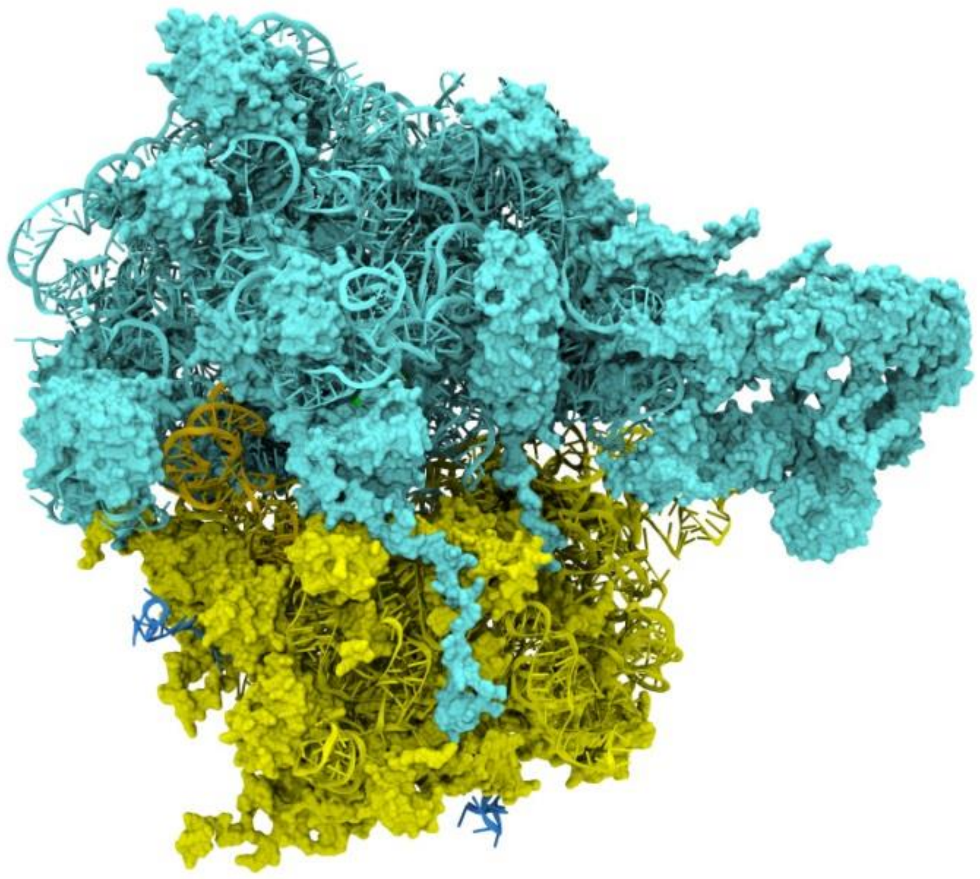

Cellular Tomography
Cryo-electron Microscopy


Whole Cell Simulations

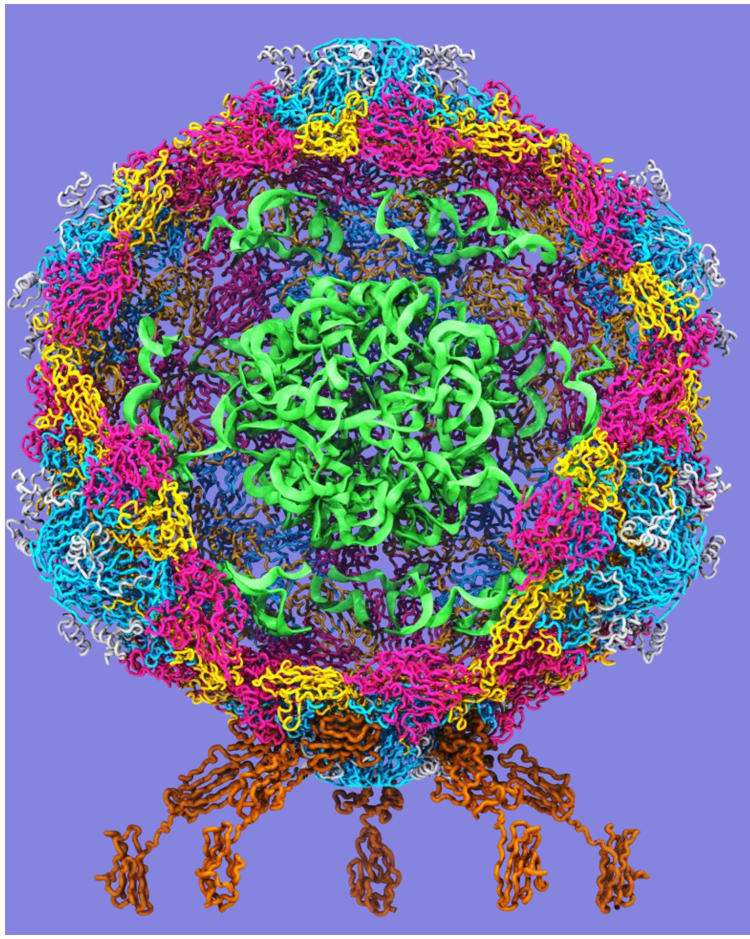
# Goal: A Computational Microscope

Study the molecular machines in living cells

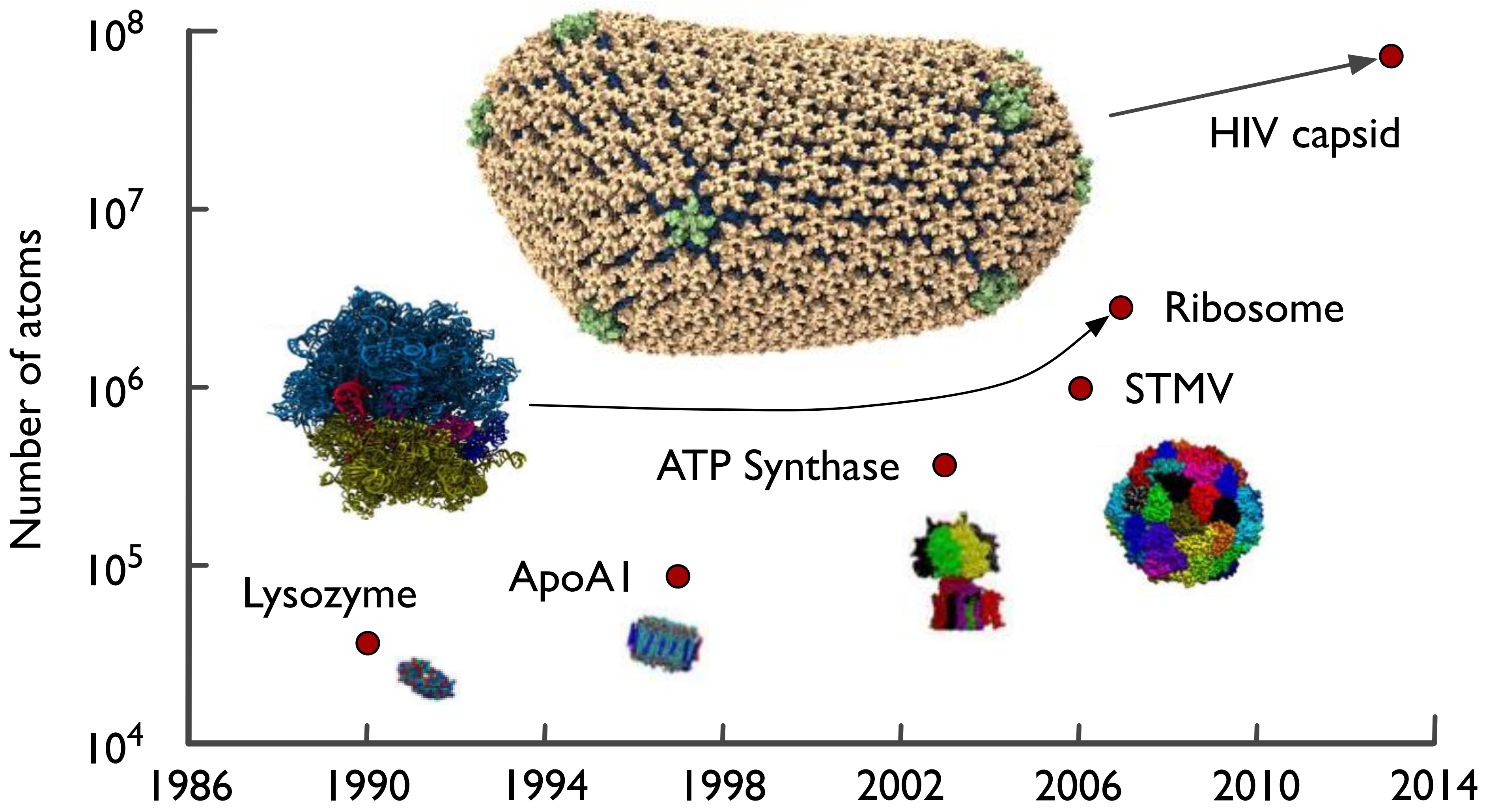
Ribosome: target for antibiotics



Poliovirus

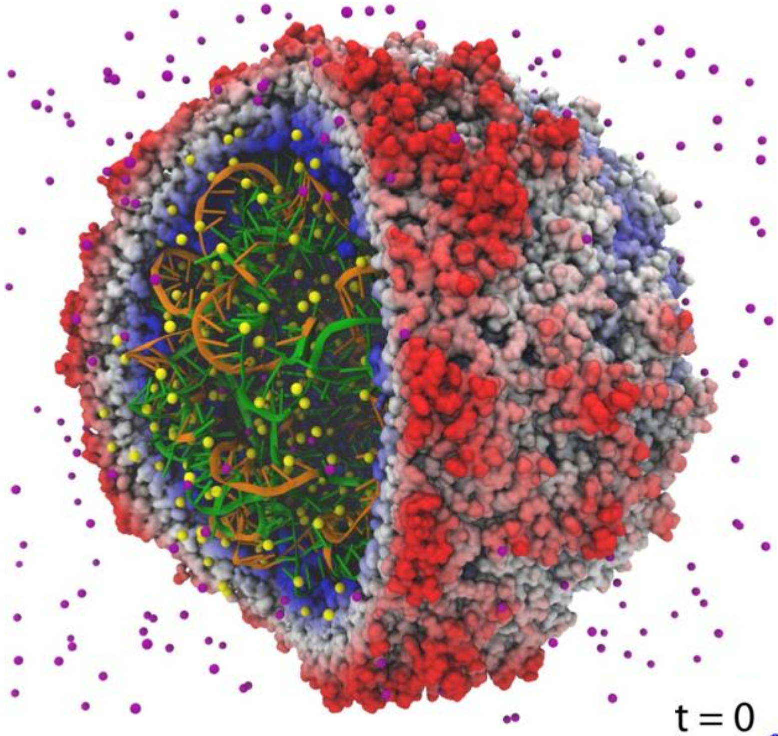


# NAMD and VMD Use GPUs & Petascale Computing to Meet Computational Biology's Insatiable Demand for Processing Power



# First Simulation of a Virus Capsid (2006)

Satellite Tobacco Mosaic Virus (STMV)

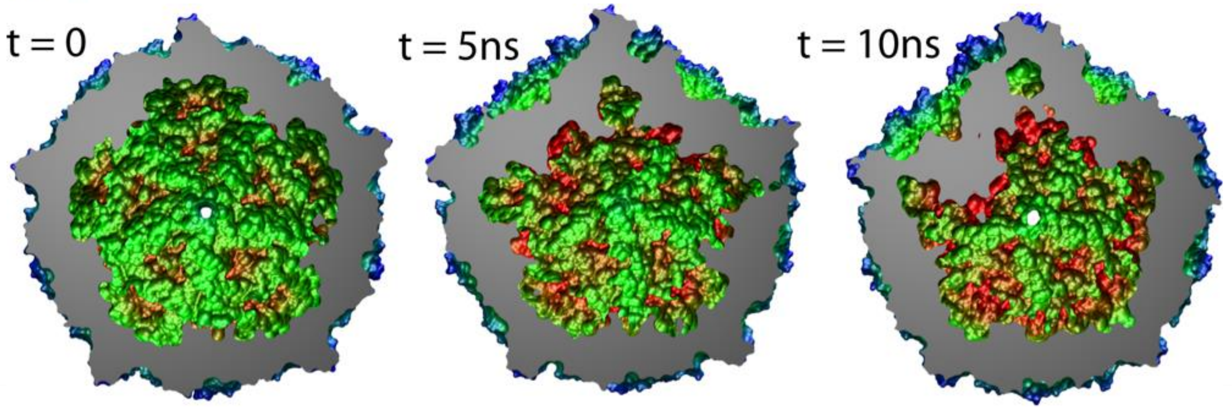


First MD simulation of a complete virus capsid

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



**1 million atoms**
**A huge system for 2006**

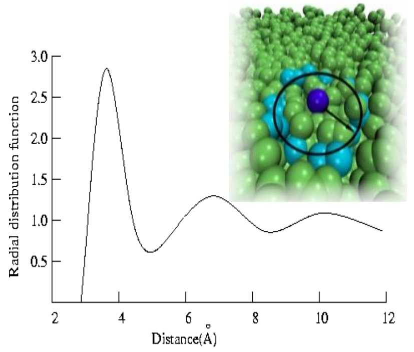
Freddolino et al., ***Structure***, **14**:437 (2006)

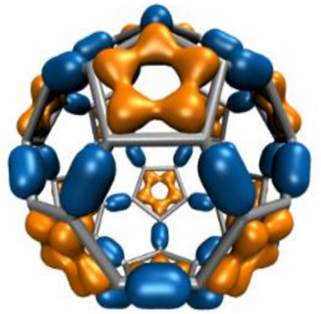
# GPU Computing

- Commodity devices, omnipresent in modern computers (over a **million** sold per **week**)
- Massively parallel hardware, hundreds of processing units, **throughput oriented architecture**
- Standard integer and floating point types supported
- Programming tools allow software to be written in dialects of familiar C/C++ and integrated into legacy software
- GPU algorithms are often multicore friendly due to attention paid to **data locality** and **data-parallel** work decomposition

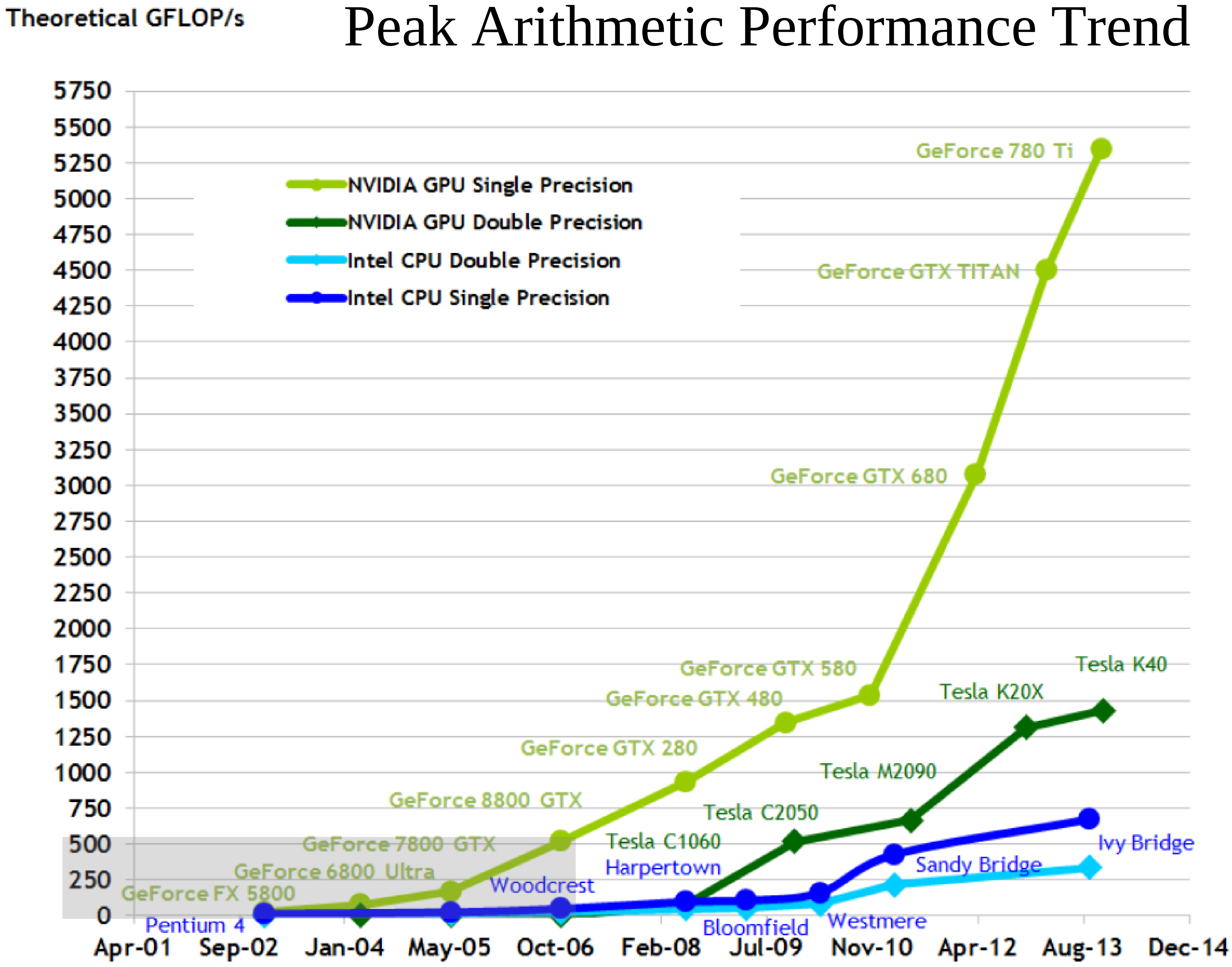
# CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

| **VMD GPU-Accelerated Feature or Kernel** | **Typical 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** | **7x** |
| 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 |

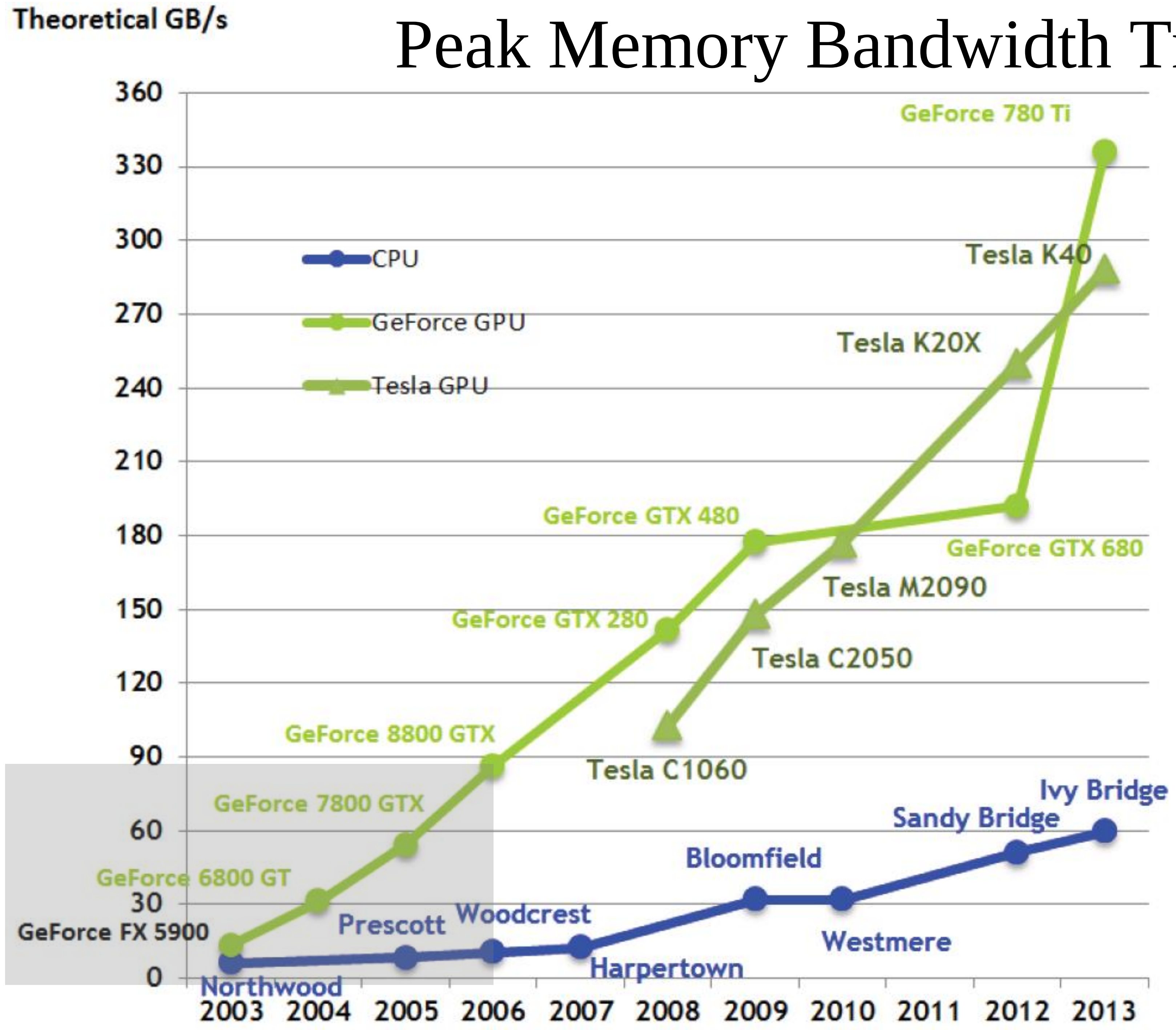




# Peak Arithmetic Performance Trend



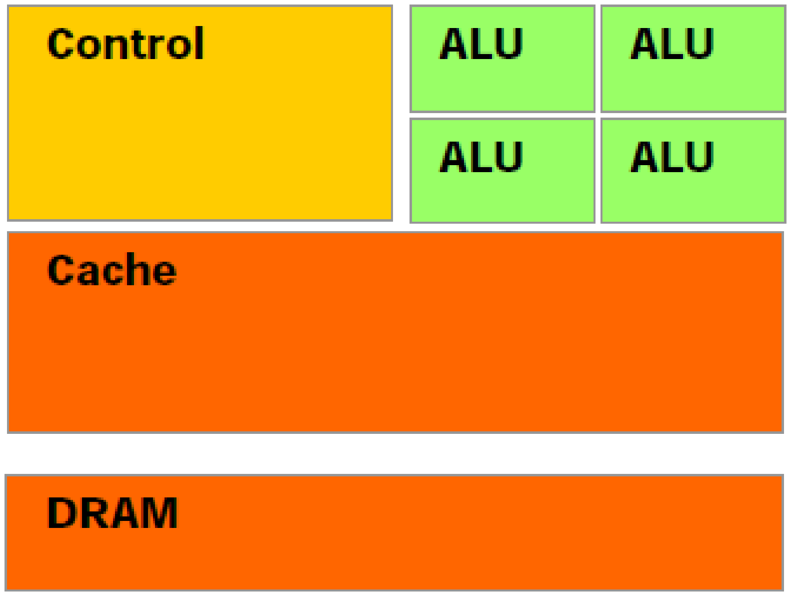
# Peak Memory Bandwidth Trend

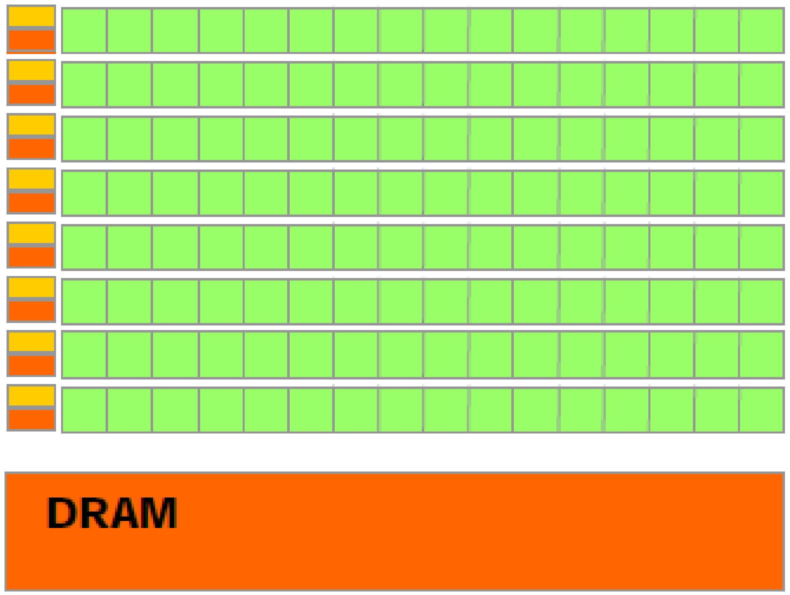


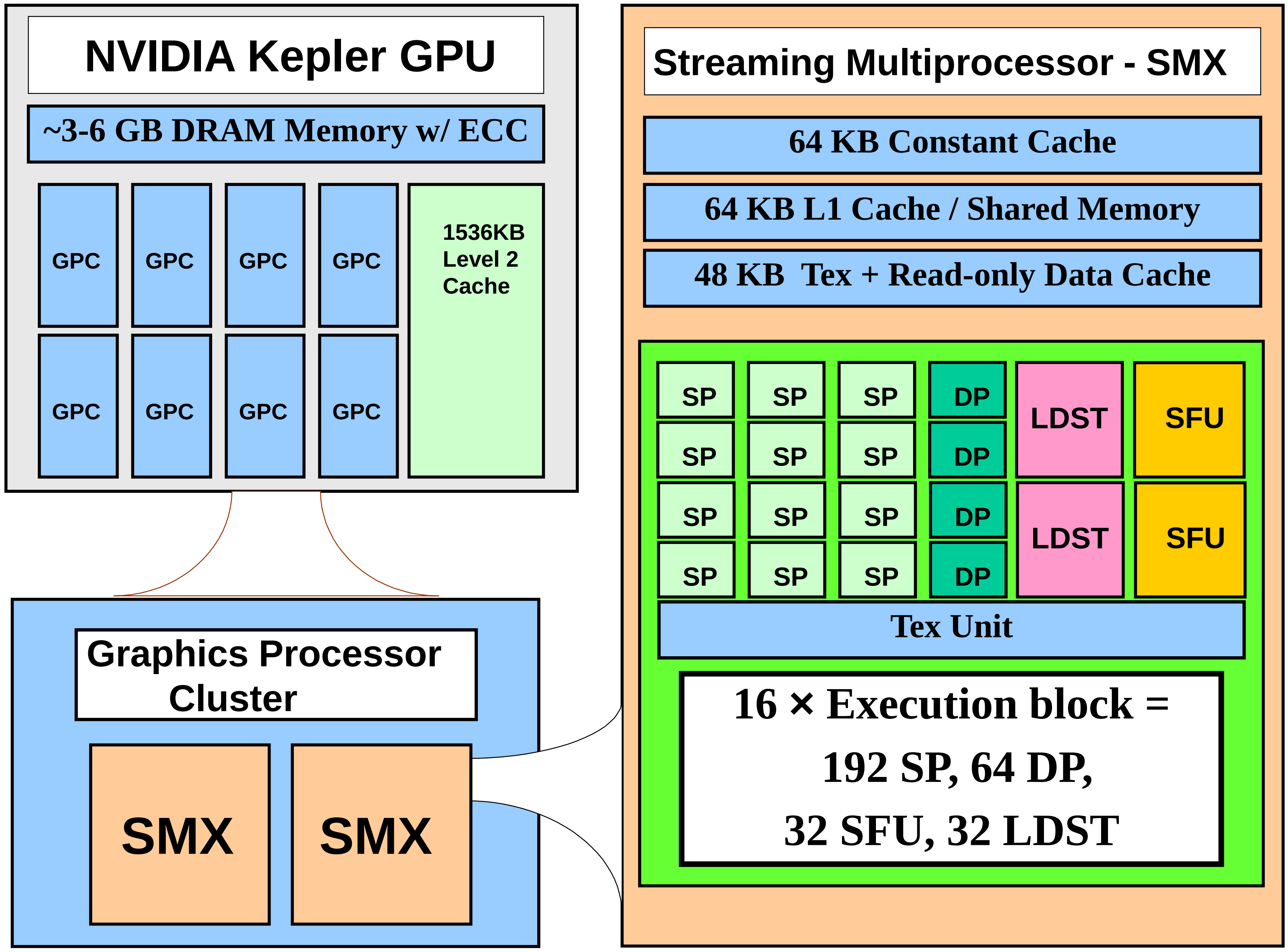
# Comparison of CPU and GPU Hardware Architecture

**CPU**: Cache heavy, focused on individual thread performance

**GPU**: ALU heavy, massively parallel, throughput oriented



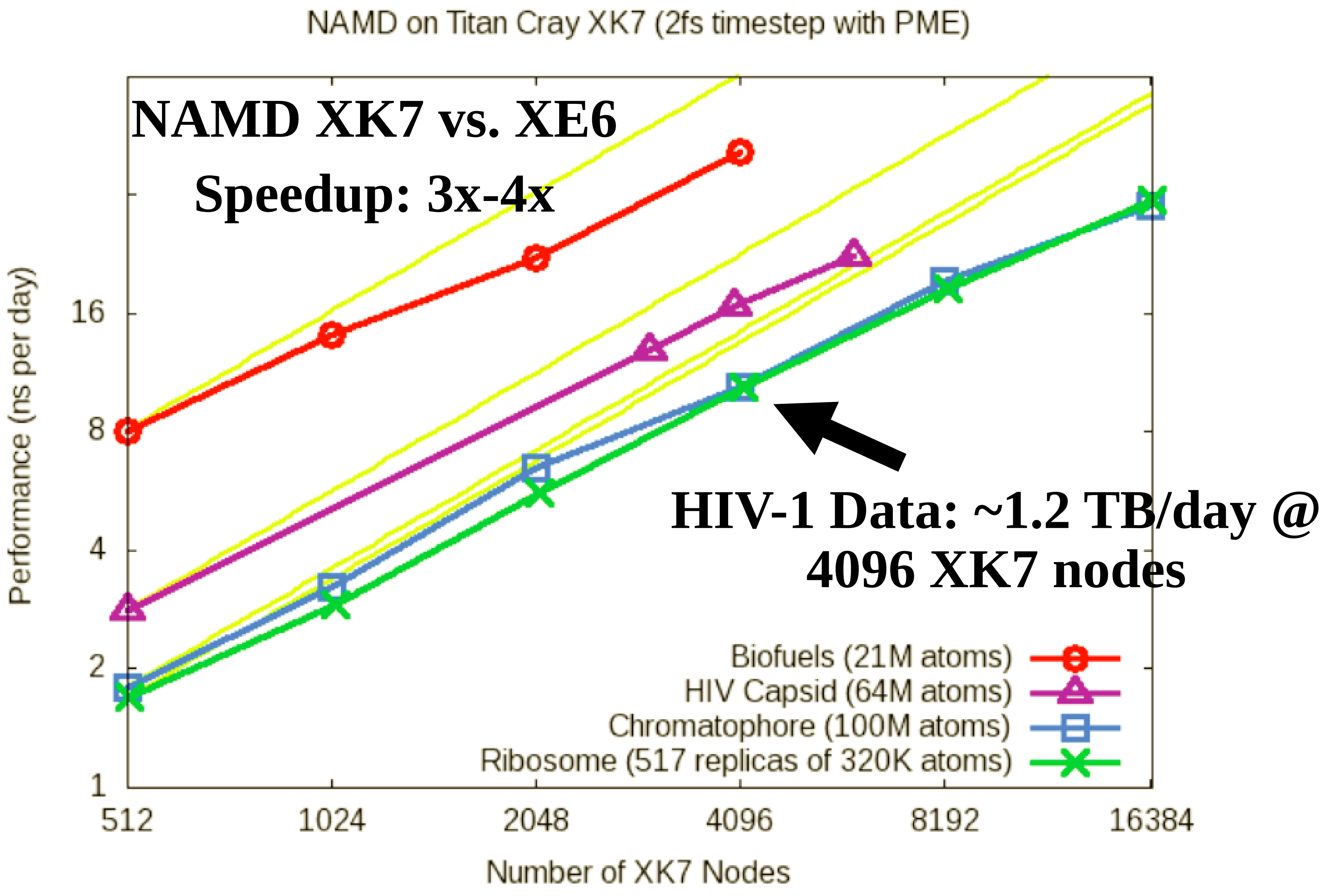



NVIDIA Kepler GPU
~3-6 GB DRAM Memory w/ ECC
GPC
GPC
GPC
GPC
GPC
GPC
GPC
GPC
1536KB Level 2 Cache
Graphics Processor Cluster
SMX
SMX
Streaming Multiprocessor - SMX
64 KB Constant Cache
64 KB L1 Cache / Shared Memory
48 KB Tex + Read-only Data Cache
SP
DP
LDST
SFU
Tex Unit
16 × Execution block = 192 SP, 64 DP, 32 SFU, 32 LDST

# GPU On-Board Global Memory

- GPU arithmetic rates dwarf memory bandwidth
- For Kepler K40 hardware:
  - ~4.3 SP TFLOPS vs. ~288 GB/sec
  - The ratio is roughly **60 FLOPS per memory reference** for single-precision floating point
- GPUs include multiple fast on-chip memories to help **narrow the gap**:
  - **Registers**
  - Constant memory (64KB)
  - **Shared memory (48KB / 16KB)**
  - Read-only data cache / Texture cache (48KB)

# NAMD Titan XK7 Performance August 2013



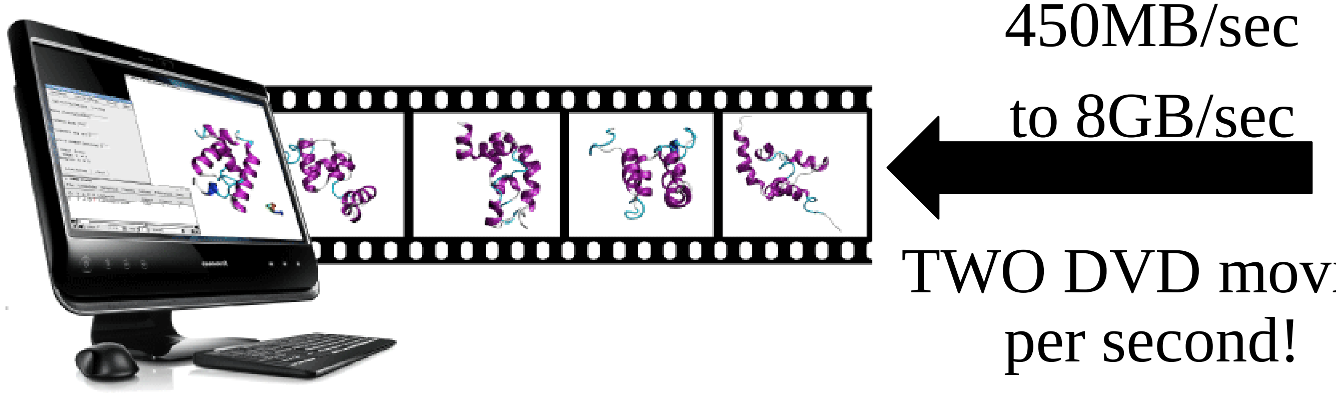
**NAMD XK7 vs. XE6**

**Speedup: 3x-4x**

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

# Interactive Display & Analysis of Terabytes of Data:

## Out-of-Core Trajectory I/O w/ Solid State Disks **and GPUs**



TWO DVD movies per second!

Commodity SSD, SSD RAID

- Timesteps loaded on-the-fly (out-of-core)
  - Eliminates memory capacity limitations, even for multi-terabyte trajectory files
  - High performance achieved by new trajectory file formats, optimized data structures, and efficient I/O
- **GPUs accelerate per-timestep calculations**
- Analyze long trajectories significantly faster using just a personal computer

**Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories.** J. Stone, K. Vandivort, and K. Schulten. *Lecture Notes in Computer Science*, 6939:1-12, 2011.

# VMD Petascale Visualization and Analysis

- Analyze/visualize large trajectories too large to transfer off-site:
  - Compute time-averaged electrostatic fields, MDFF quality-of-fit, etc.
  - User-defined parallel analysis operations, data types
  - Parallel ray tracing, movie making
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 nodes – can read in **231 TB in 15 minutes!**
- Multi-level dynamic load balancing tested with up to 262,144 CPU cores
- **Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis usage**

NCSA Blue Waters Hybrid Cray XE6 / XK7 Supercomputer

22,640 XE6 CPU nodes

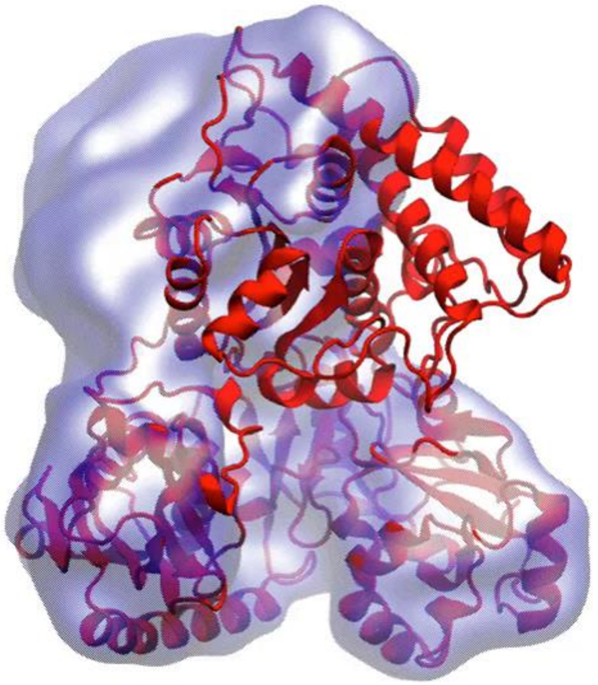
4,224 XK7 nodes w/ GPUs support fast VMD OpenGL movie rendering and visualization

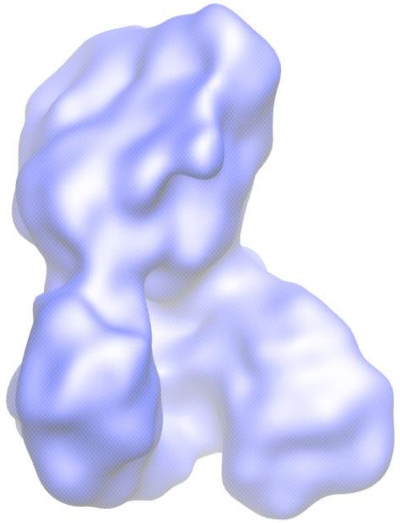
# Molecular Dynamics Flexible Fitting (MDFF)

$$\begin{tikzcd}
\text{X-ray crystallography} \arrow[r] & \text{MDFF} & \text{Electron microscopy} \arrow[l]
\end{tikzcd}$$

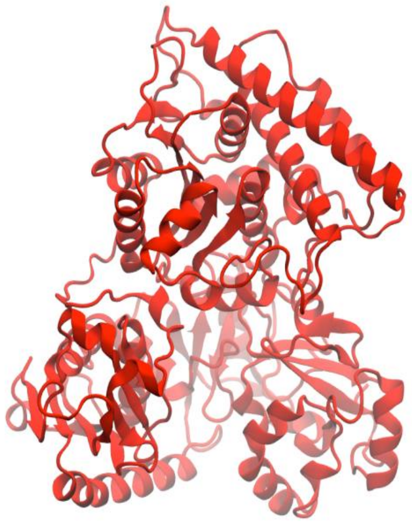
APS at Argonne

FEI microscope





ORNL Titan


Acetyl - CoA Synthase

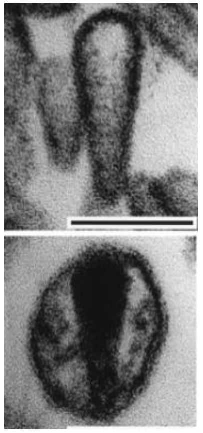
**Flexible fitting of atomic structures into electron microscopy maps using molecular dynamics.**
**L. Trabuco, E. Villa, K. Mitra, J. Frank, and K. Schulten. Structure, 16:673-683, 2008.**

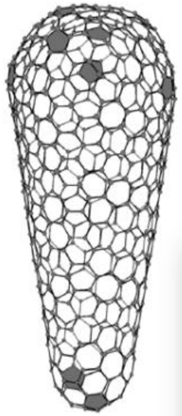
# Structural Route to the all-atom HIV-1 Capsid

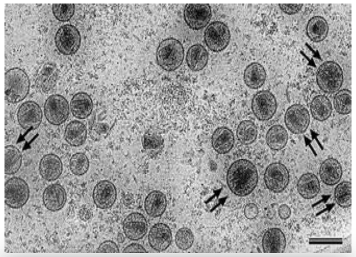
1st TEM (1999)

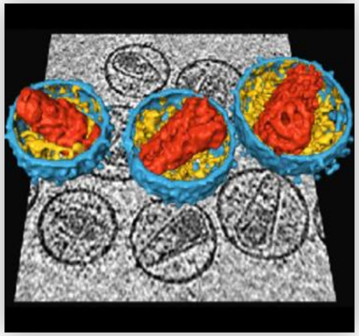
1st tomography (2003)

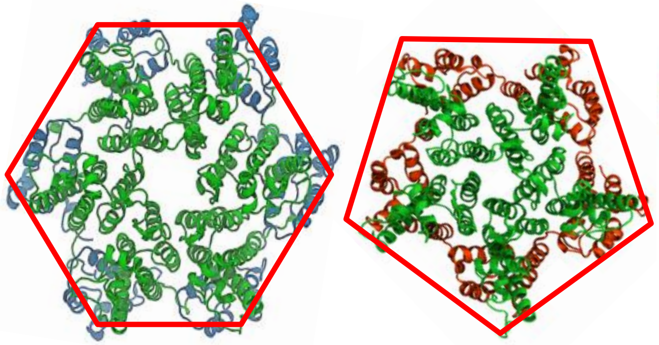
Crystal structures of separated hexamer and pentamer

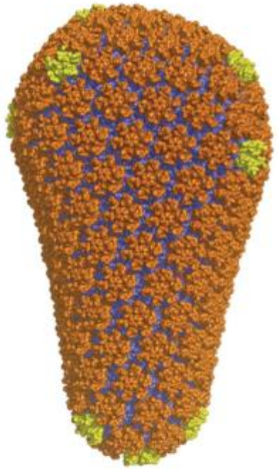












**Ganser et al. *Science*, 1999**

**Briggs et al. *EMBO J*, 2003**

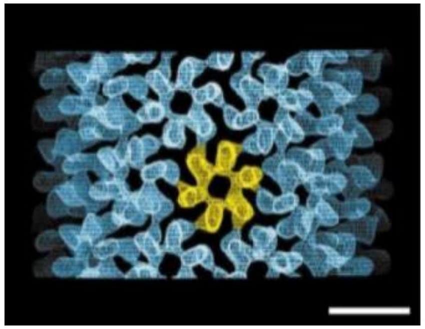
**Briggs et al. *Structure*, 2006**

cryo-ET (2006)

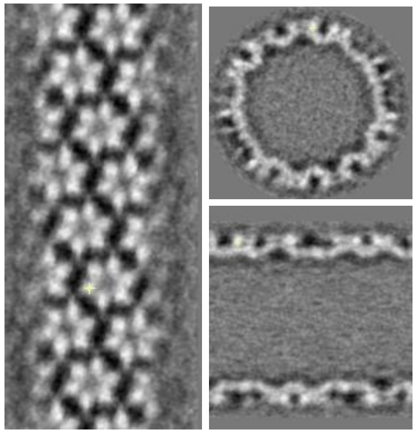
**Pornillos et al. , *Cell* 2009, *Nature* 2011**

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

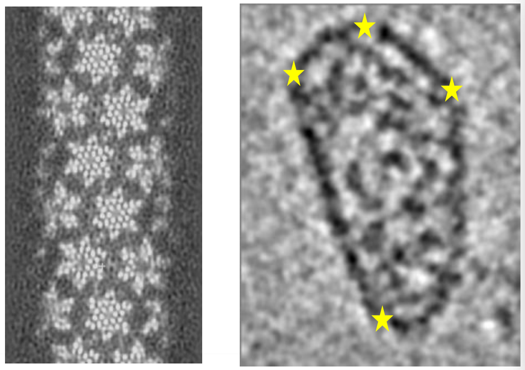
hexameric tubule



**Li et al., *Nature*, 2000**



**Byeon et al., *Cell* 2009**

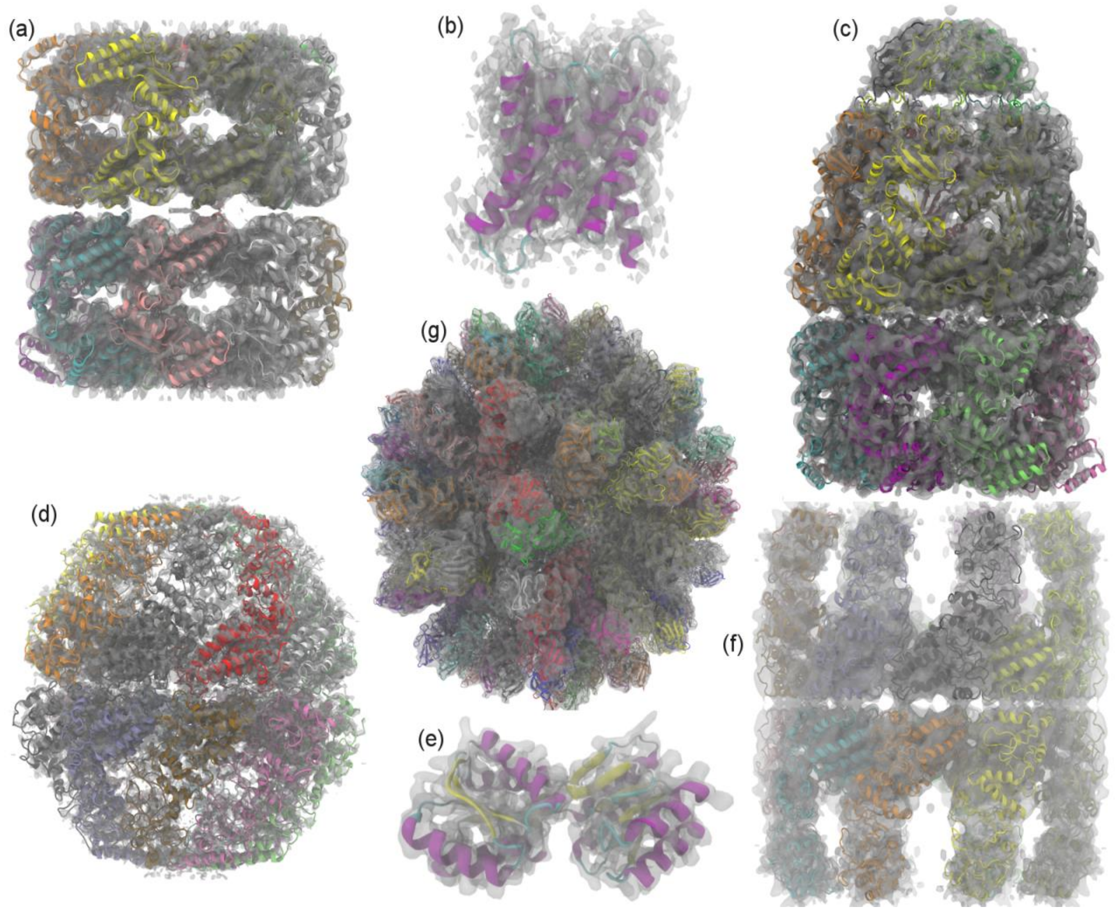


nature
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
THE HIV-1 CAPSID
Atomic structure of the AIDS pathogen's protein coat

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

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

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

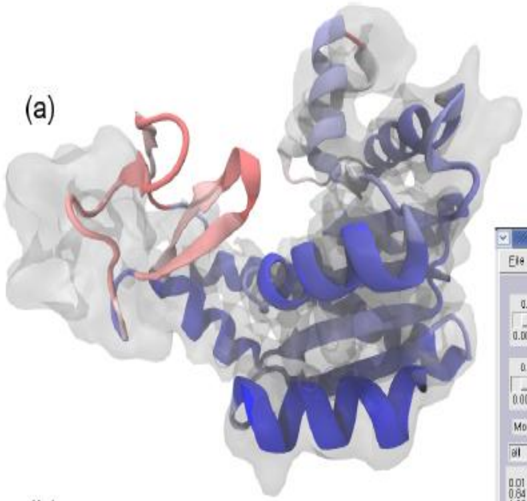


# GPUs Can Reduce Trajectory Analysis Runtimes from Hours to Minutes

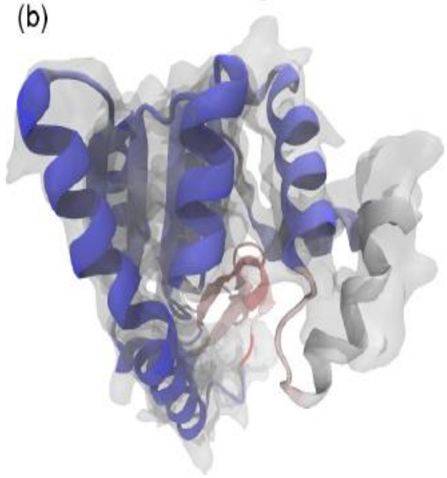
GPUs enable laptops and desktop workstations to handle tasks that would have previously required a cluster, or a very long wait…

GPU-accelerated petascale supercomputers enable analyses were previously impractical, allowing detailed study of very large structures such as viruses

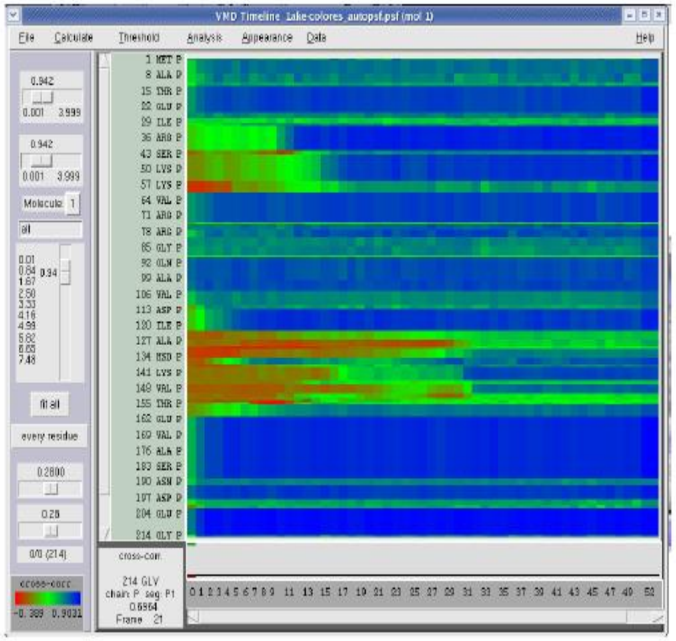
(a)



(b)



(c)



**GPU-accelerated MDFF Cross Correlation Timeline**

**Regions with poor fit** **Regions with good fit**

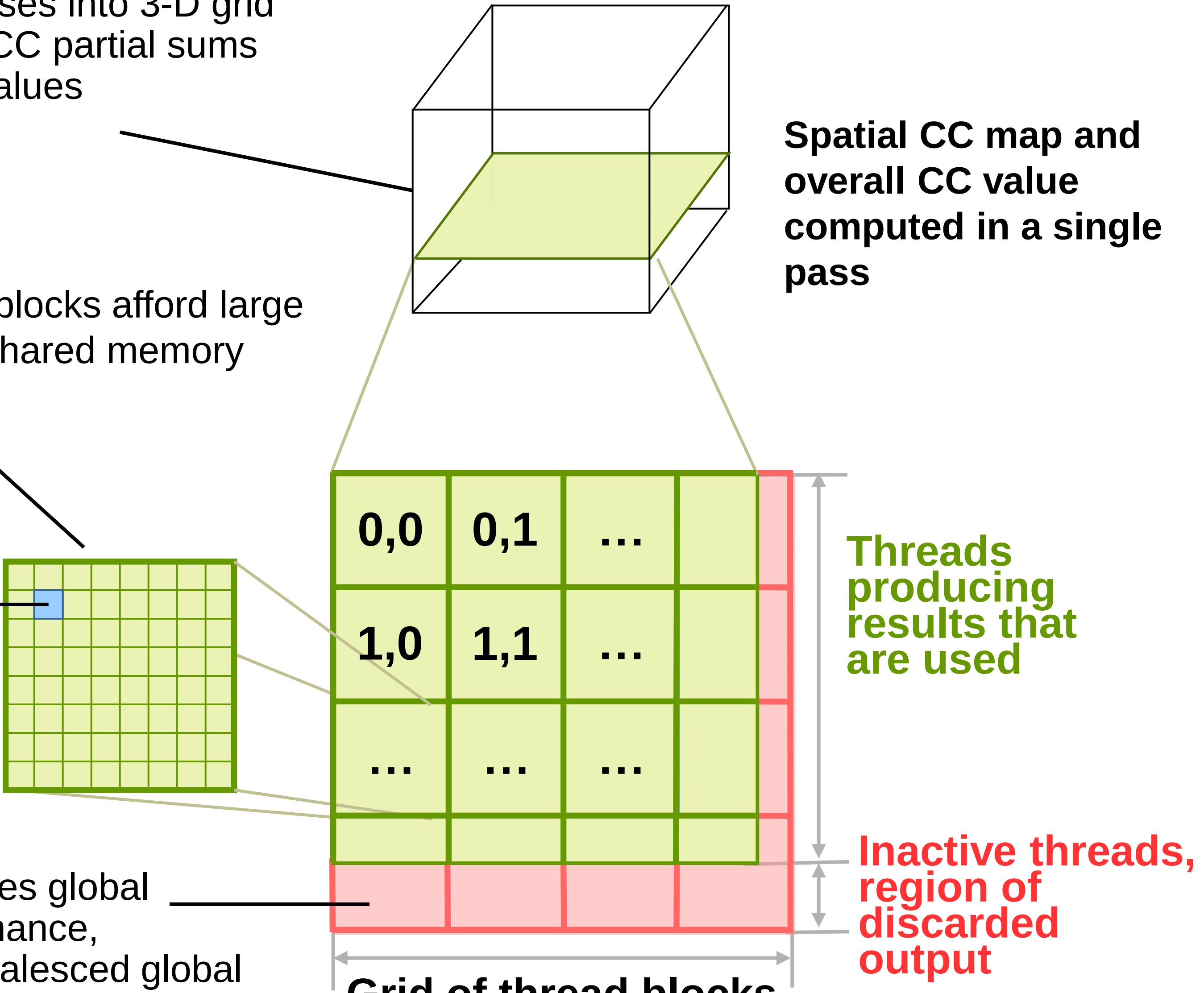
# Single-Pass MDFF GPU Cross-Correlation

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

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

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

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



0,0
0,1
…
1,0
1,1
…
…
…
…
Threads producing results that are used
Inactive threads, region of discarded output
Grid of thread blocks

Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

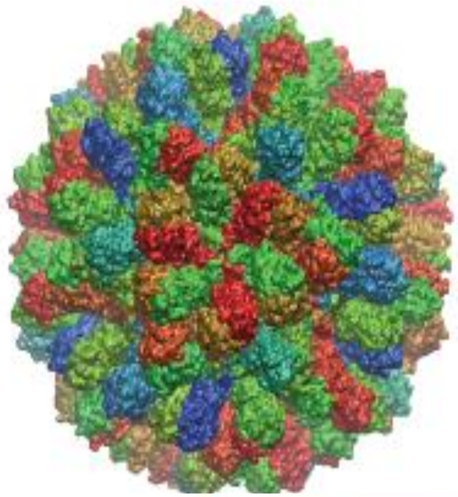
# VMD GPU Cross Correlation Performance

| | **RHDV** | **Mm-cpn open** | **GroEL** | **Aquaporin** |
|---|---|---|---|---|
| **Resolution (Å)** | **6.5** | **8** | **4** | **3** |
| **Atoms** | **702K** | **61K** | **54K** | **1.6K** |
| **VMD-CUDA**<br>**Quadro K6000** | **0.458s**<br>**34.6x** | **0.06s**<br>**25.7x** | **0.034s**<br>**36.8x** | **0.007s**<br>**55.7x** |
| VMD-CPU-SSE<br>32-threads, 2x Xeon E5-2687W | 0.779s<br>20.3x | 0.085s<br>18.1x | 0.159s<br>7.9x | 0.033s<br>11.8x |
| **Chimera**<br>**1-thread Xeon E5-2687W** | **15.86s**<br>**1.0x** | **1.54s**<br>**1.0x** | **1.25s**<br>**1.0x** | **0.39s**<br>**1.0x** |
| **VMD CPU-SEQ (plugin)**<br>1-thread Xeon E5-2687W | 62.89s<br>0.25x | 2.9s<br>0.53x | 1.57s<br>0.79x | 0.04s<br>9.7x |

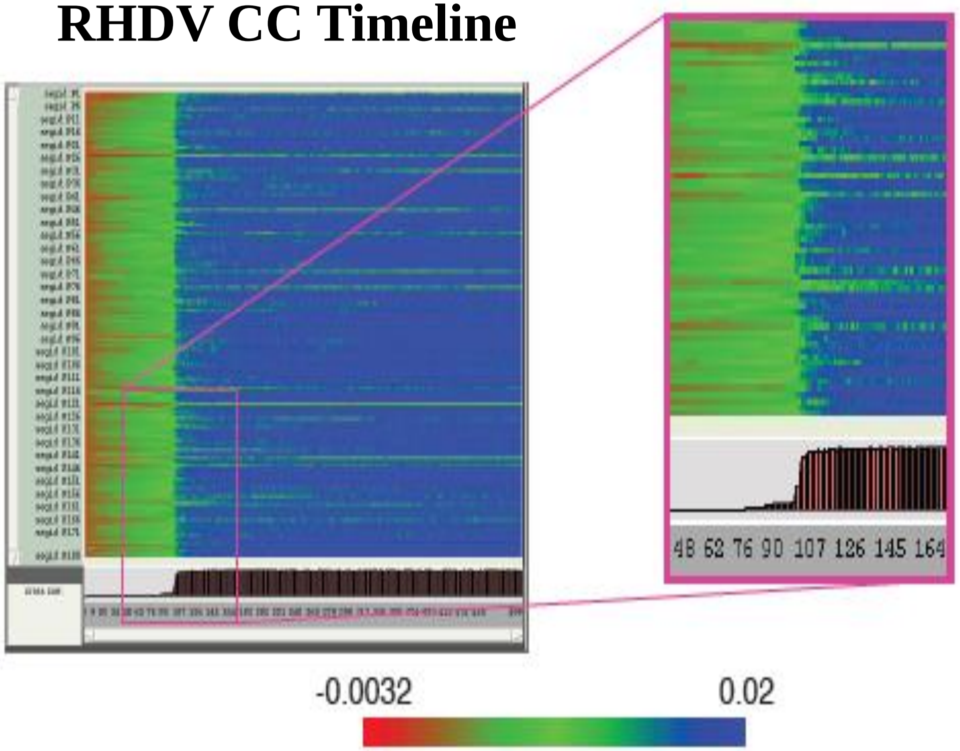
# VMD RHDV Cross Correlation Timeline on Cray XK7

| | **RHDV** |
|---|---|
| **Atoms** | **702K** |
| **Traj. Frames** | **10,000** |
| **Component Selections** | **720** |
| **Single-node XK7 (projected)** | **336 hours (14 days)** |
| **128-node XK7** | **3.2 hours<br>105x speedup** |
| **2048-node XK7** | **19.5 minutes<br>1035x speedup** |

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

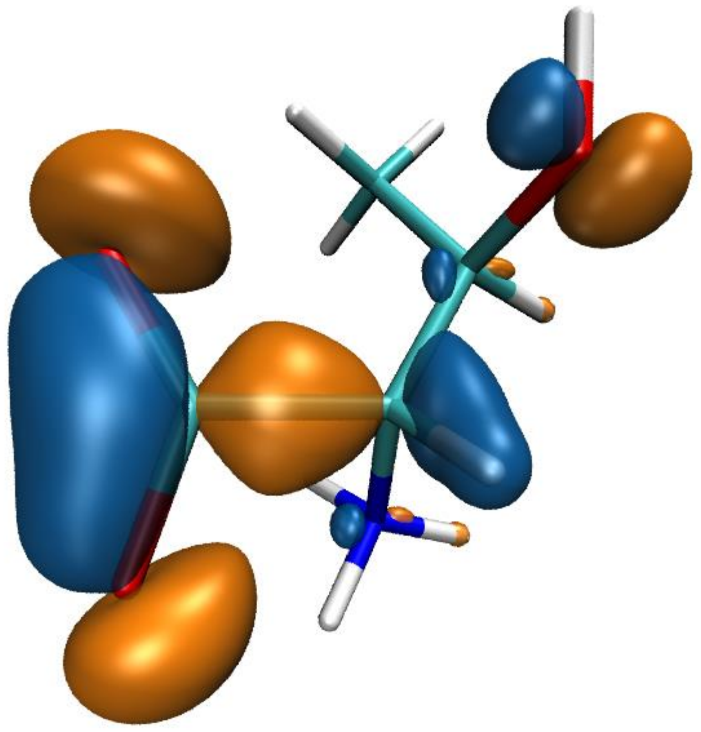


**RHDV CC Timeline**



# Animating Molecular Orbitals

- Animation of (classical mechanics) molecular dynamics trajectories provides insight into simulation results
- To do the same for QM or QM/MM simulations one must compute MOs at ~**10 FPS** or more
- **>100x** speedup (GPU) over existing tools now makes this possible!



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.

# MO Kernel for One Grid Point  (Naive C)

```
…
for (at=0; at<numatoms; at++) {
  int prim_counter = atom_basis[at];
  calc_distances_to_atom(&atompos[at], &xdist, &ydist, &zdist, &dist2, &xdiv);
  for (contracted_gto=0.0f, shell=0; shell < num_shells_per_atom[at]; shell++) {
    int shell_type = shell_symmetry[shell_counter];
    for (prim=0; prim < num_prim_per_shell[shell_counter];  prim++) {
      float exponent       = basis_array[prim_counter      ];
      float contract_coeff = basis_array[prim_counter + 1];
      contracted_gto += contract_coeff * expf(-exponent*dist2);
      prim_counter += 2;
    }
    for (tmpshell=0.0f, j=0, zdp=1.0f; j<=shell_type; j++, zdp*=zdist) {
      int imax = shell_type - j;
      for (i=0, ydp=1.0f, xdp=pow(xdist, imax); i<=imax; i++, ydp*=ydist, xdp*=xdiv)
        tmpshell += wave_f[ifunc++] * xdp * ydp * zdp;
    }
    value += tmpshell * contracted_gto;
    shell_counter++;
  }
} …..
```

Loop over atoms

Loop over shells

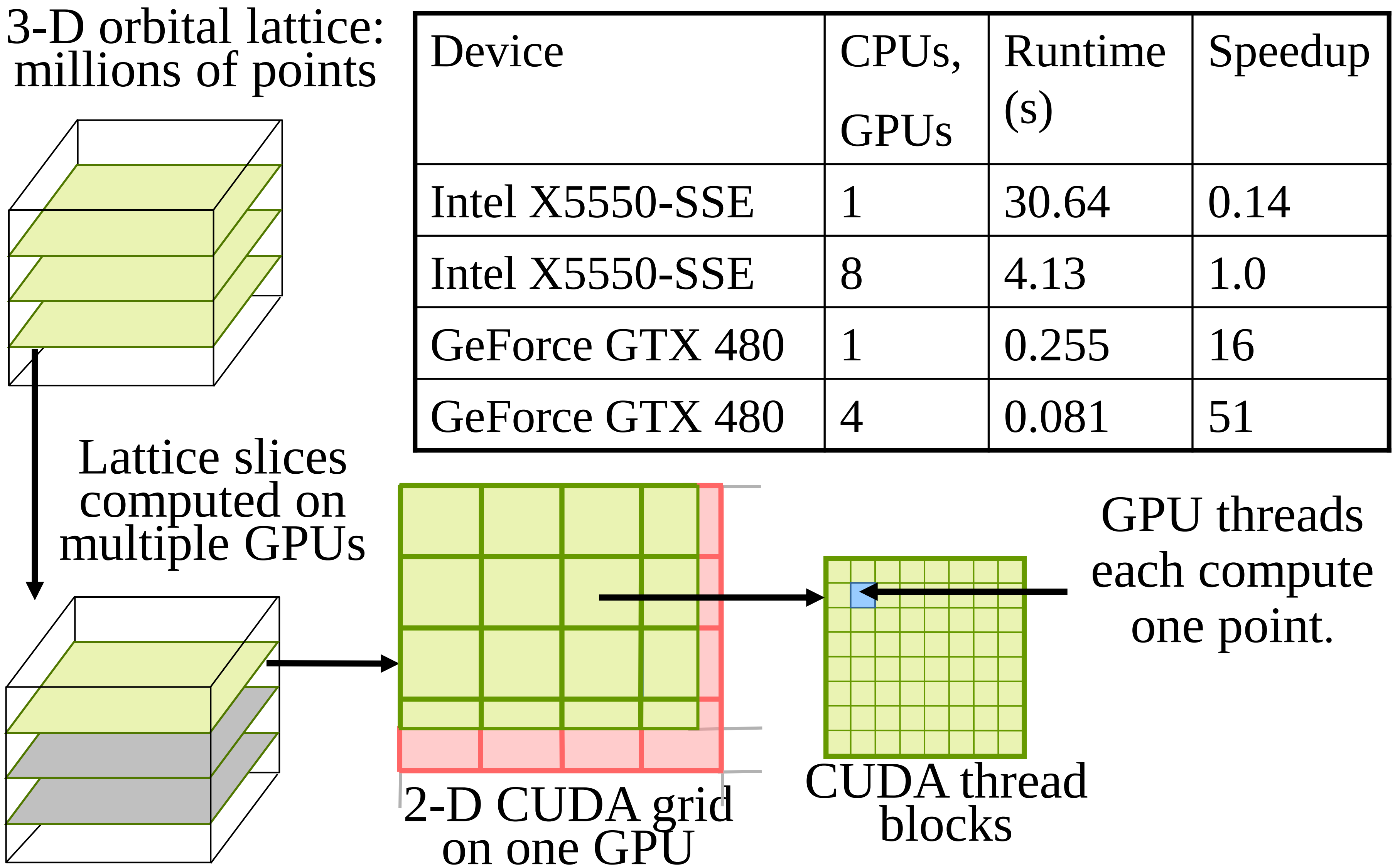
Loop over primitives: largest component of runtime, due to expf()

Loop over angular momenta

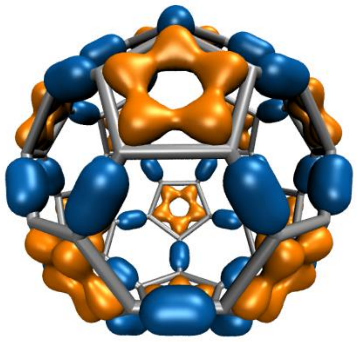
(unrolled in real code)

# GPU Solution: Computing $C_{60}$ Molecular Orbitals

| Device | CPUs, GPUs | Runtime (s) | Speedup |
|---|---|---|---|
| Intel X5550-SSE | 1 | 30.64 | 0.14 |
| Intel X5550-SSE | 8 | 4.13 | 1.0 |
| GeForce GTX 480 | 1 | 0.255 | 16 |
| GeForce GTX 480 | 4 | 0.081 | 51 |


3-D orbital lattice: millions of points
Lattice slices computed on multiple GPUs
2-D CUDA grid on one GPU
CUDA thread blocks
GPU threads each compute one point.

## Molecular Orbital Inner Loop, Hand-Coded x86 SSE
## Hard to Read, Isn't It? (And this is the "pretty" version!)

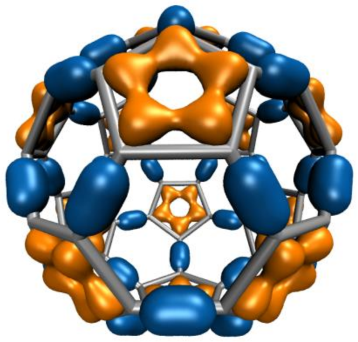


```
for (shell=0; shell < maxshell; shell++) {
    __m128 Cgto = _mm_setzero_ps();
    for (prim=0; prim<num_prim_per_shell[shell_counter]; prim++) {
        float exponent        = -basis_array[prim_counter     ];
        float contract_coeff =  basis_array[prim_counter + 1];
        __m128 expval = _mm_mul_ps(_mm_load_ps1(&exponent), dist2);
        __m128 ctmp = _mm_mul_ps(_mm_load_ps1(&contract_coeff), exp_ps(expval));
        Cgto = _mm_add_ps(contracted_gto, ctmp);
        prim_counter += 2;
    }
    __m128 tshell = _mm_setzero_ps();
    switch (shell_types[shell_counter]) {
        case S_SHELL:
            value = _mm_add_ps(value, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), Cgto));    break;
        case P_SHELL:
            tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), xdist));
            tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), ydist));
            tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), zdist));
            value = _mm_add_ps(value, _mm_mul_ps(tshell, Cgto));      break;
```

Writing SSE kernels for CPUs requires assembly language, compiler intrinsics, various libraries, or a really smart autovectorizing compiler **and lots of luck...**

# Molecular Orbital Inner Loop in CUDA

```
for (shell=0; shell < maxshell; shell++) {
    float contracted_gto = 0.0f;
    for (prim=0; prim<num_prim_per_shell[shell_counter]; prim++) {
      float exponent       = const_basis_array[prim_counter    ];
      float contract_coeff = const_basis_array[prim_counter + 1];
      contracted_gto += contract_coeff * exp2f(-exponent*dist2);
      prim_counter += 2;
    }
    float tmpshell=0;
    switch (const_shell_symmetry[shell_counter]) {
      case S_SHELL:
        value += const_wave_f[ifunc++] * contracted_gto;   break;
      case P_SHELL:
        tmpshell += const_wave_f[ifunc++] * xdist;
        tmpshell += const_wave_f[ifunc++] * ydist
        tmpshell += const_wave_f[ifunc++] * zdist;
        value += tmpshell * contracted_gto;   break;
```

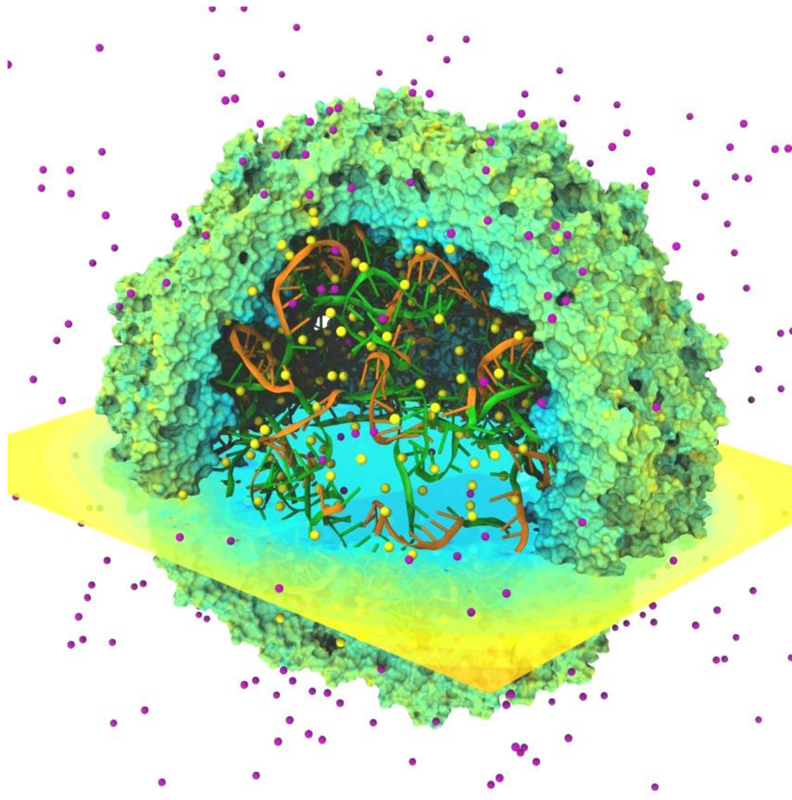


Aaaaahhhh….

Data-parallel CUDA kernel looks like normal C code for the most part….

# Time-Averaged Electrostatics Analysis on Energy-Efficient GPU Cluster

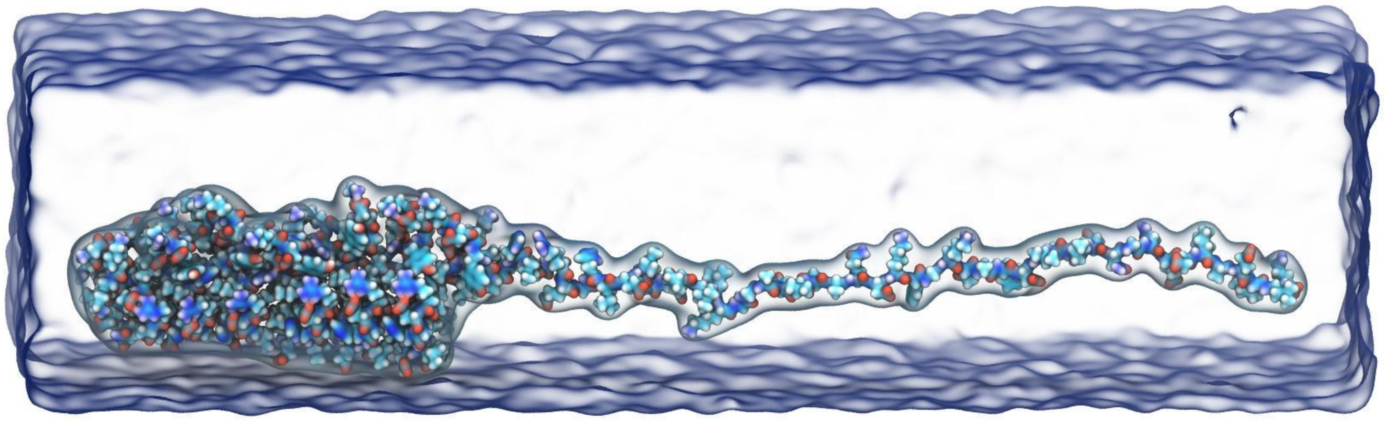
- **1.5 hour** job (CPUs) reduced to **3 min** (CPUs+GPU)
- Electrostatics of thousands of trajectory frames averaged
- Per-node power consumption on NCSA "AC" GPU cluster:
  - CPUs-only: 448 Watt-hours
  - CPUs+GPUs: 43 Watt-hours
- GPU Speedup: **25.5x**
- Power efficiency gain: **10.5x**



**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. *The Work in Progress in Green Computing*, pp. 317-324, 2010.

# VMD "QuickSurf" Representation

- Displays continuum of structural detail:
  - All-atom models
  - Coarse-grained models
  - Cellular scale models
  - Multi-scale models: All-atom + CG,  Brownian + Whole Cell
  - Smoothly variable between full detail, and reduced resolution representations of very large complexes

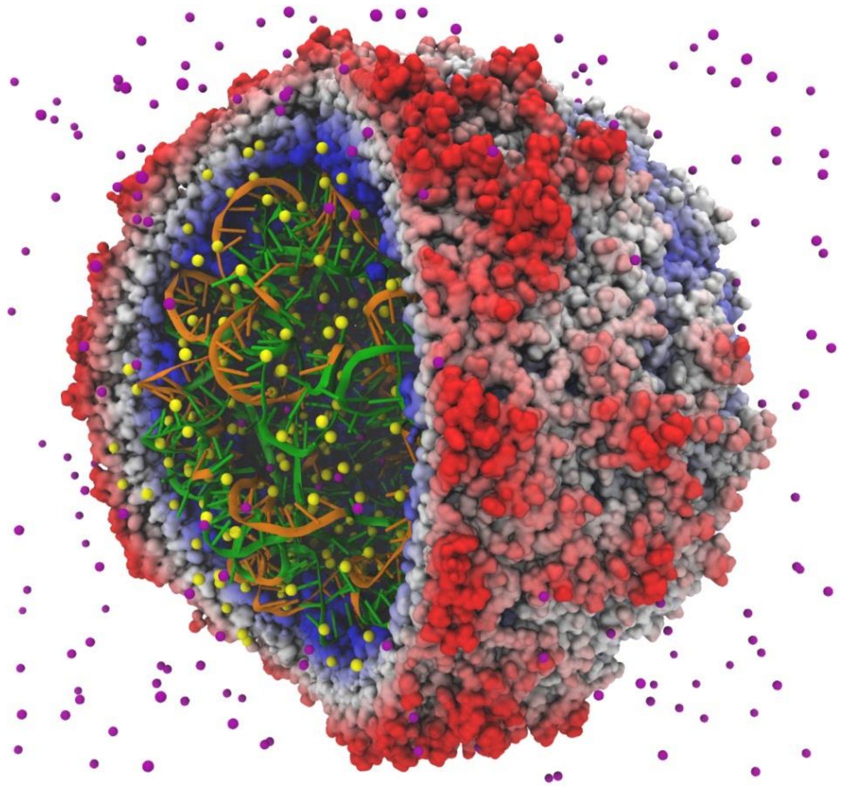


**Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.**

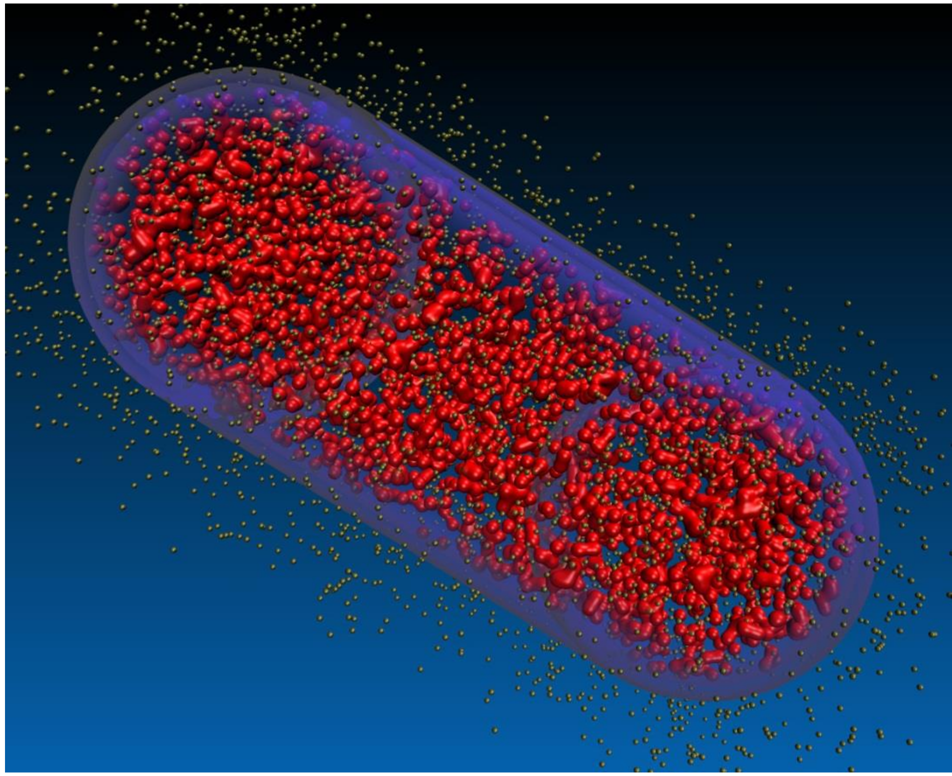
M. Krone, J. E. Stone, T. Ertl, K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012

# VMD "QuickSurf" Representation

- Uses multi-core CPUs and GPU acceleration to enable **smooth real-time animation** of MD trajectories
- Linear-time algorithm, scales to millions of particles, as limited by memory capacity



**Satellite Tobacco Mosaic Virus**



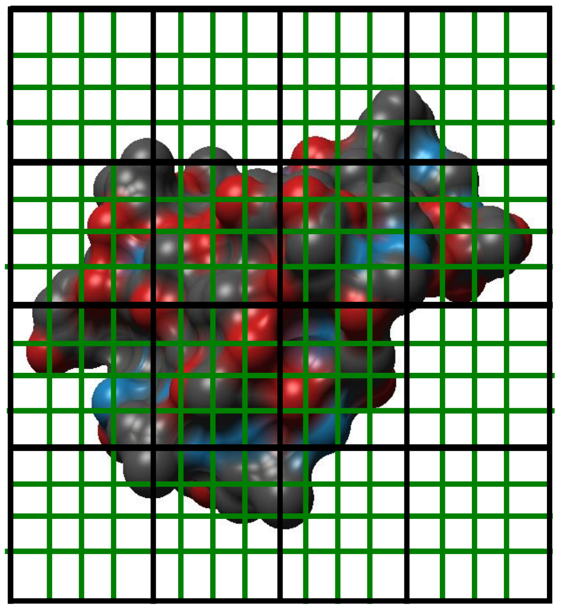
**Lattice Cell Simulations**

# QuickSurf Algorithm Overview

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

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

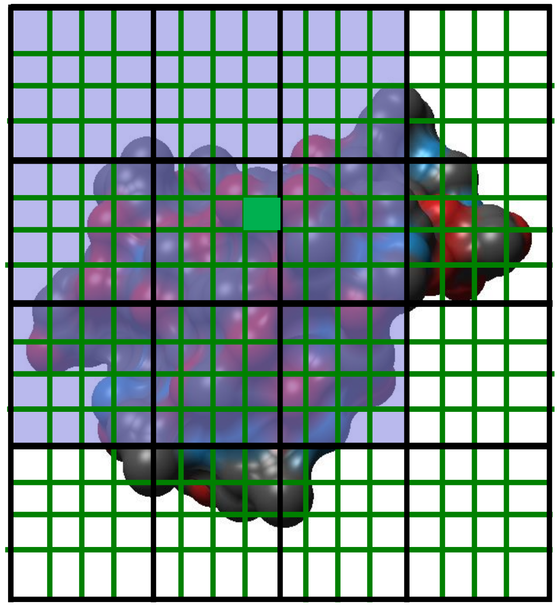
- Extract isosurface for a user-defined density value



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

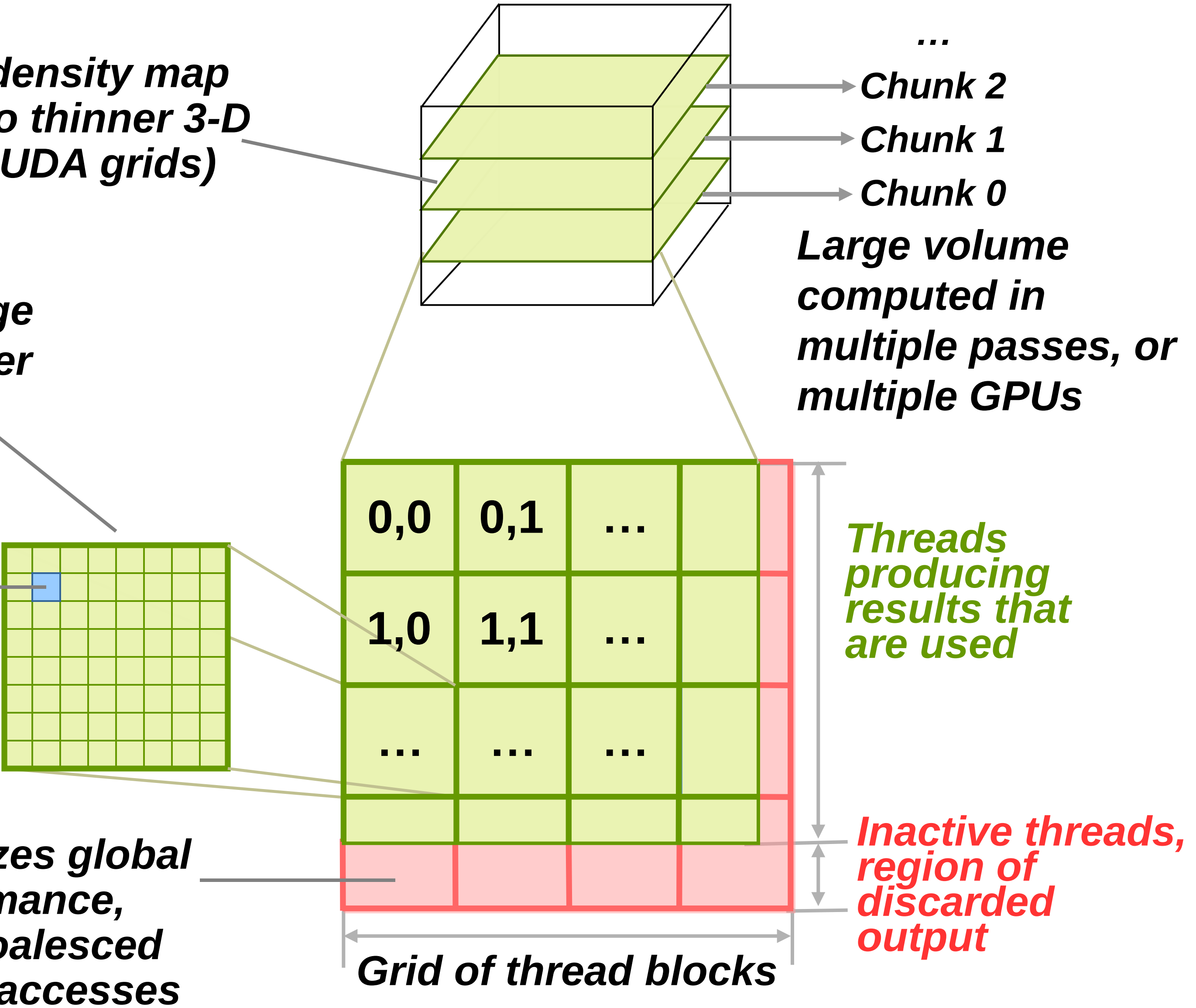
# QuickSurf Density Map Algorithm

- Spatial acceleration grid cells are sized to match the cutoff radius for the exponential, beyond which density contributions are negligible
- Density map lattice points computed by summing density contributions from particles in 3x3x3 grid of neighboring spatial acceleration cells
- Volumetric texture map is computed by summing particle colors normalized by their individual density contribution



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

# QuickSurf Density Parallel Decomposition



...
Chunk 2
Chunk 1
Chunk 0
0,0
0,1
...
1,0
1,1
...
...
...
...
Threads producing results that are used
Inactive threads, region of discarded output
Grid of thread blocks

*QuickSurf 3-D density map decomposes into thinner 3-D slabs/slices (CUDA grids)*

*Large volume computed in multiple passes, or multiple GPUs*

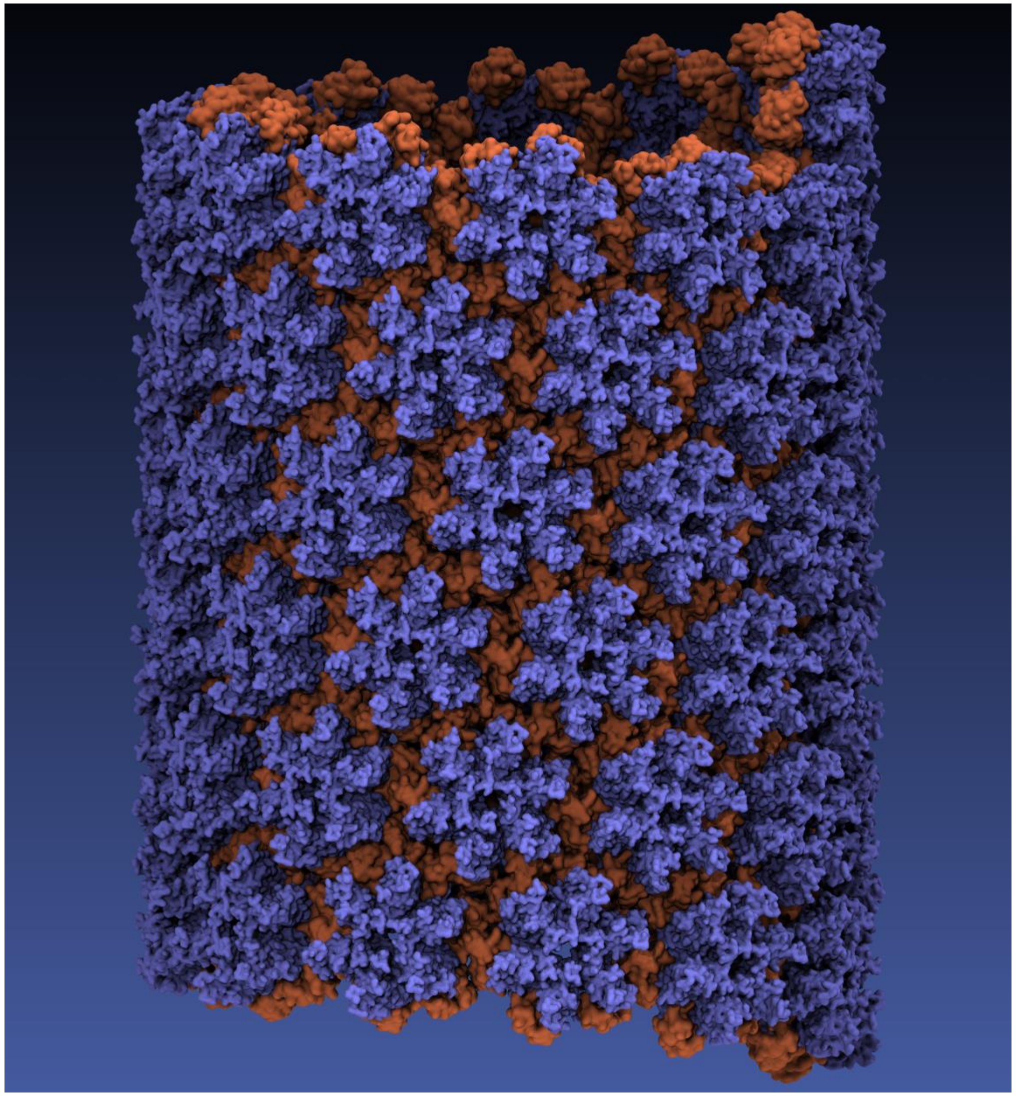
*Small 8x8 thread blocks afford large per-thread register count, shared memory*

*Each thread computes one or more density map lattice points*

*Padding optimizes global memory performance, guaranteeing coalesced global memory accesses*

## Challenge: Support GPU-accelerated QuickSurf for **Large** Biomolecular Complexes

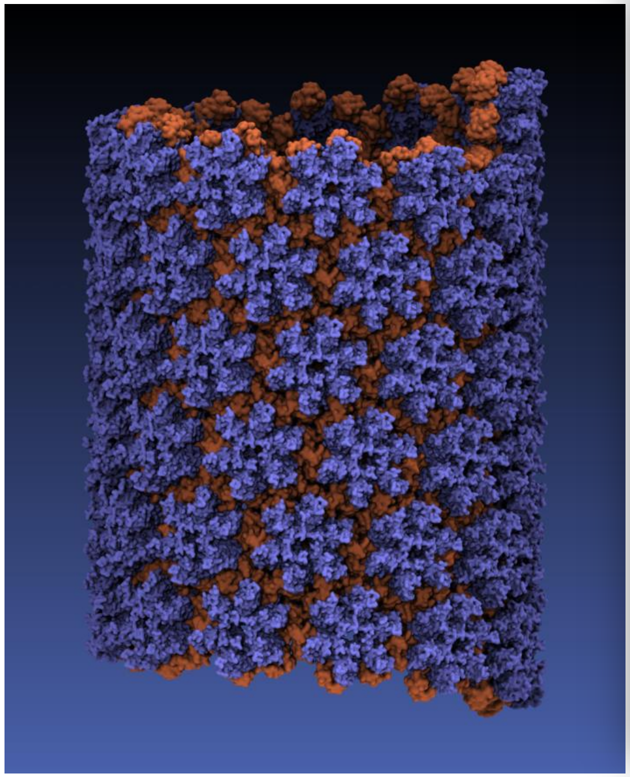
- Structures such as HIV initially needed all XK7 GPU memory to generate detailed surface renderings
- Goals and approach:
  - **Avoid slow CPU-fallback!**
  - Incrementally change algorithm phases to use more compact data types, while maintaining performance
  - Specialize code for different precision/performance/memory capacity cases



## Net Result of QuickSurf Memory Efficiency Optimizations

- **Halved** overall GPU memory use
- Achieved **1.5x to 2x performance gain**:
  - The "gather" density map algorithm keeps type conversion operations out of the innermost loop
  - Density map global memory writes reduced to half
  - Multiple stages of Marching Cubes operate on smaller input and output data types
  - Same code path supports multiple precisions
- Users now get full GPU-accelerated QuickSurf in many cases that previously triggered CPU-fallback, all platforms (laptop/desk/super) benefit!

# VMD "QuickSurf" Representation, Ray Tracing



nature
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Atomic structure of the AIDS pathogen's protein coat
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ANTICANCER DRUGS
A SITTING TARGET
An indirect hit on 'undruggable' KRAS protein
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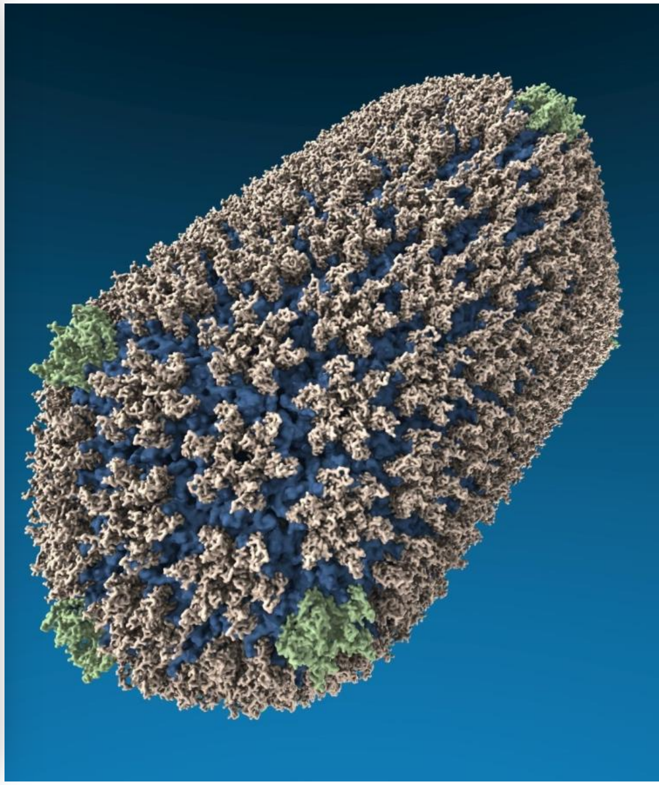
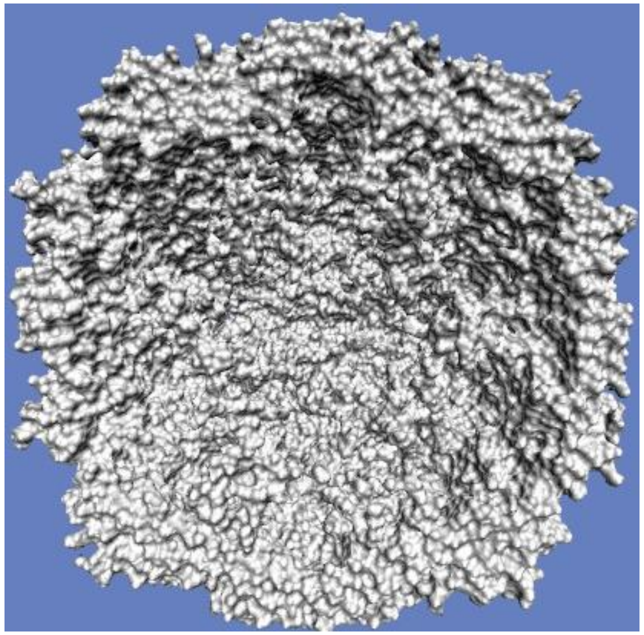
30 May 2013

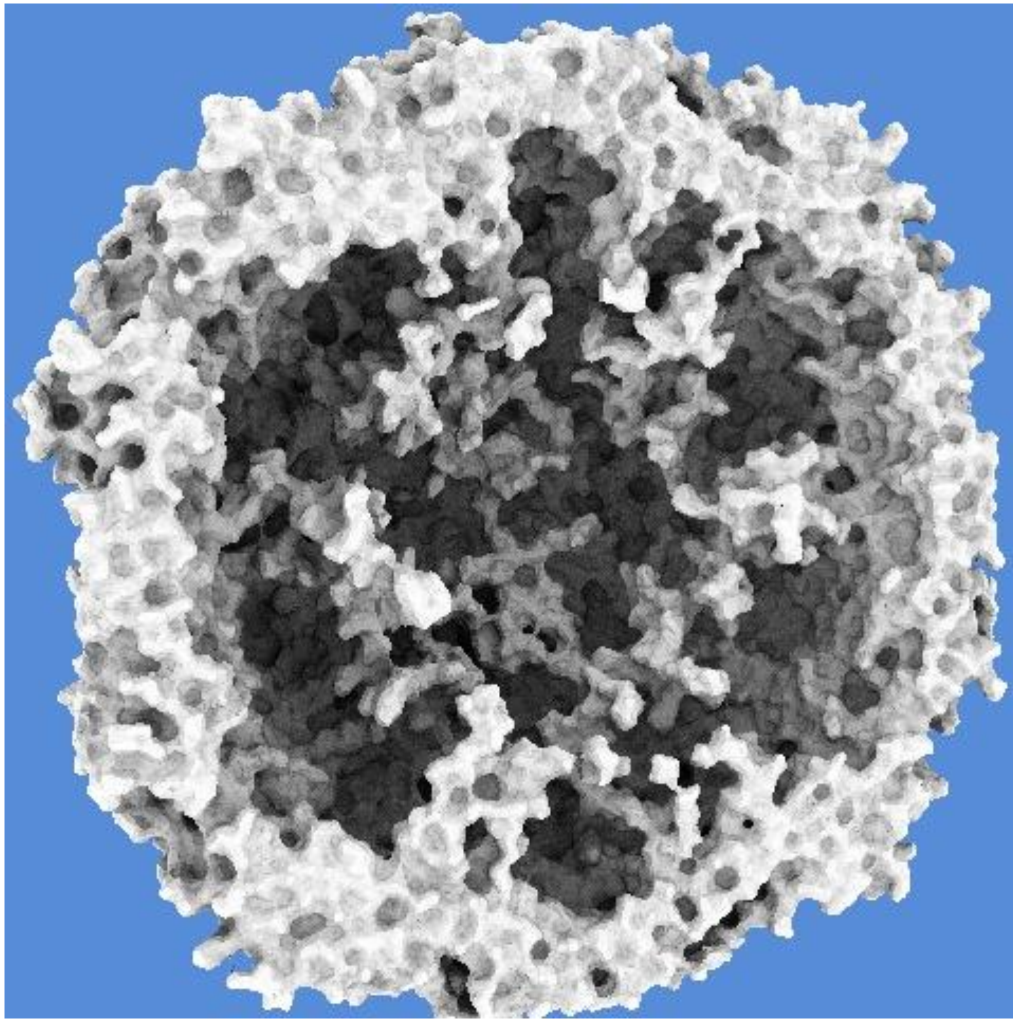


**All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters**

## Ray Tracing Molecular Graphics

- Ambient occlusion lighting, shadows, reflections, transparency, and more…
- Satellite tobacco mosaic virus capsid w/ ~75K atoms


Standard OpenGL rasterization

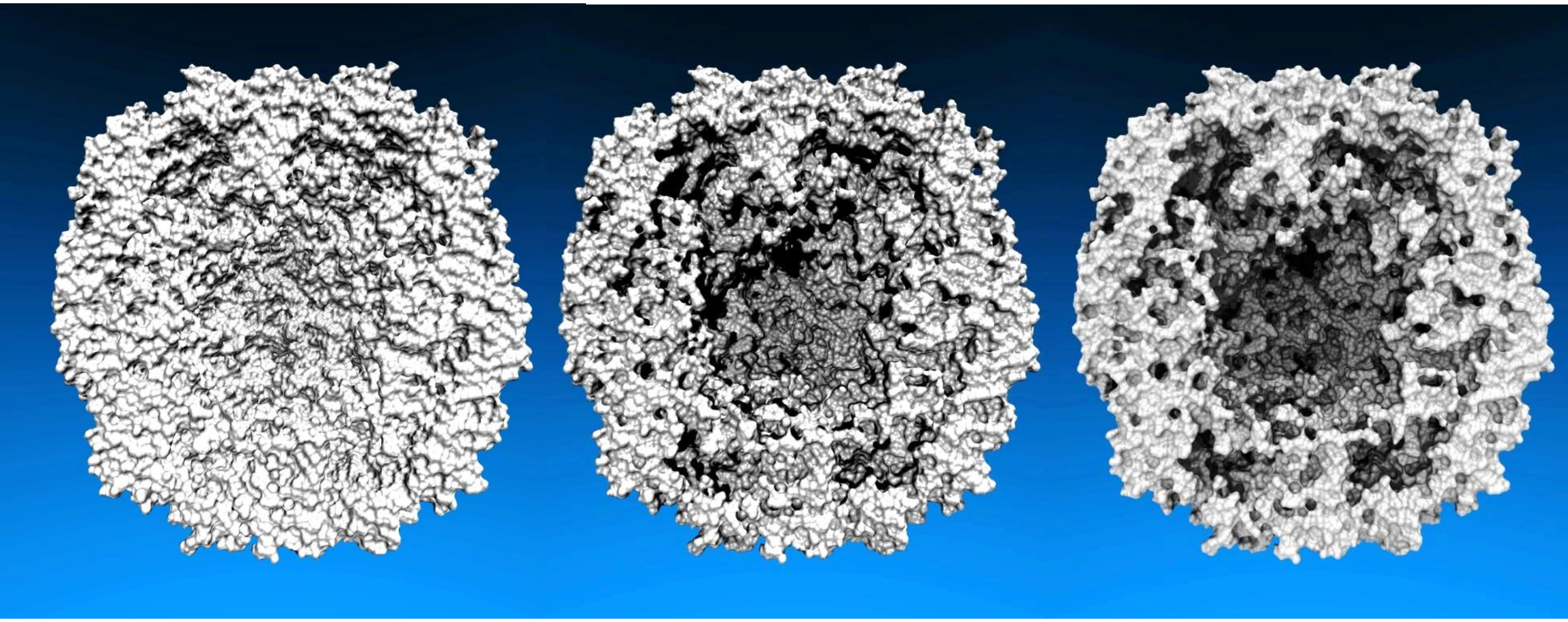

VMD w/ new GPU ray tracing engine based on CUDA + OptiX

# Lighting Comparison

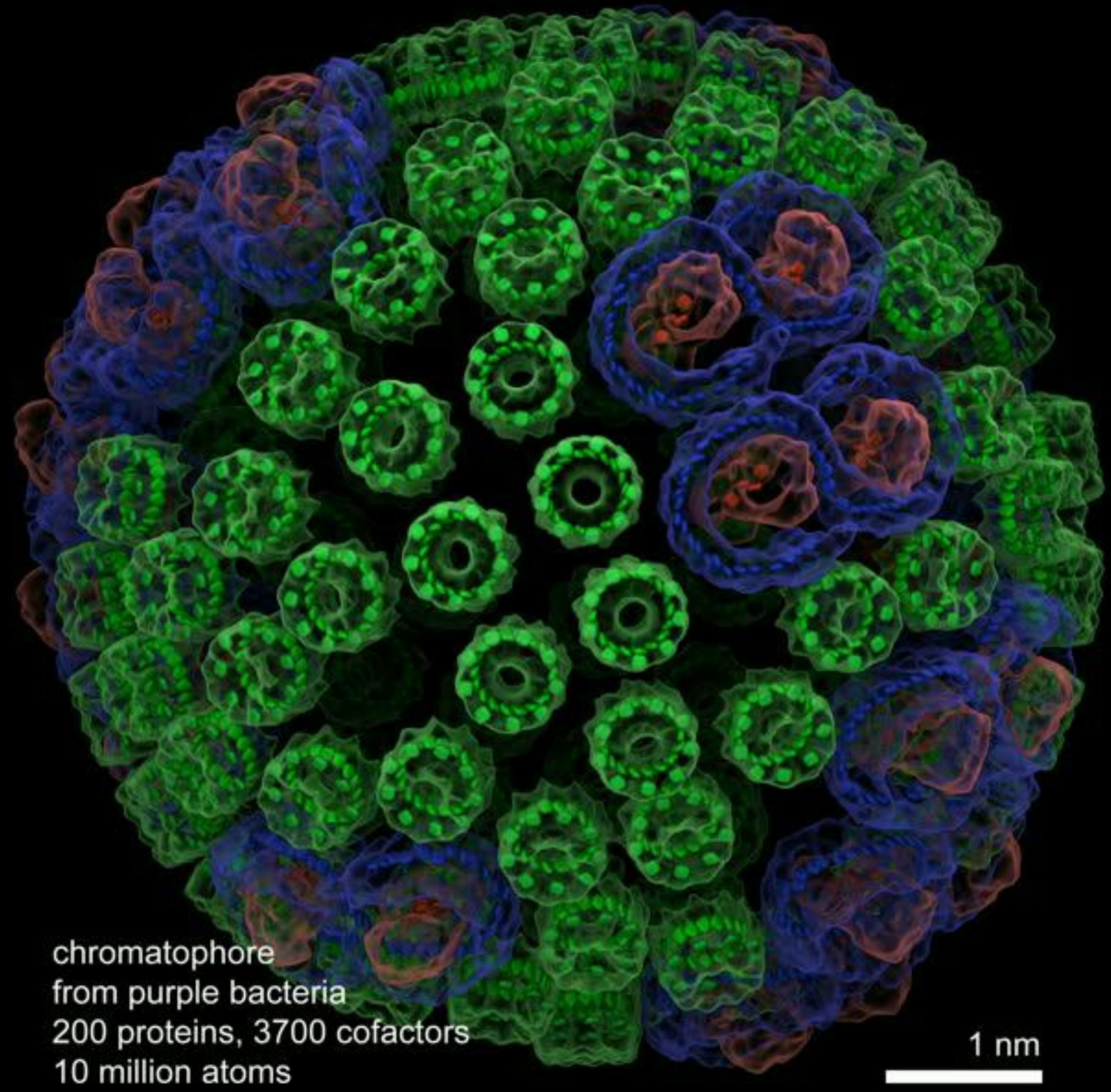
**Two lights, no shadows**

**Two lights, hard shadows, 1 shadow ray per light**

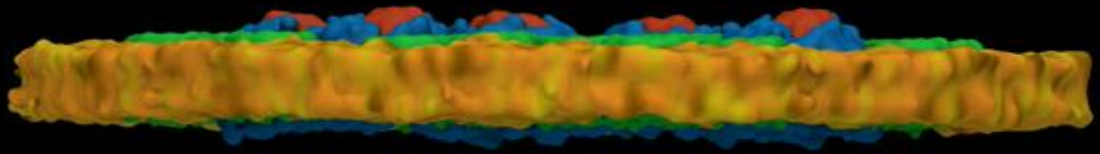
**Ambient occlusion + two lights, 144 AO rays/hit**



## BW VMD/Tachyon Movie Generation



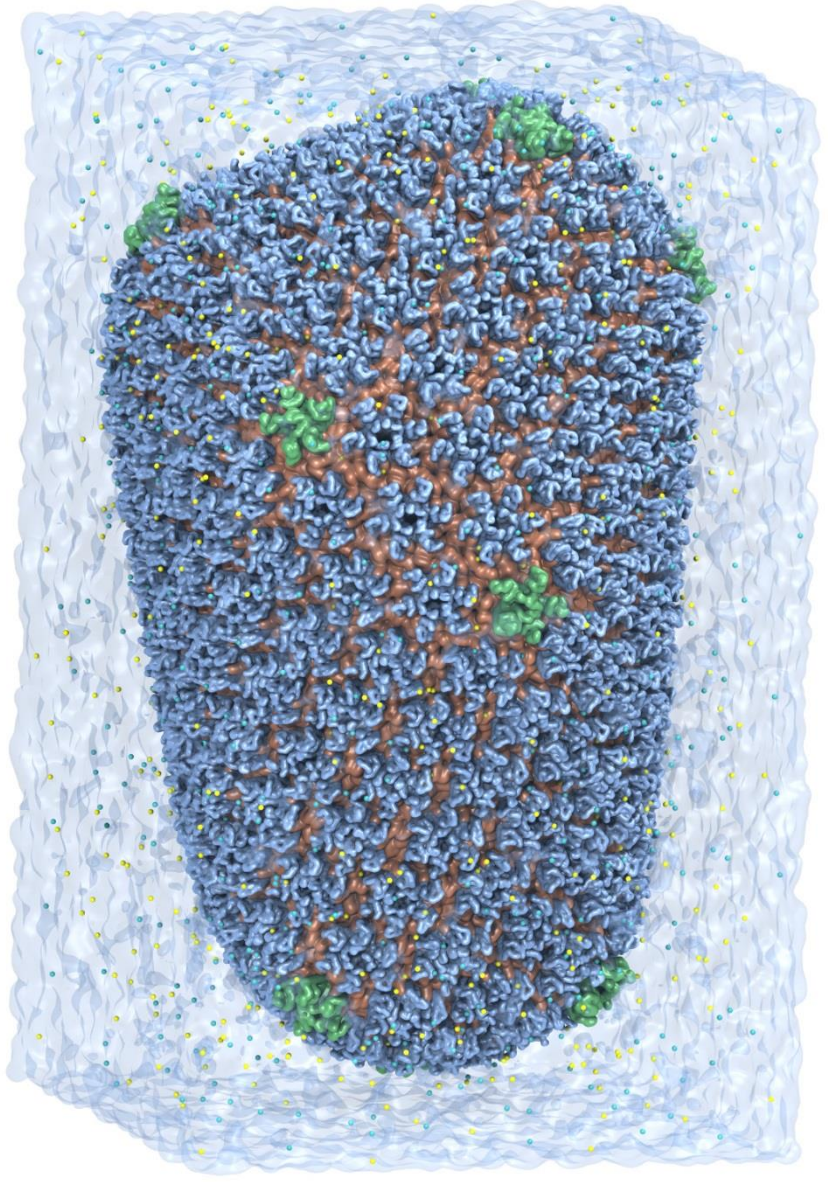
## BW VMD/Tachyon Movie Generation



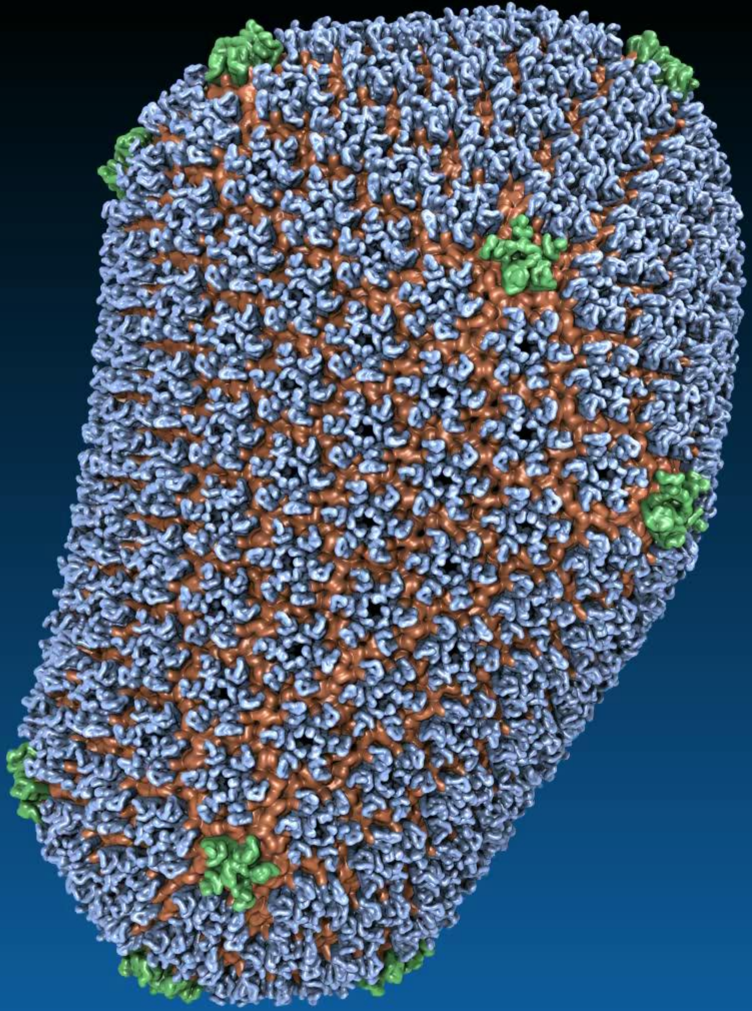
20 M atom chromatophore patch

# GPU Ray Tracing of HIV-1 on Blue Waters

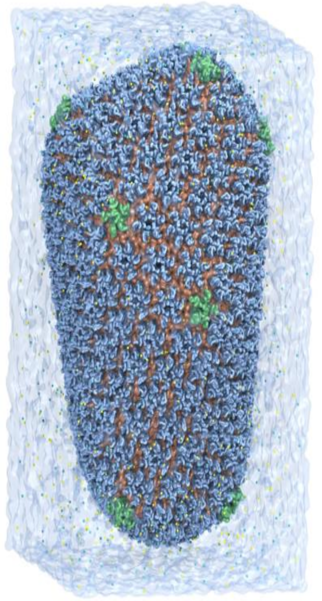
- **Ambient occlusion lighting**, shadows, transparency, antialiasing, depth cueing, **144 rays/pixel minimum**
- 64 million atom virus simulation
- 1000+ movie frames
- Surface generation and ray tracing stages each use >= 75% of GPU memory



# VMD GPU Ray Tracing of HIV-1 Capsid



# 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

Cray XE6: 2x Opteron 62xx CPUs (32-cores)

Cray XK7: 1x Opteron 62xx CPU (16-cores) + NVIDIA Tesla K20X

| **Node Type and Count** | **Script Load Time** | **State Load Time** | **Geometry + Ray Tracing** | **Total Time** |
|---|---|---|---|---|
| **256 XE6 CPU nodes** | 7 s | 160 s | **1,374 s** | **1,541 s** |
| 512 XE6 CPU nodes | 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.

## Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
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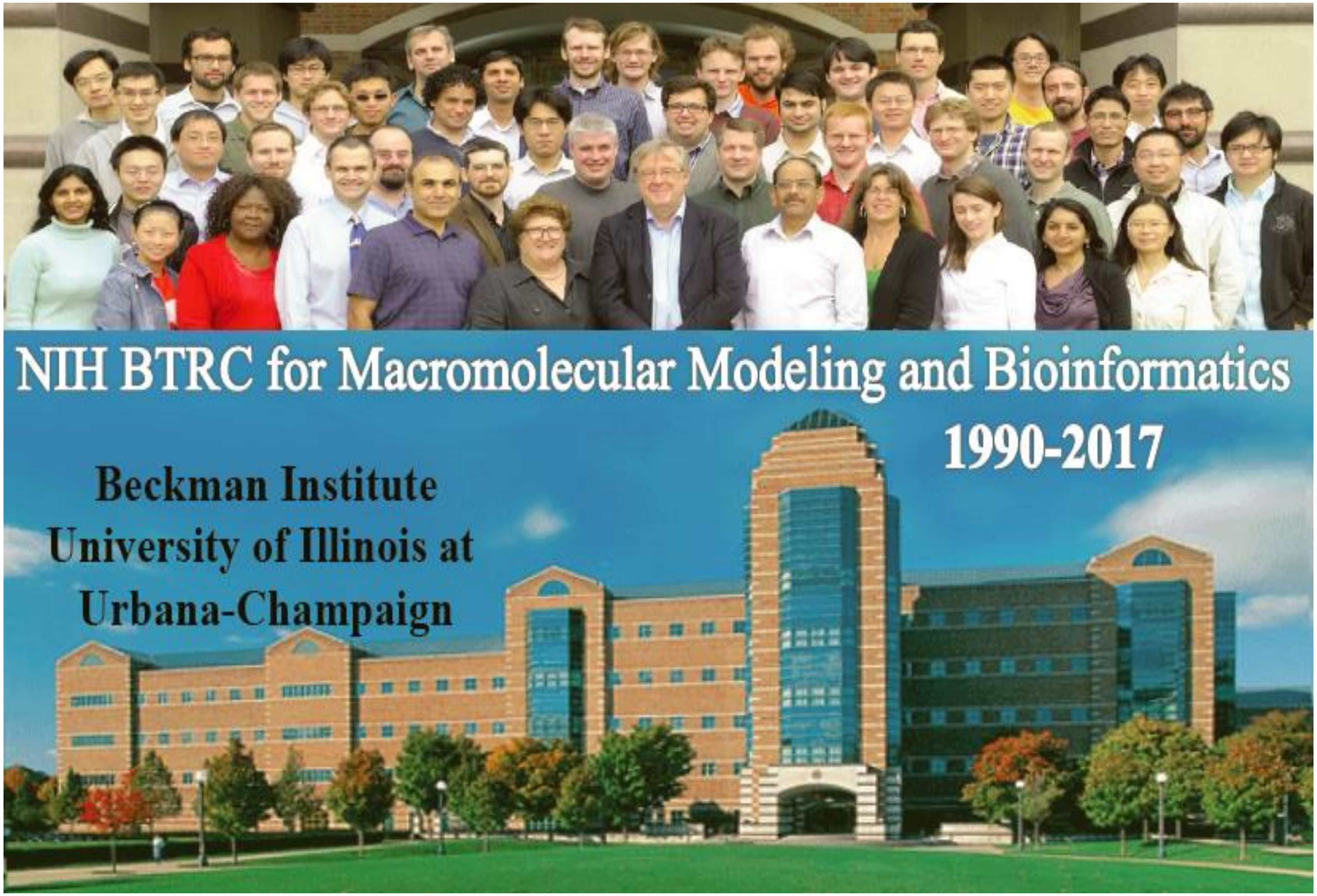
  - NSF OCI 07-25070
  - NSF PRAC "The Computational Microscope"
  - NIH support: 9P41GM104601, 5R01GM098243-02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# GPU Computing Publications

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

- **Runtime and Architecture Support for Efficient Data Exchange in Multi-Accelerator Applications** Javier Cabezas, Isaac Gelado, John E. Stone, Nacho Navarro, David B. Kirk, and Wen-mei Hwu. IEEE Transactions on Parallel and Distributed Systems, 2014. (Accepted)
- **Unlocking the Full Potential of the Cray XK7 Accelerator** Mark Klein and John E. Stone. Cray Users Group, 2014. (In press)
- **Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations** Michael J. Hallock, John E. Stone, Elijah Roberts, Corey Fry, and Zaida Luthey-Schulten. Journal of Parallel Computing, 2014. (In press)
- **GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting** John E. Stone, Ryan McGreevy, Barry Isralewitz, and Klaus Schulten. Faraday Discussion 169, 2014. (In press)
- **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. 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**.**

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- **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.
- **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.
- **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.
- **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.

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

- **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 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.

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## 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.