GPU-Accelerated Visualization and Analysis of Biomolecular Complexes

John E. Stone

Theoretical and Computational Biophysics Group

Beckman Institute for Advanced Science and Technology

University of Illinois at Urbana-Champaign

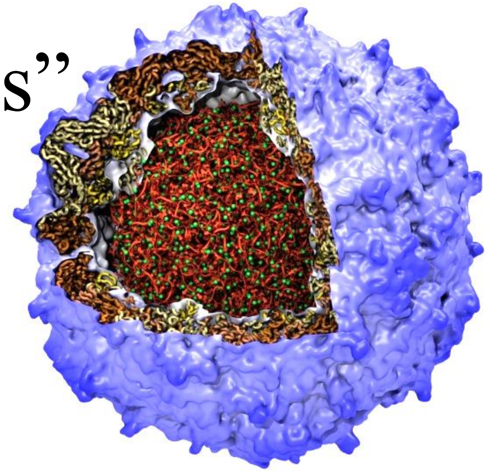
http://www.ks.uiuc.edu/Research/vmd/

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

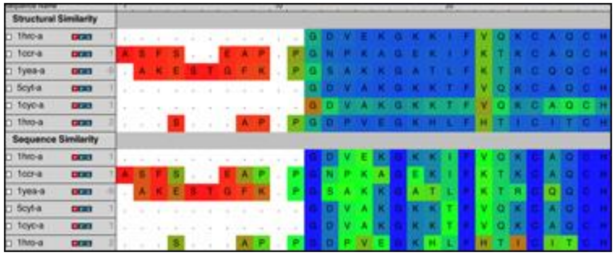
Oxford University, May 12, 2014

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/

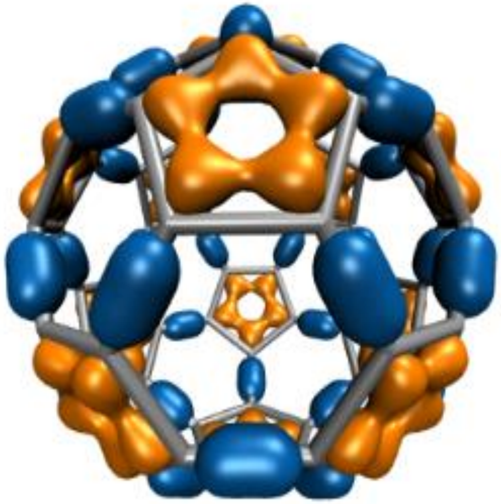


Poliovirus

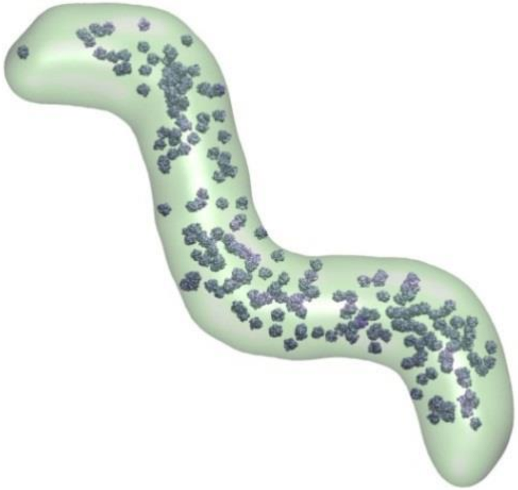


```
Sequence Name
Structural Similarity
□ 1hrc-a   1  . . . . . . . . . . . G D V E K G K K I F V Q K C A Q C H
□ 1ccr-a   1  A S F S . . E A P . P G N P K A G E K I F K T K C A Q C H
□ 1yea-a      . A K E S T G F K . P G S A K K G A T L F K T R C Q Q C H
□ 5cyt-a   1  . . . . . . . . . . . G D V A K G K K T F V Q K C A Q C H
□ 1cyc-a   1  . . . . . . . . . . . G D V A K G K K T F V Q K C A Q C H
□ 1hro-a      . . . S . . . A P . P G D P V E G K H L F H T I C I T C H
Sequence Similarity
□ 1hrc-a   1  . . . . . . . . . . . G D V E K G K K I F V Q K C A Q C H
□ 1ccr-a   1  A S F S . . E A P . P G N P K A G E K I F K T K C A Q C H
□ 1yea-a      . A K E S T G F K . P G S A K K G A T L F K T R C Q Q C H
□ 5cyt-a   1  . . . . . . . . . . . G D V A K G K K T F V Q K C A Q C H
□ 1cyc-a   1  . . . . . . . . . . . G D V A K G K K T F V Q K C A Q C H
□ 1hro-a      . . . S . . . A P . P G D P V E G K H L F H T I C I T C H
```

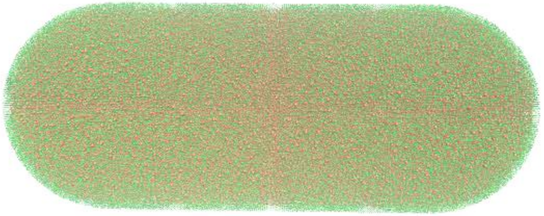
Ribosome Sequences



Electrons in
Vibrating Buckyball



Cellular Tomography
Cryo-electron Microscopy

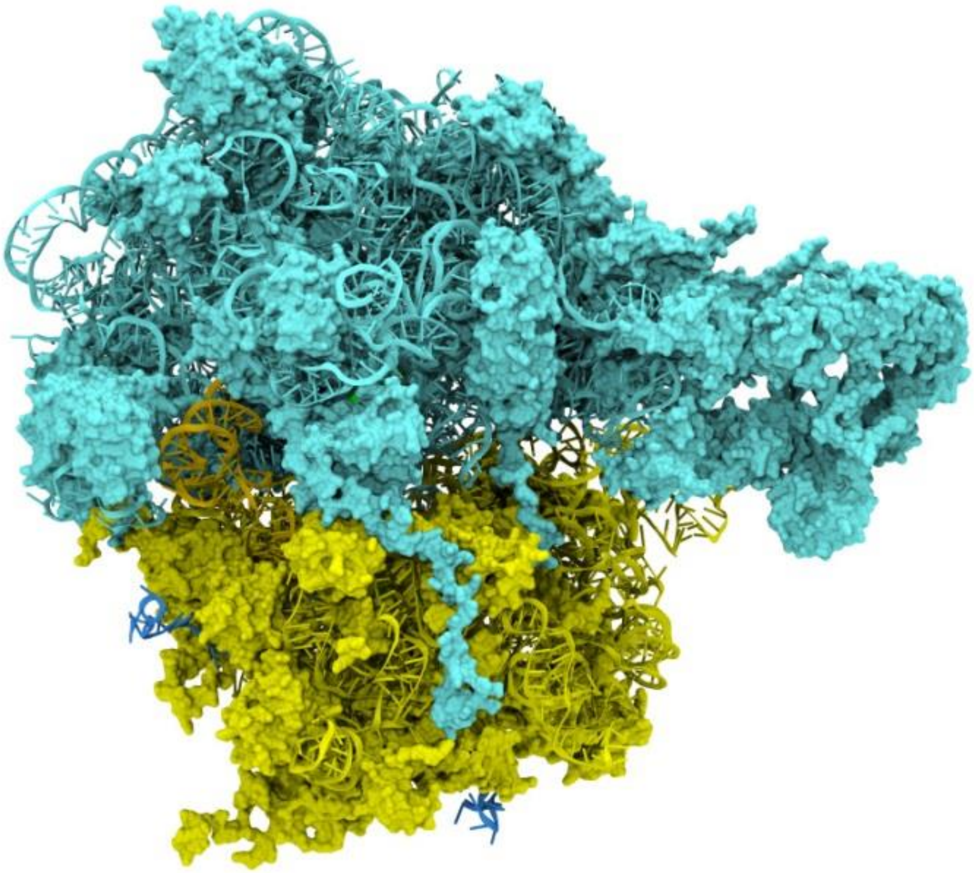


Whole Cell Simulations

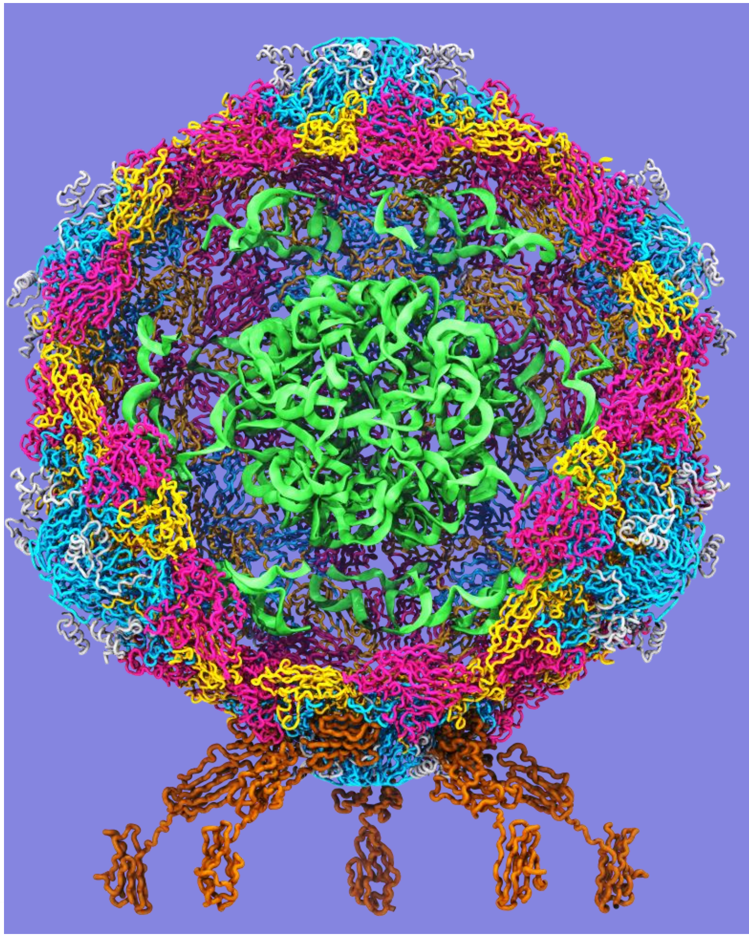
Goal: A Computational Microscope

Study the molecular machines in living cells

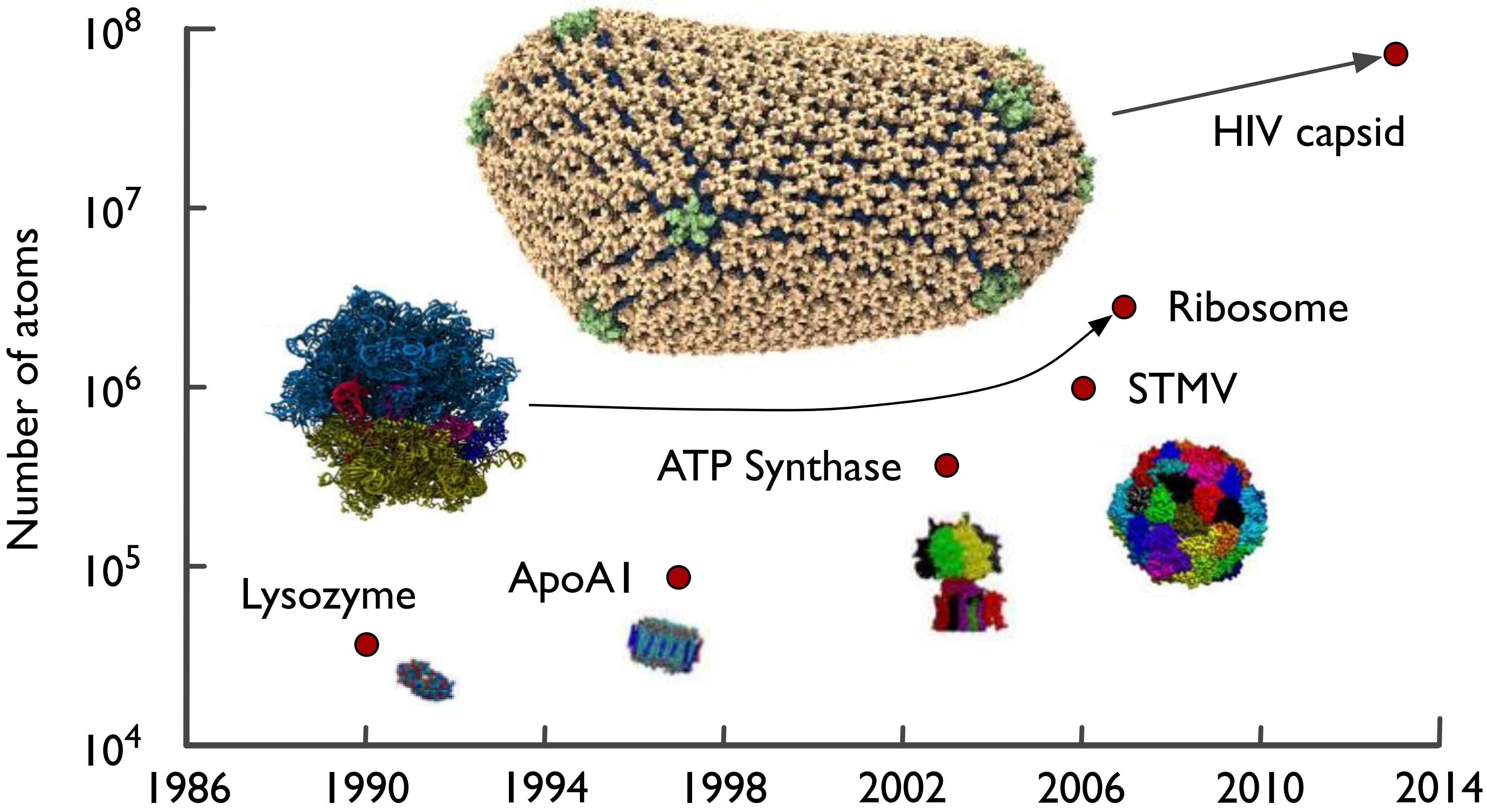
Ribosome: target for antibiotics



Poliovirus



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

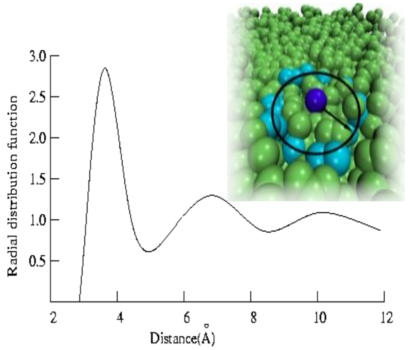


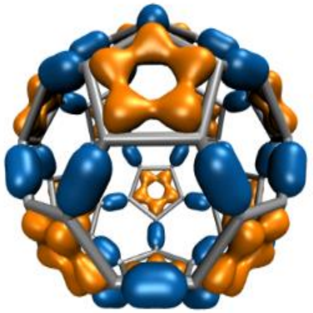
GPU Computing

- 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

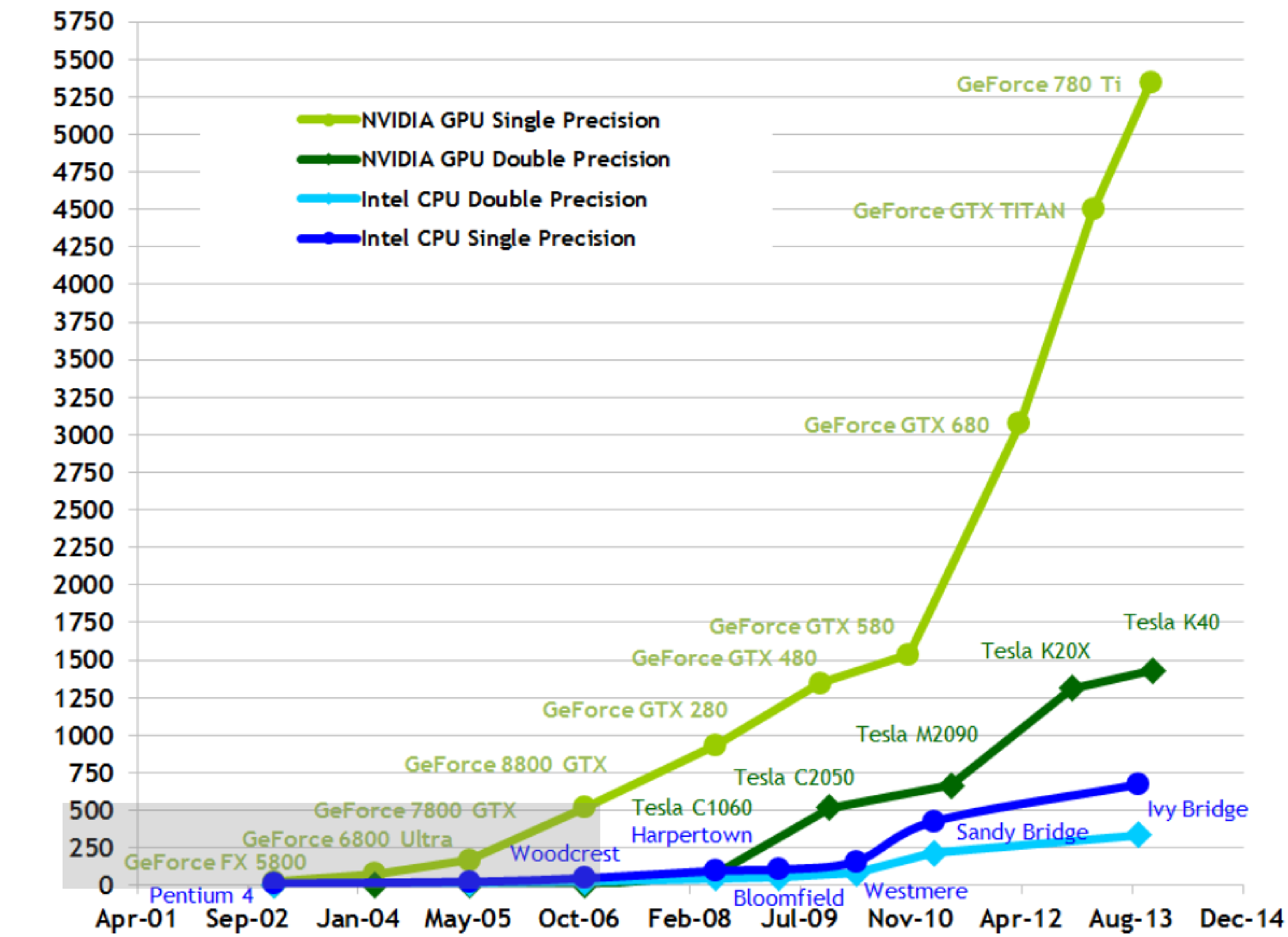
CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

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

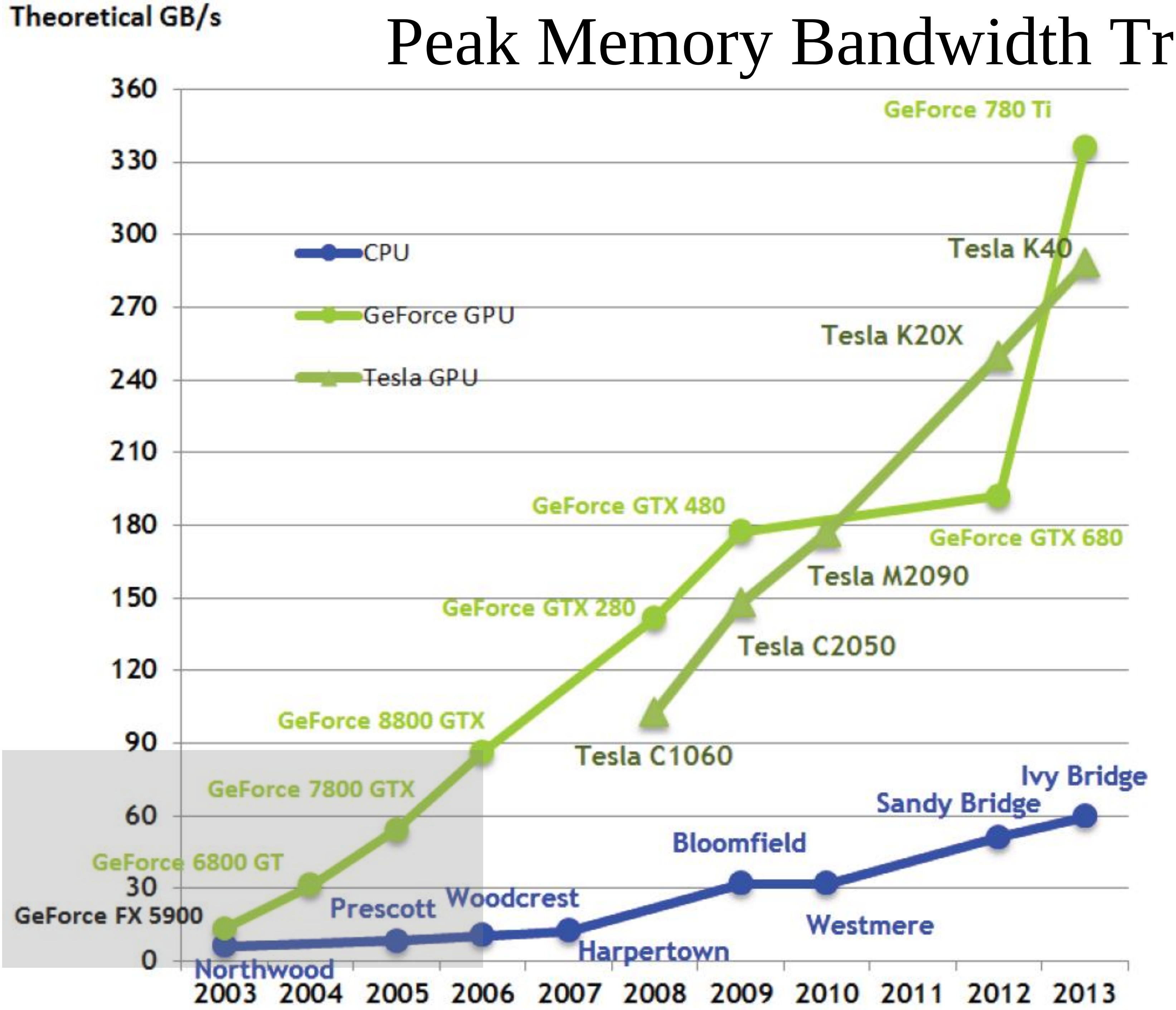




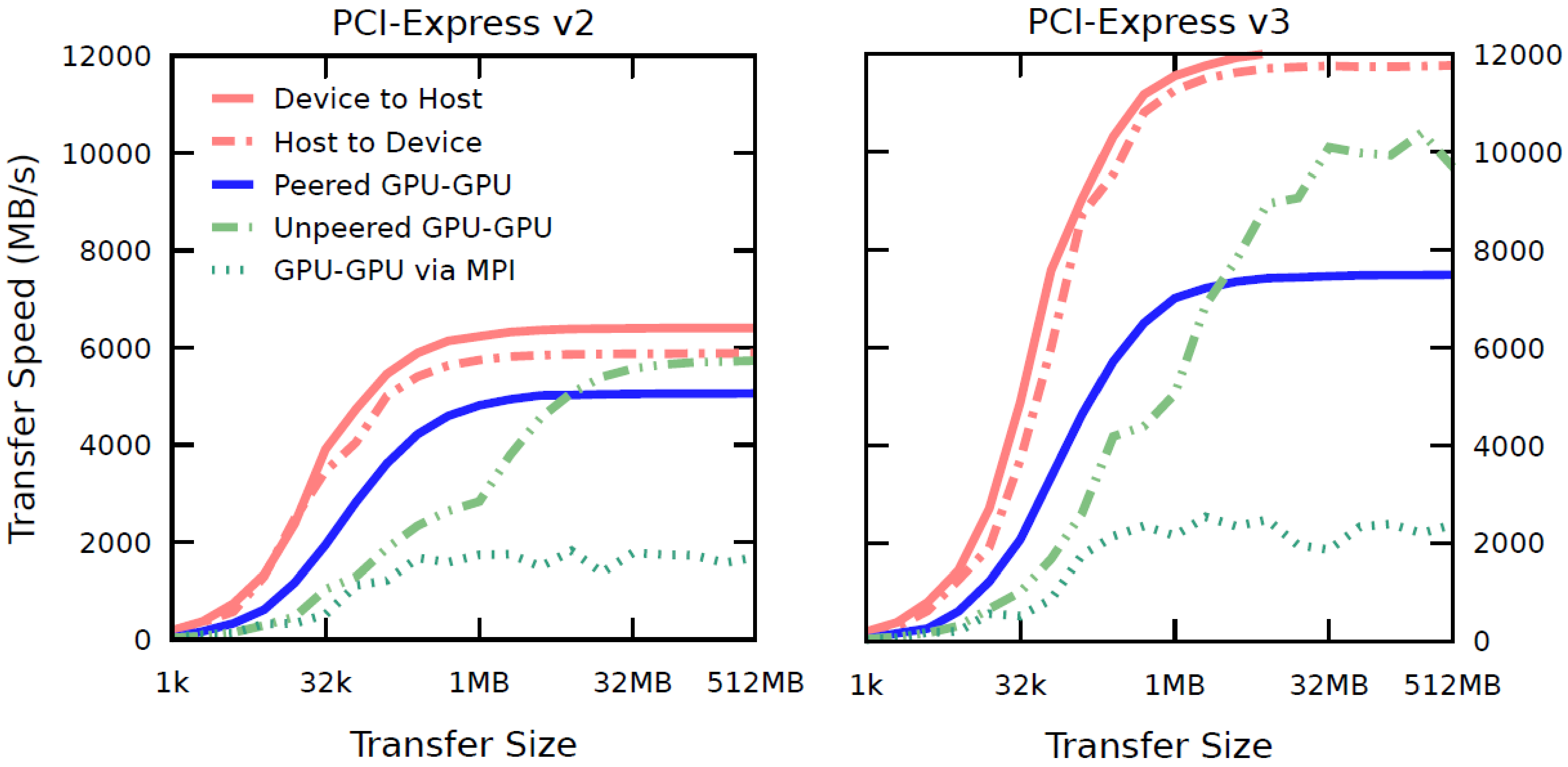
Peak Arithmetic Performance Trend



Peak Memory Bandwidth Trend



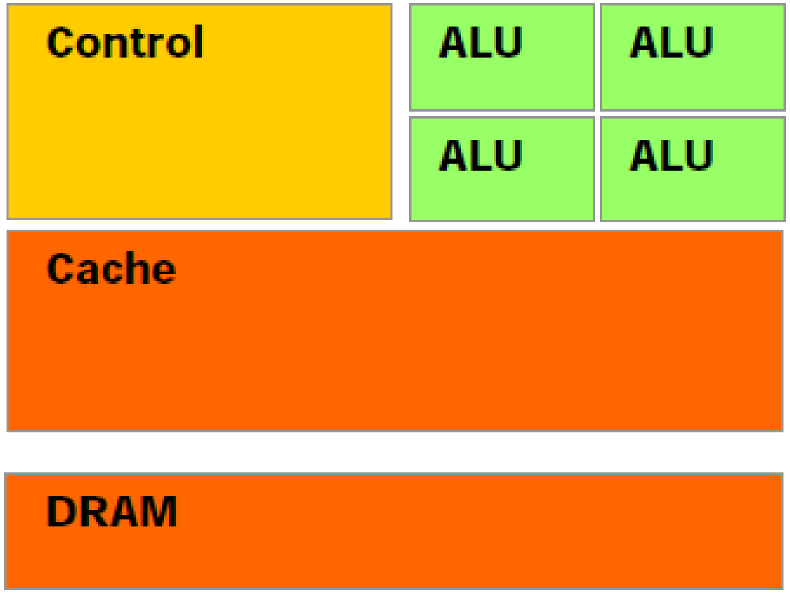
GPU PCI-Express DMA



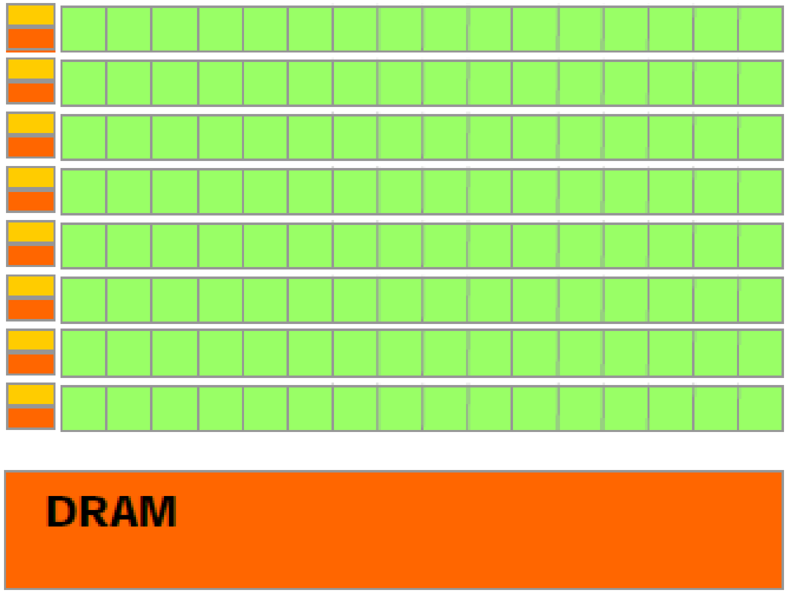
Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations
Michael J. Hallock, John E. Stone, Elijah Roberts, Corey Fry, and Zaida Luthey-Schulten.
Journal of Parallel Computing, 2014. **(In press)**
http://dx.doi.org/10.1016/j.parco.2014.03.009

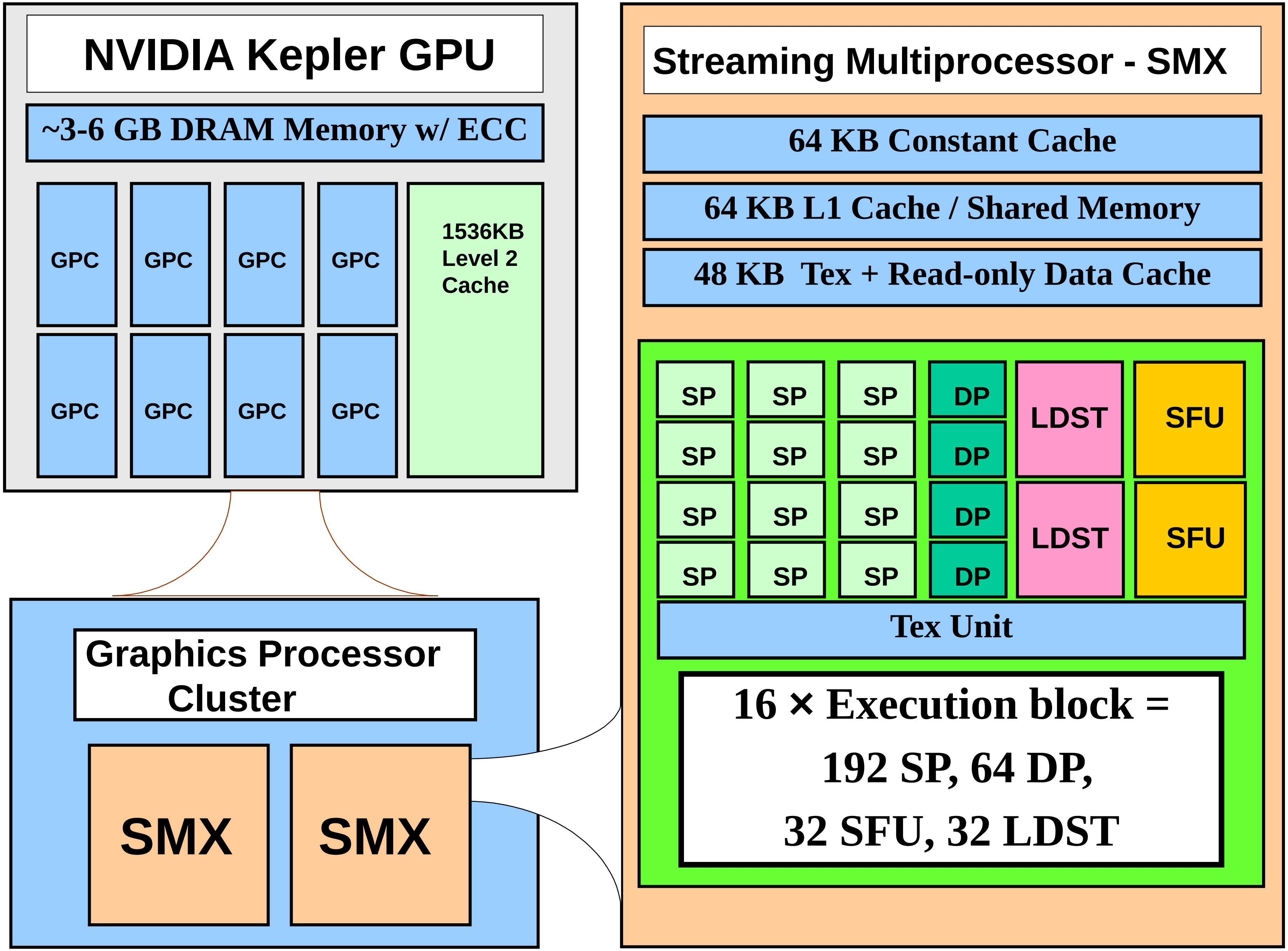
Comparison of CPU and GPU Hardware Architecture

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 SP SP DP

SP SP SP DP

SP SP SP DP

SP SP SP DP

LDST SFU

LDST SFU

Tex Unit

16 × Execution block =

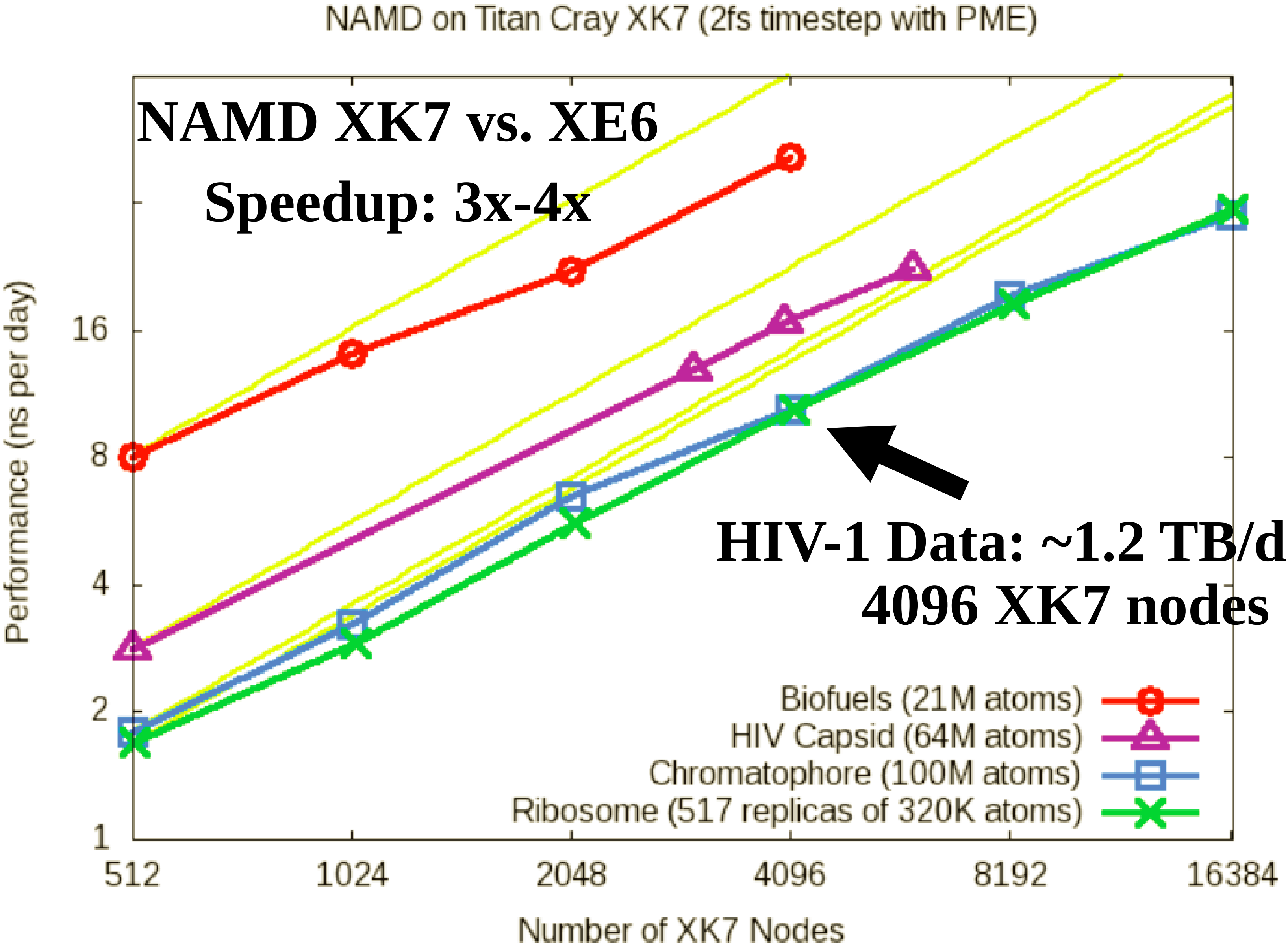
192 SP, 64 DP,

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**

450MB/sec

to 8GB/sec

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

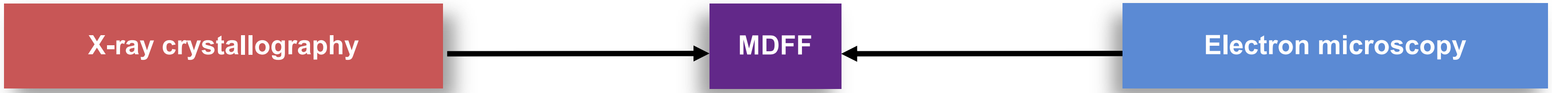
- Analyze/visualize large trajectories too large to transfer off-site:
  - Compute time-averaged electrostatic fields, MDFF quality-of-fit, etc.
  - User-defined parallel analysis operations, data types
  - Parallel ray tracing, movie making
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 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)

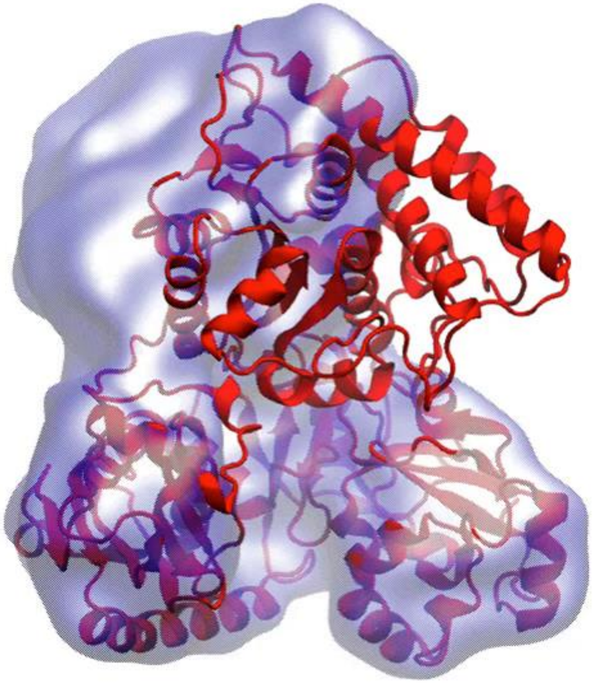

X-ray crystallography

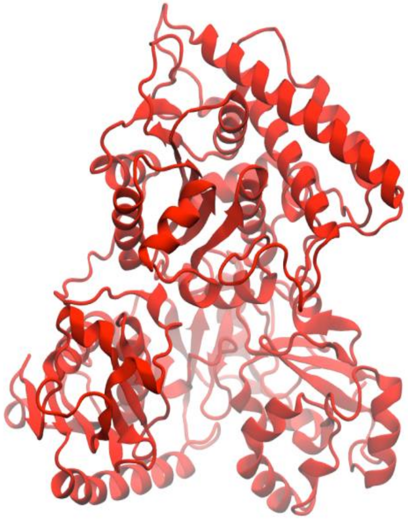
MDFF

Electron microscopy

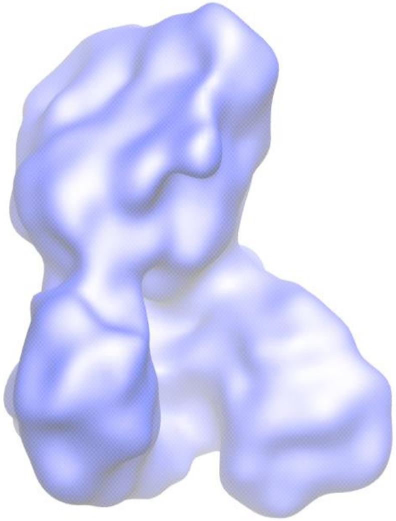
APS at Argonne

FEI microscope



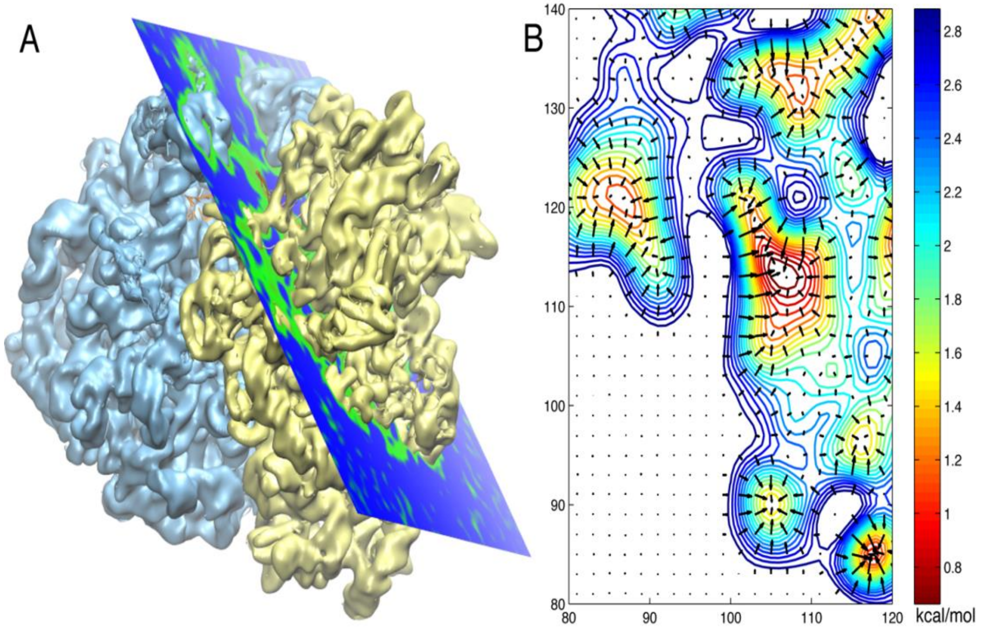

Acetyl - CoA Synthase

ORNL Titan



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.

Molecular Dynamics Flexible Fitting - Theory



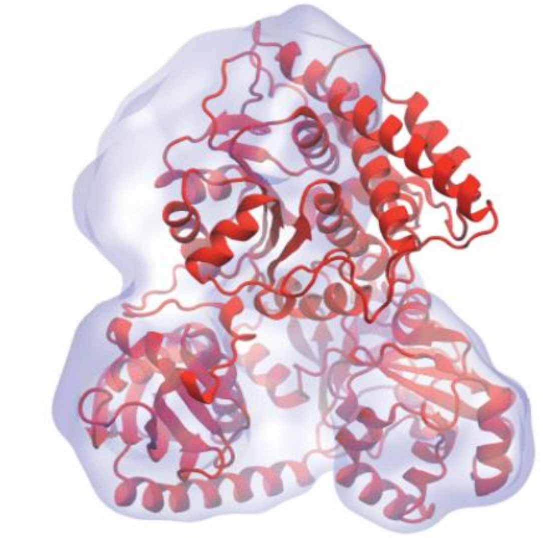
Two terms are added to the MD potential

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

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

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

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

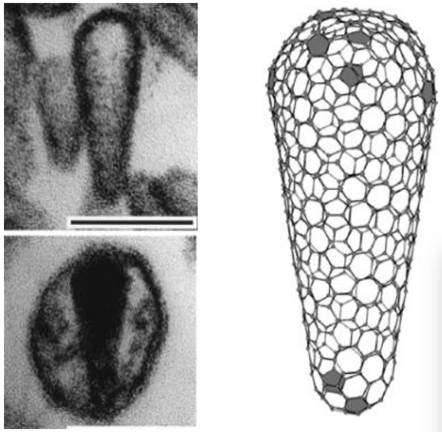


A mass-weighted force is then applied to each atom

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

Structural Route to the all-atom HIV-1 Capsid

1st TEM (1999)

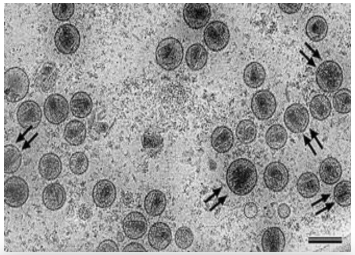


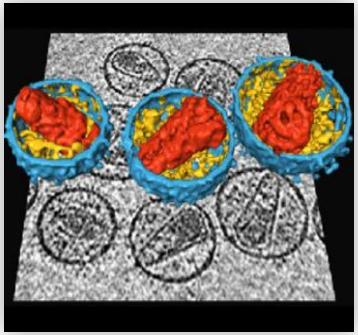
Ganser et al. *Science*, 1999

Briggs et al. *EMBO J*, 2003

Briggs et al. *Structure*, 2006

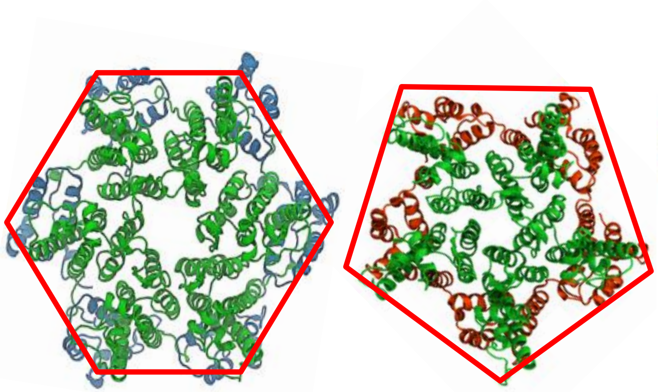
1st tomography (2003)



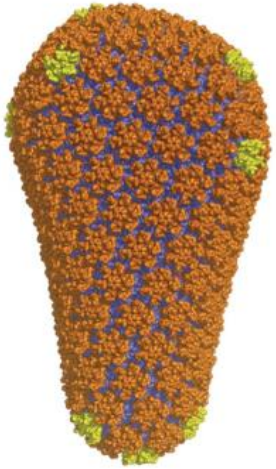


cryo-ET (2006)

Crystal structures of separated hexamer and pentamer

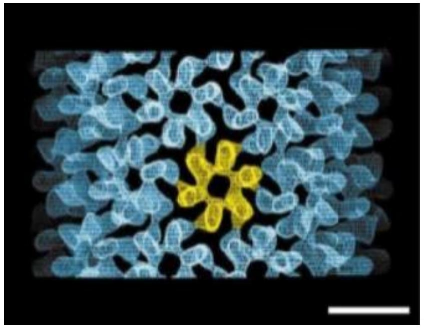


Pornillos et al. , *Cell* 2009, *Nature* 2011

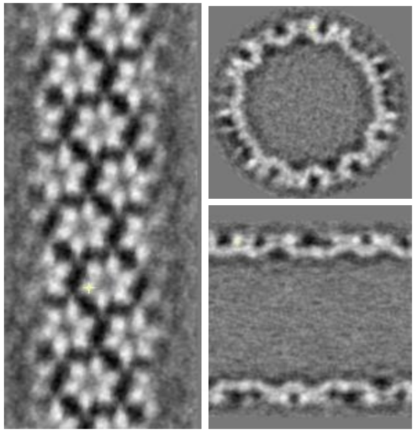


High res. EM of hexameric tubule, tomography of capsid,
all-atom model of capsid by MDFF w/ NAMD & VMD,
NSF/NCSA Blue Waters computer at Illinois

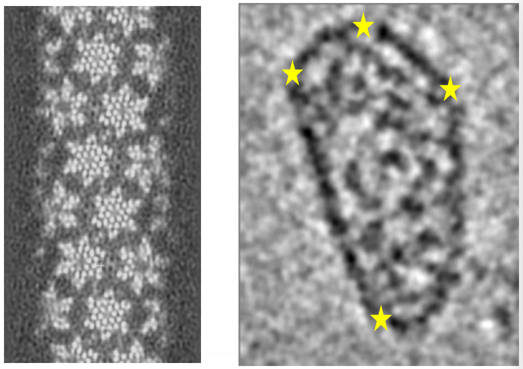
hexameric tubule



Li et al., *Nature*, 2000



Byeon et al., *Cell* 2009

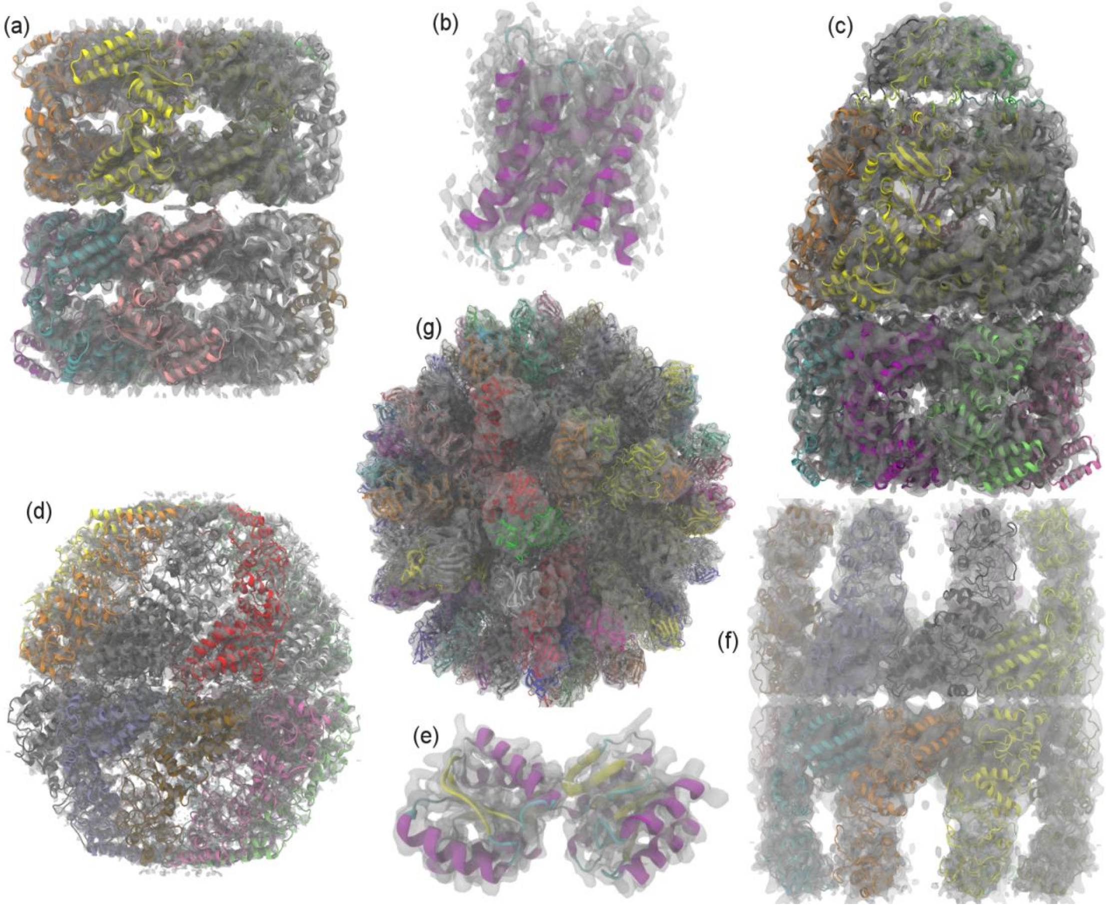


nature
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
THE HIV-1 CAPSID
Atomic structure of the AIDS pathogen's protein coat
PAGE 643

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

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

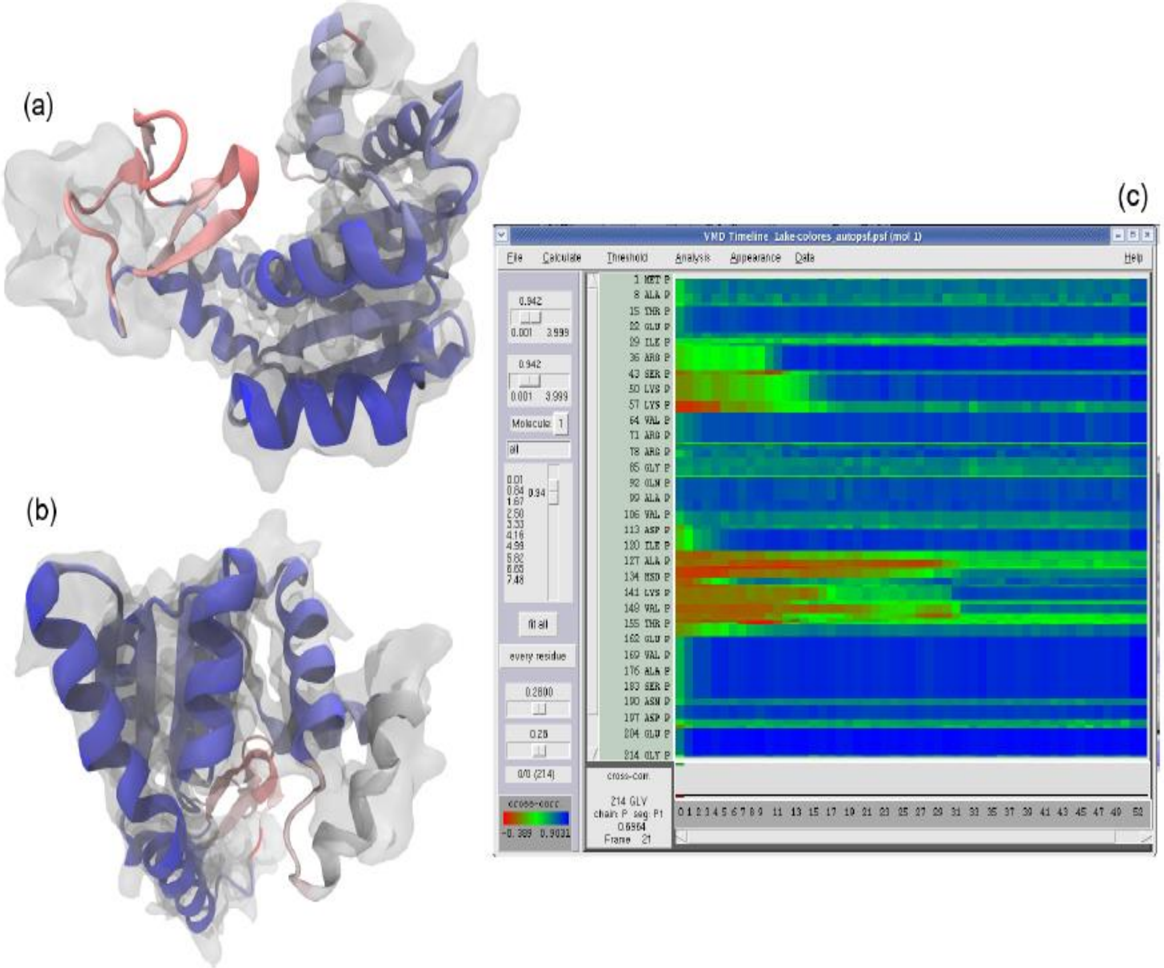
Compute Pearson correlation to evaluate the fit of a reference cryo-EM density map with a **simulated density map** produced from an **all-atom structure**.



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



GPU-accelerated MDFF Cross Correlation Timeline

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

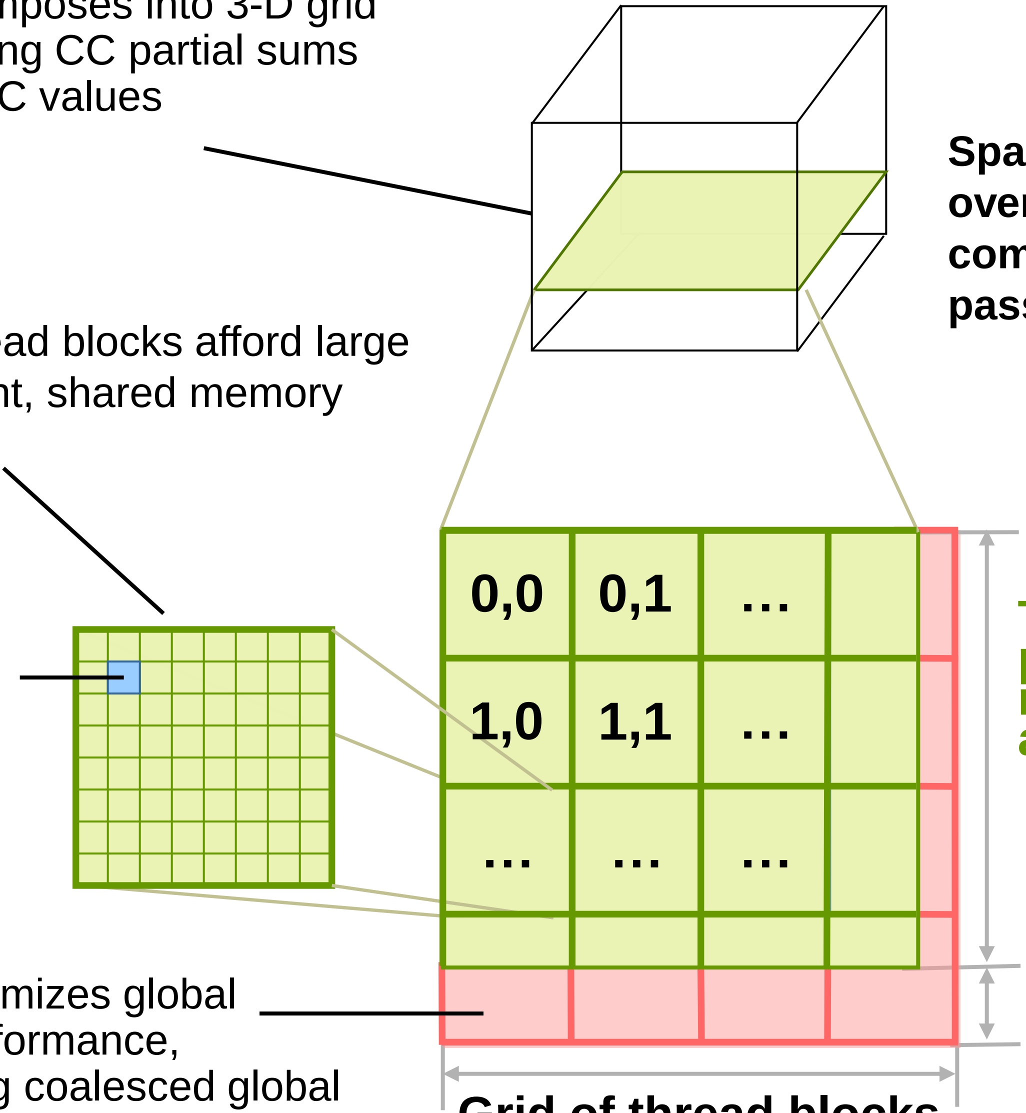
Single-Pass MDFF GPU Cross-Correlation

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



Threads producing results that are used

Inactive threads, region of discarded output

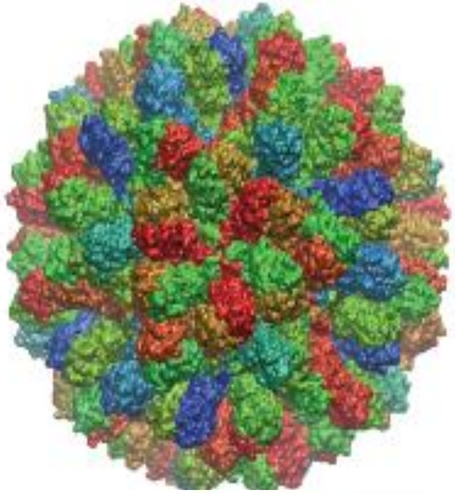
Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

Grid of thread blocks

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 **Quadro K6000**	**0.458s** **34.6x**	**0.06s** **25.7x**	**0.034s** **36.8x**	**0.007s** **55.7x**
VMD-CPU-SSE 32-threads, 2x Xeon E5-2687W	0.779s 20.3x	0.085s 18.1x	0.159s 7.9x	0.033s 11.8x
Chimera **1-thread Xeon E5-2687W**	**15.86s** **1.0x**	**1.54s** **1.0x**	**1.25s** **1.0x**	**0.39s** **1.0x**
VMD CPU-SEQ (plugin) 1-thread Xeon E5-2687W	62.89s 0.25x	2.9s 0.53x	1.57s 0.79x	0.04s 9.7x

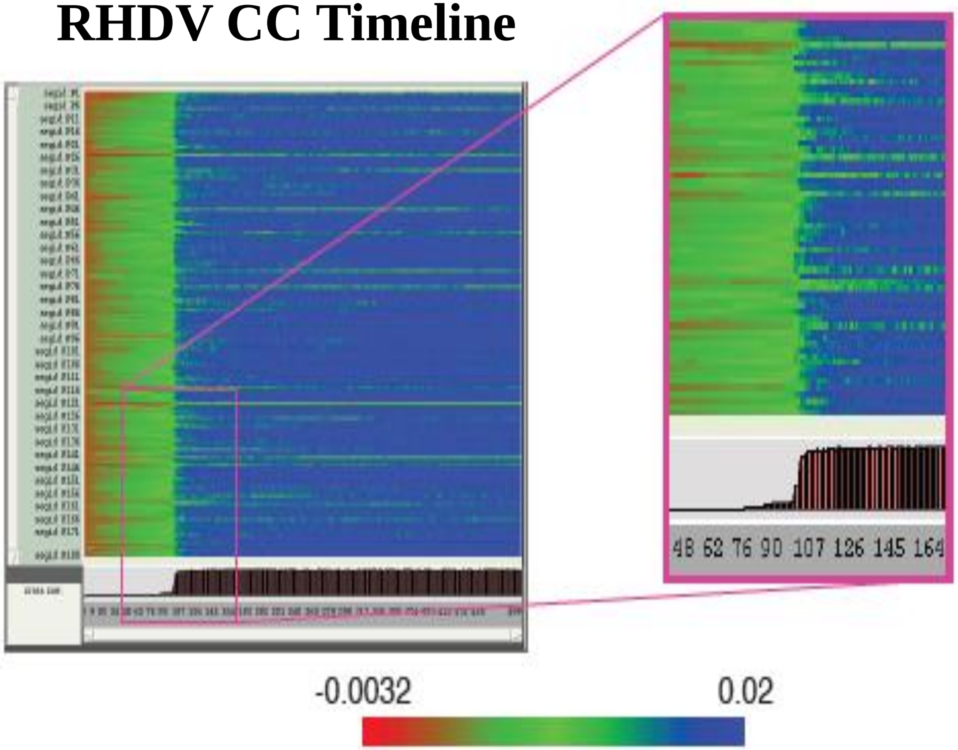
VMD RHDV Cross Correlation Timeline on Cray XK7



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

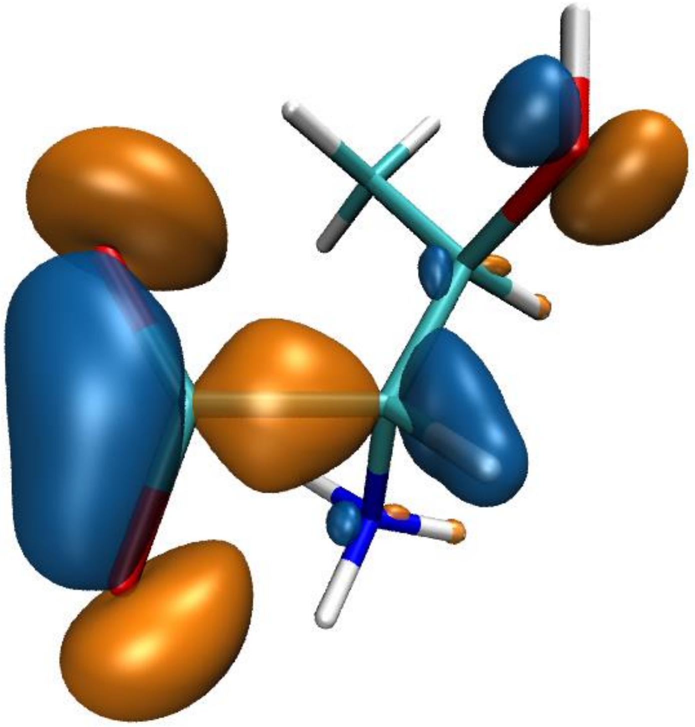
Calculation would take **5 years** using original serial VMD CC plugin on a workstation!

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

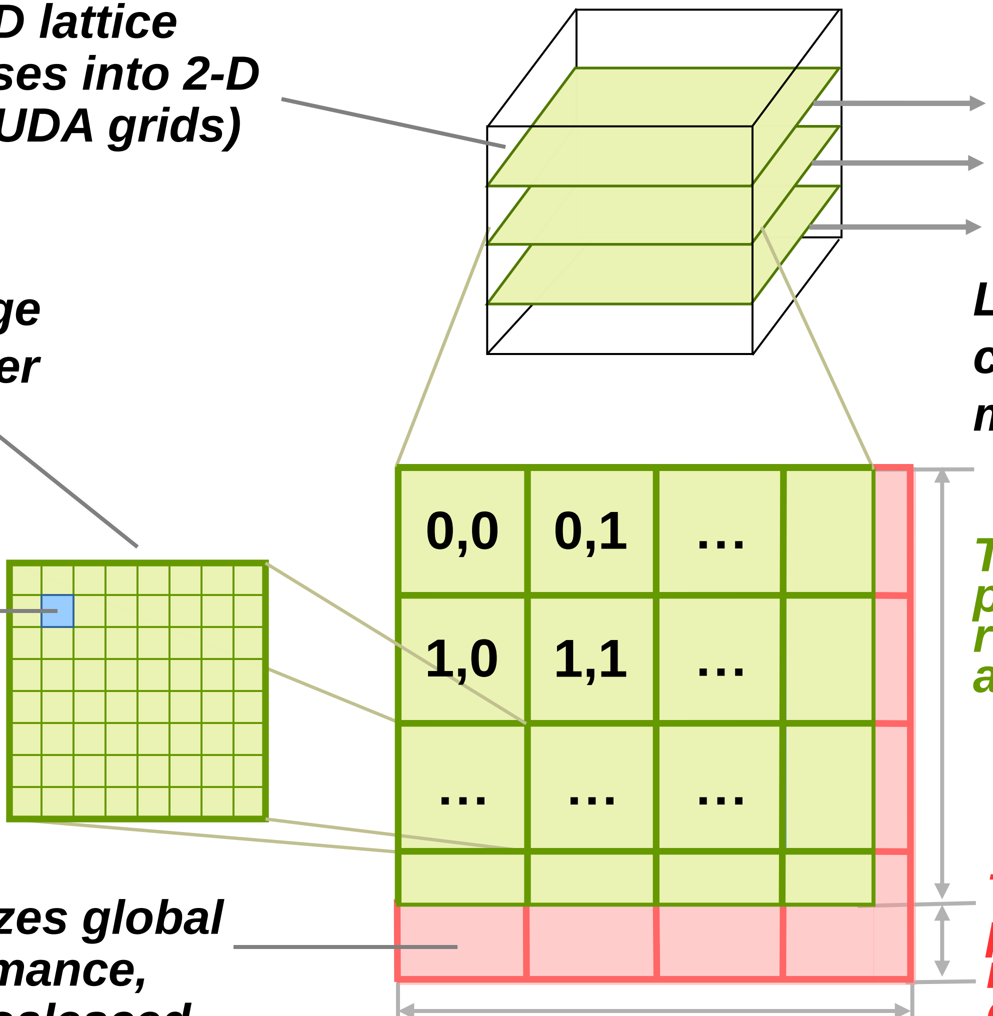
Loop over shells

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

Loop over angular momenta

(unrolled in real code)

MO GPU Parallel Decomposition



MO 3-D lattice decomposes into 2-D slices (CUDA grids)

Lattice can be computed using multiple GPUs

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

Each thread computes one MO lattice point.

Threads producing results that are used

Threads producing results that are discarded

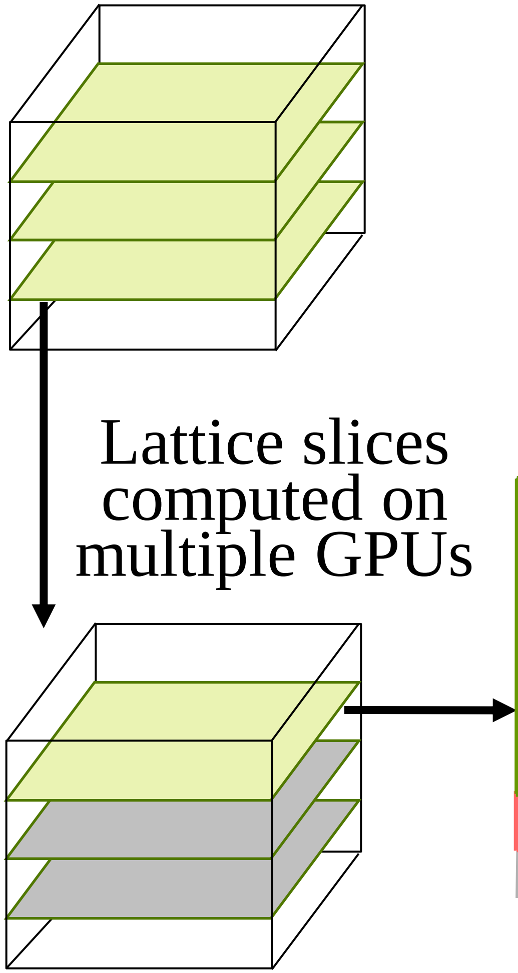
Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

Grid of thread blocks

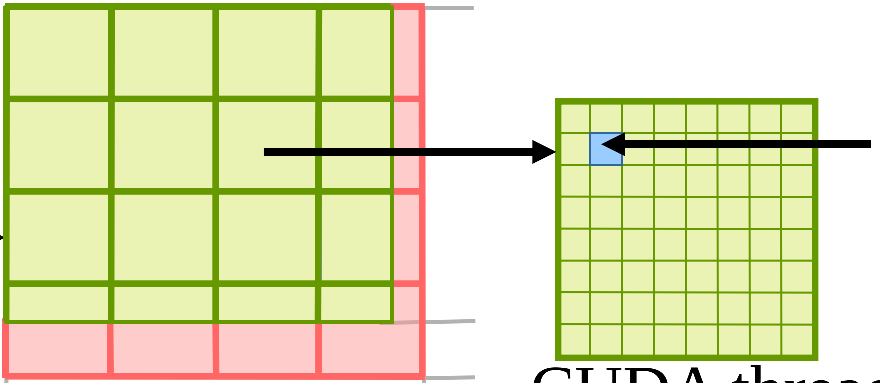
GPU Solution: Computing C_{60} Molecular Orbitals

3-D orbital lattice: millions of points

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



Lattice slices computed on multiple GPUs

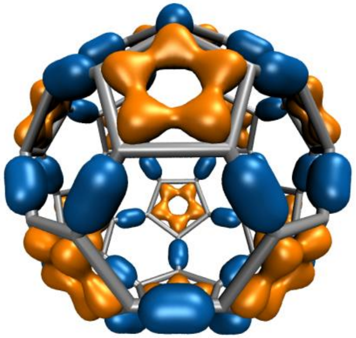


2-D CUDA grid on one GPU

CUDA thread blocks

GPU threads each compute one point.

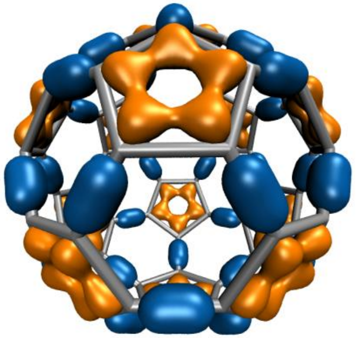
Molecular Orbital Inner Loop, Hand-Coded x86 SSE
Hard to Read, Isn't It? (And this is the "pretty" version!)



```
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



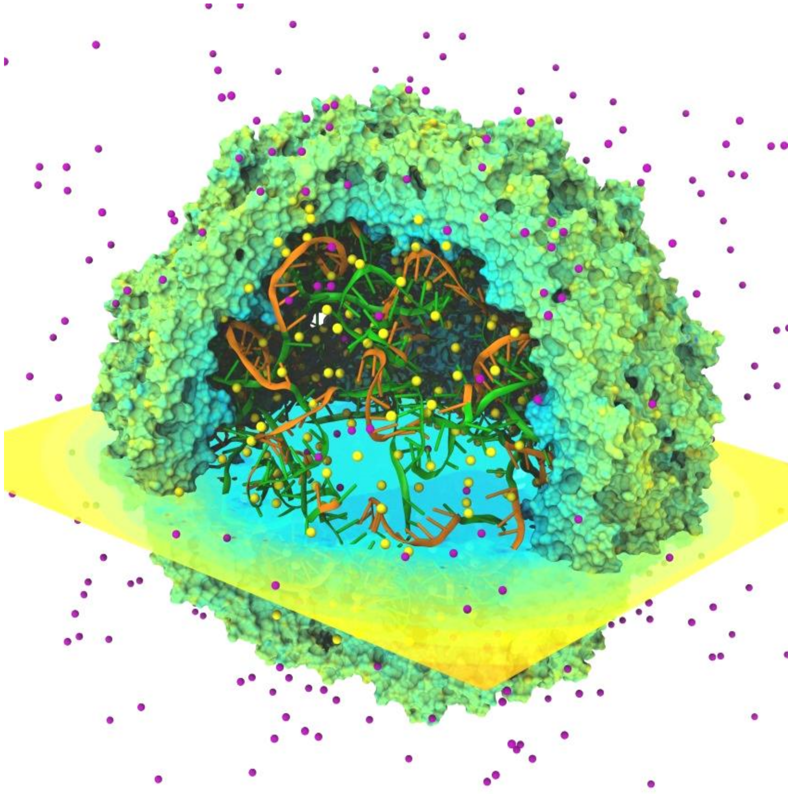
```
for (shell=0; shell < maxshell; shell++) {
    float contracted_gto = 0.0f;
    for (prim=0; prim<num_prim_per_shell[shell_counter]; prim++) {
      float exponent         = const_basis_array[prim_counter     ];
      float contract_coeff = const_basis_array[prim_counter + 1];
      contracted_gto += 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.

Time-Averaged Electrostatics Analysis on NCSA Blue Waters

NCSA Blue Waters Node Type	**Seconds per trajectory frame for one compute node**
Cray XE6 Compute Node: 32 CPU cores (2xAMD 6200 CPUs)	9.33
Cray XK6 GPU-accelerated Compute Node: 16 CPU cores + **NVIDIA X2090 (Fermi) GPU**	2.25
Speedup for GPU XK6 nodes vs. CPU XE6 nodes	**XK6 nodes are 4.15x faster overall**
Tests on XK7 nodes indicate MSM is CPU-bound with the Kepler K20X GPU. **Performance is not much faster (yet) than Fermi X2090** **Need to move spatial hashing, prolongation, interpolation onto the GPU…**	**In progress….** **XK7 nodes 4.3x faster overall**

Preliminary performance for VMD time-averaged electrostatics w/ Multilevel Summation Method on the NCSA Blue Waters Early Science System

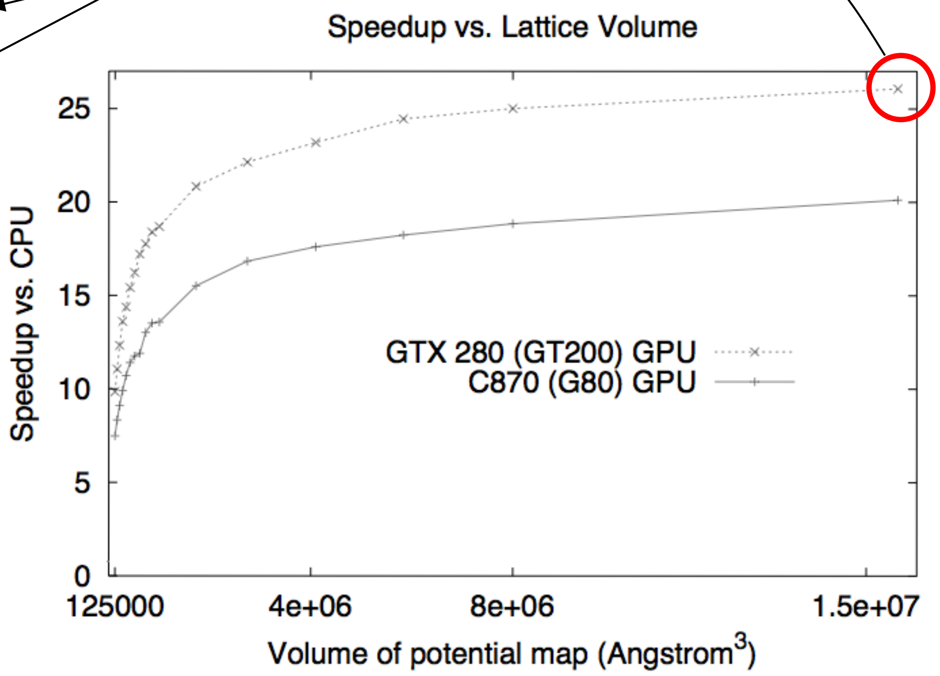
Multilevel Summation on the GPU

Accelerate **short-range cutoff** and **lattice cutoff** parts

Performance profile for 0.5 Å map of potential for 1.5 M atoms.

Hardware platform is Intel QX6700 CPU and NVIDIA GTX 280.

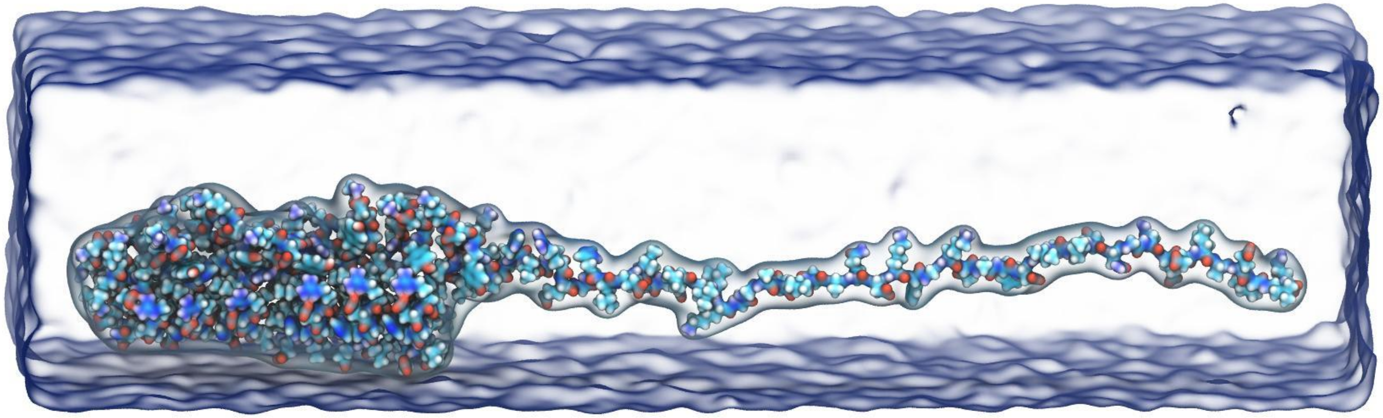
Computational steps	CPU (s)	w/ GPU (s)	Speedup
Short-range cutoff	480.07	14.87	32.3
Long-range anterpolation	0.18		
restriction	0.16		
lattice cutoff	49.47	1.36	36.4
prolongation	0.17		
interpolation	3.47		
Total	533.52	20.21	26.4



Multilevel summation of electrostatic potentials using graphics processing units. D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

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

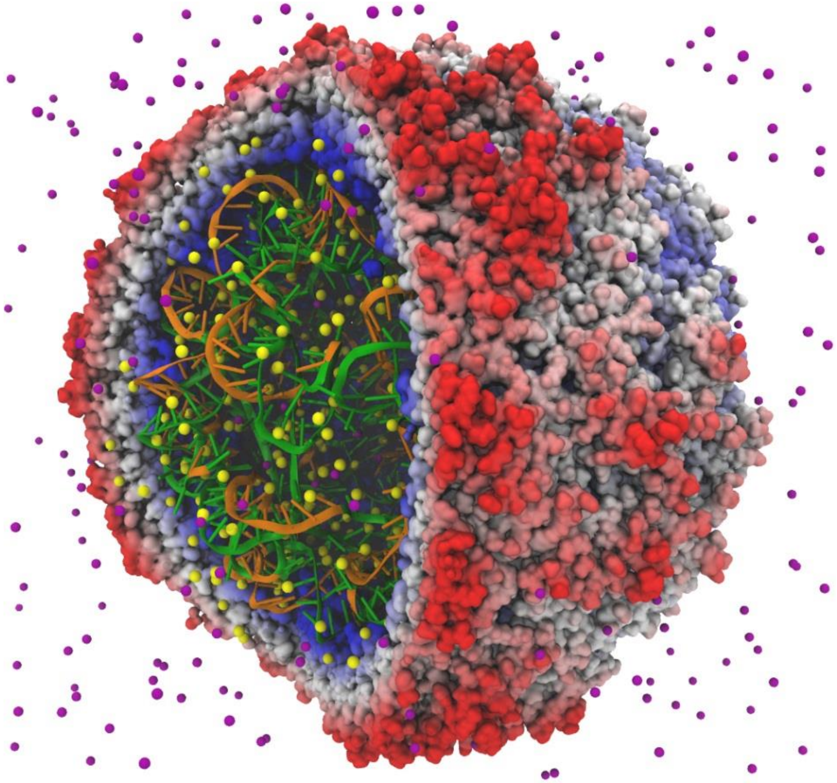


Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.

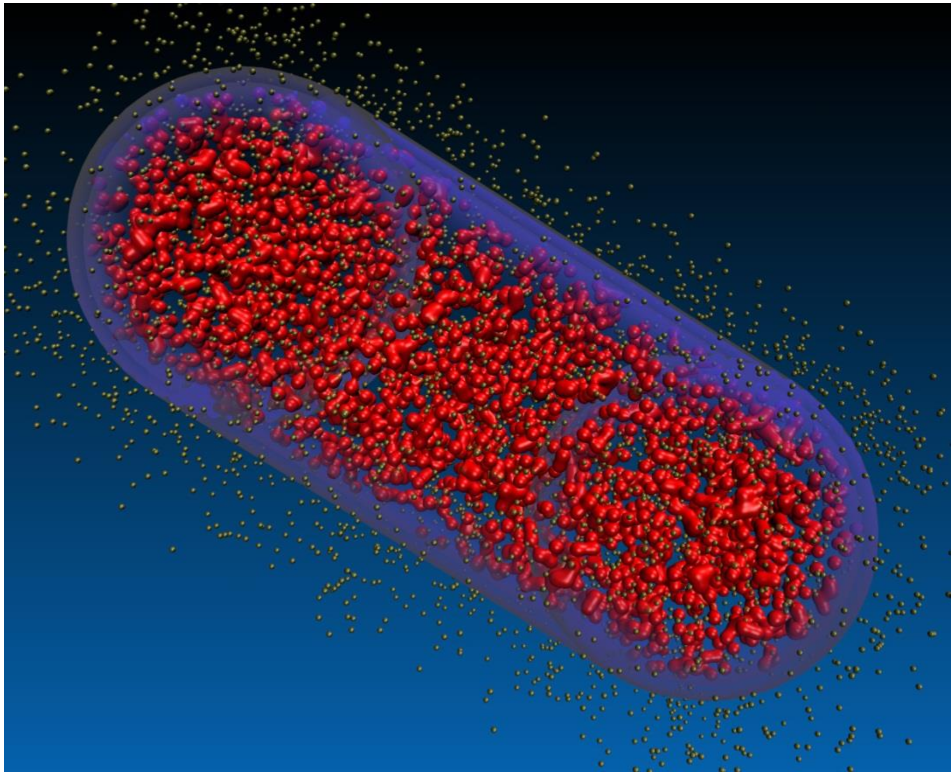
M. Krone, J. E. Stone, T. Ertl, K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012

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



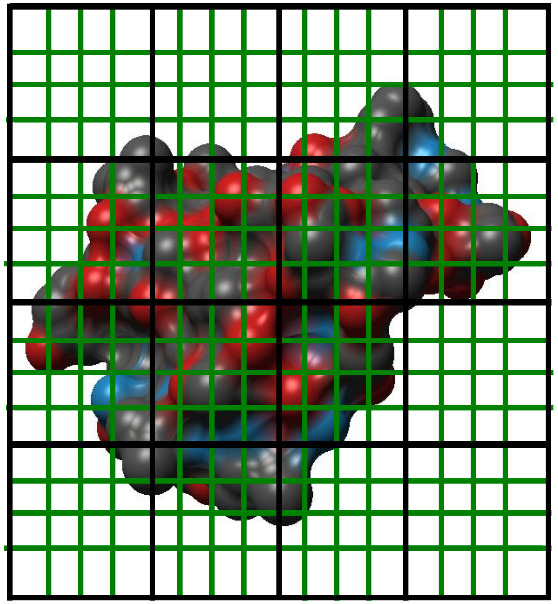
Lattice Cell Simulations

QuickSurf Algorithm Overview

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

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

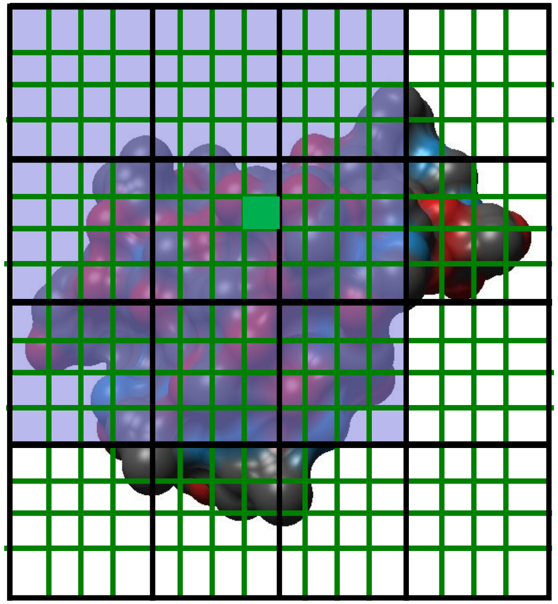
- Extract isosurface for a user-defined density value



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

QuickSurf Density Map Algorithm

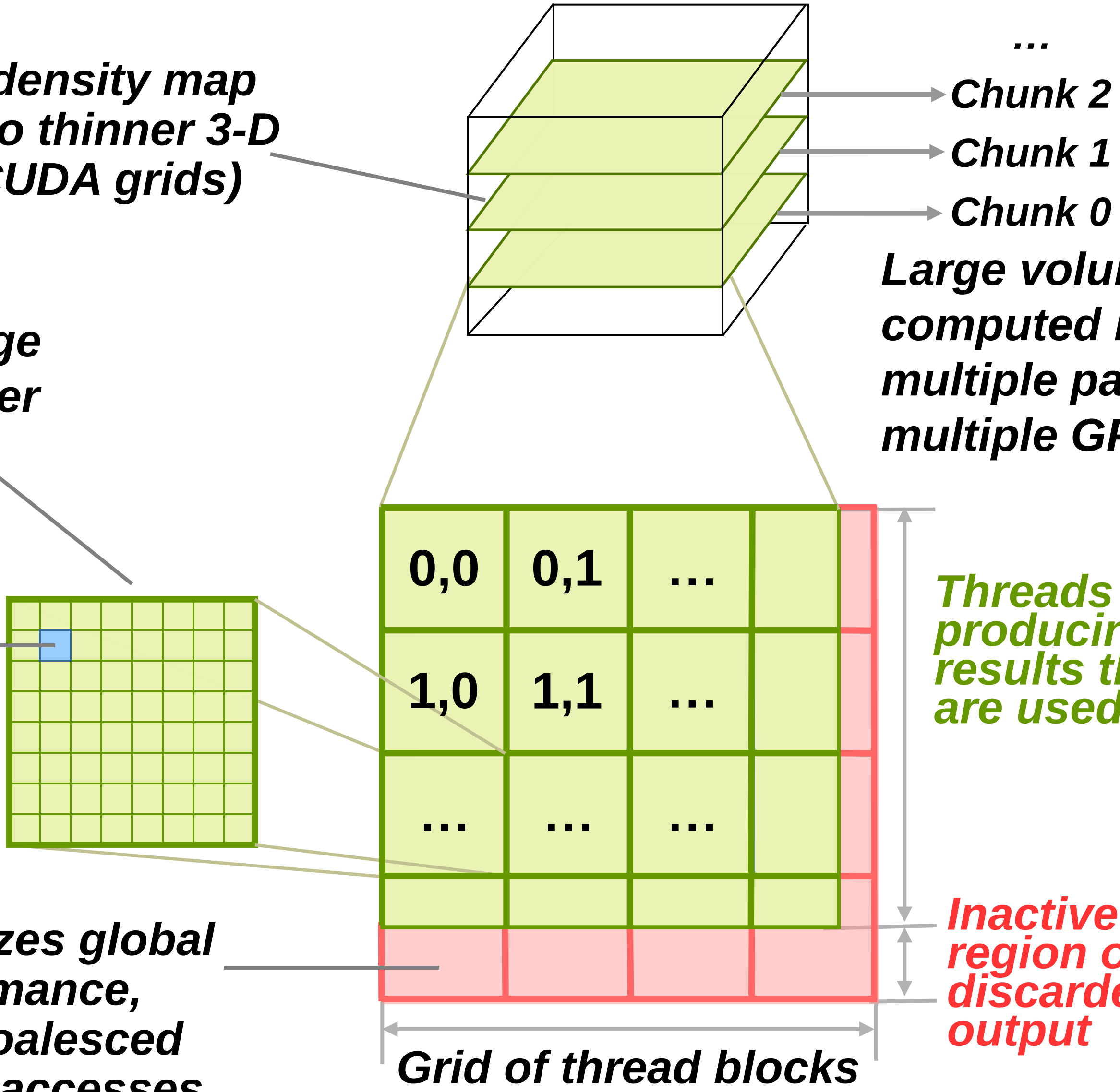
- Spatial acceleration grid cells are sized to match the cutoff radius for the exponential, beyond which density contributions are negligible
- Density map lattice points computed by summing density contributions from particles in 3x3x3 grid of neighboring spatial acceleration cells
- Volumetric texture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

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

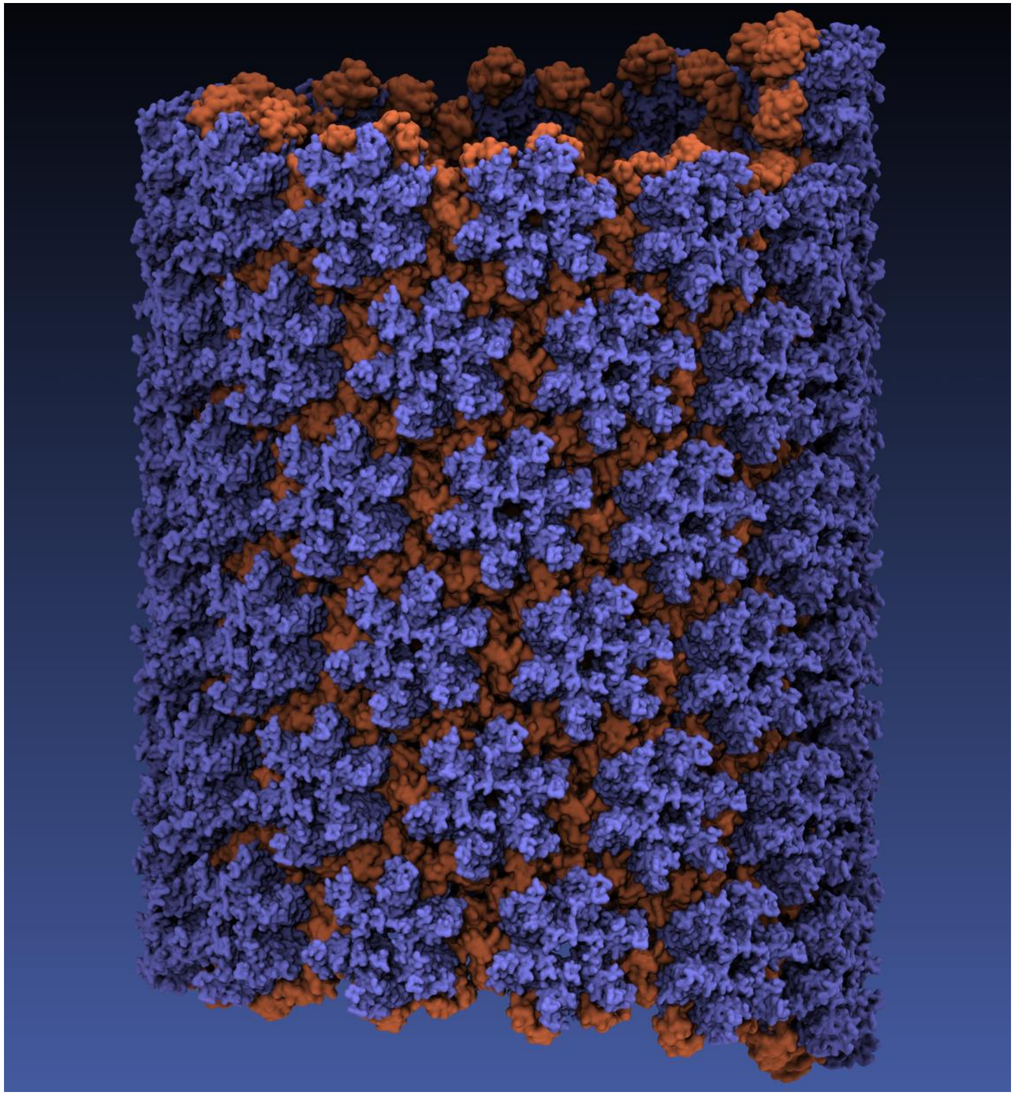
Threads producing results that are used

Inactive threads, region of discarded output

Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

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

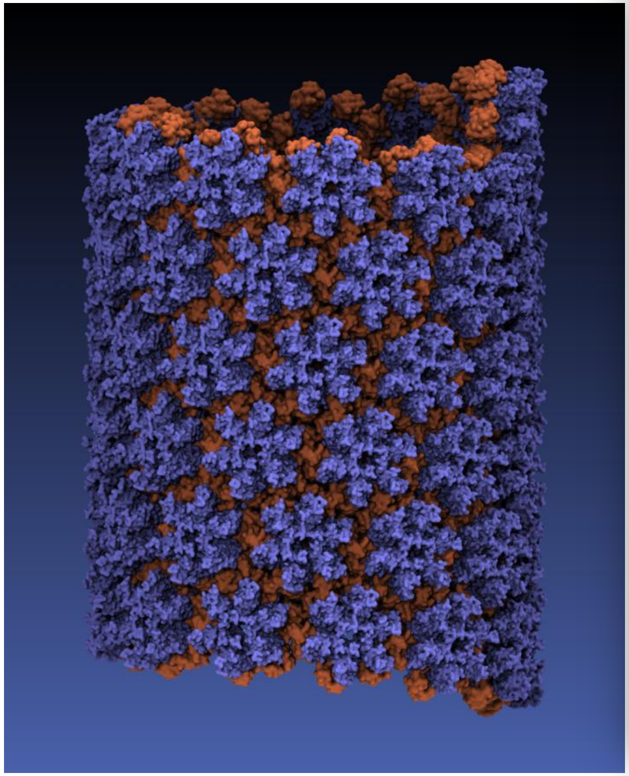
- Structures such as HIV initially needed all XK7 GPU memory to generate detailed surface renderings
- Goals and approach:
  - **Avoid slow CPU-fallback!**
  - Incrementally change algorithm phases to use more compact data types, while maintaining performance
  - Specialize code for different precision/performance/memory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

THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE

THE HIV-1 CAPSID

Atomic structure of the AIDS pathogen's protein coat

PAGE 643

COSMOLOGY

THE FIRST LIGHT

In pursuit of the most distant galaxies

PAGE 554

CITATION

CROSSING THE BORDERS

International collaborations make the most impact

PAGE 557

ANTICANCER DRUGS

A SITTING TARGET

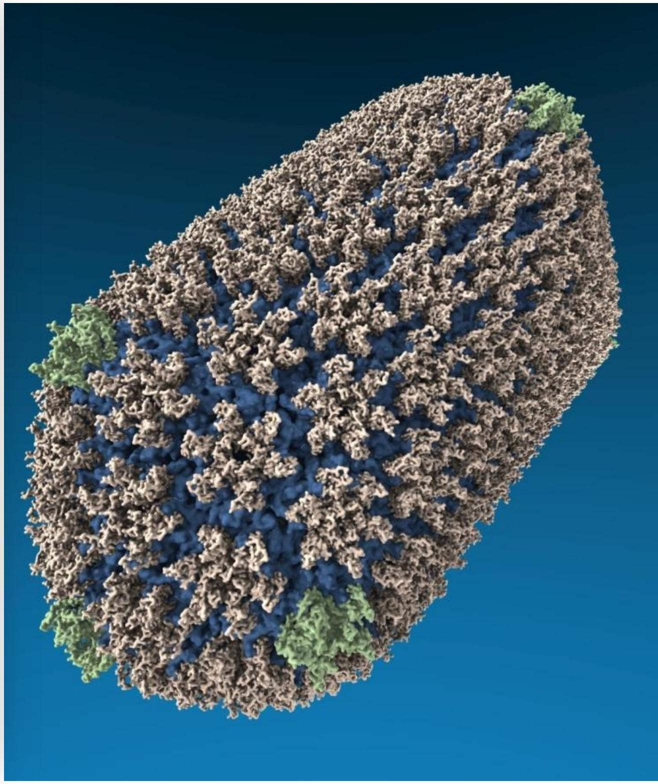
An indirect hit on 'undruggable' KRAS protein

PAGES 577 & 638

NATURE.COM/NATURE

30 May 2013

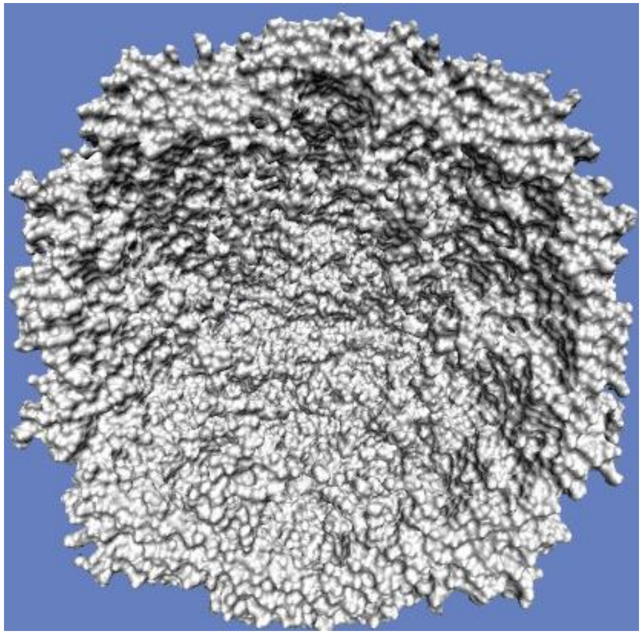
$10.00US $12.99CAN



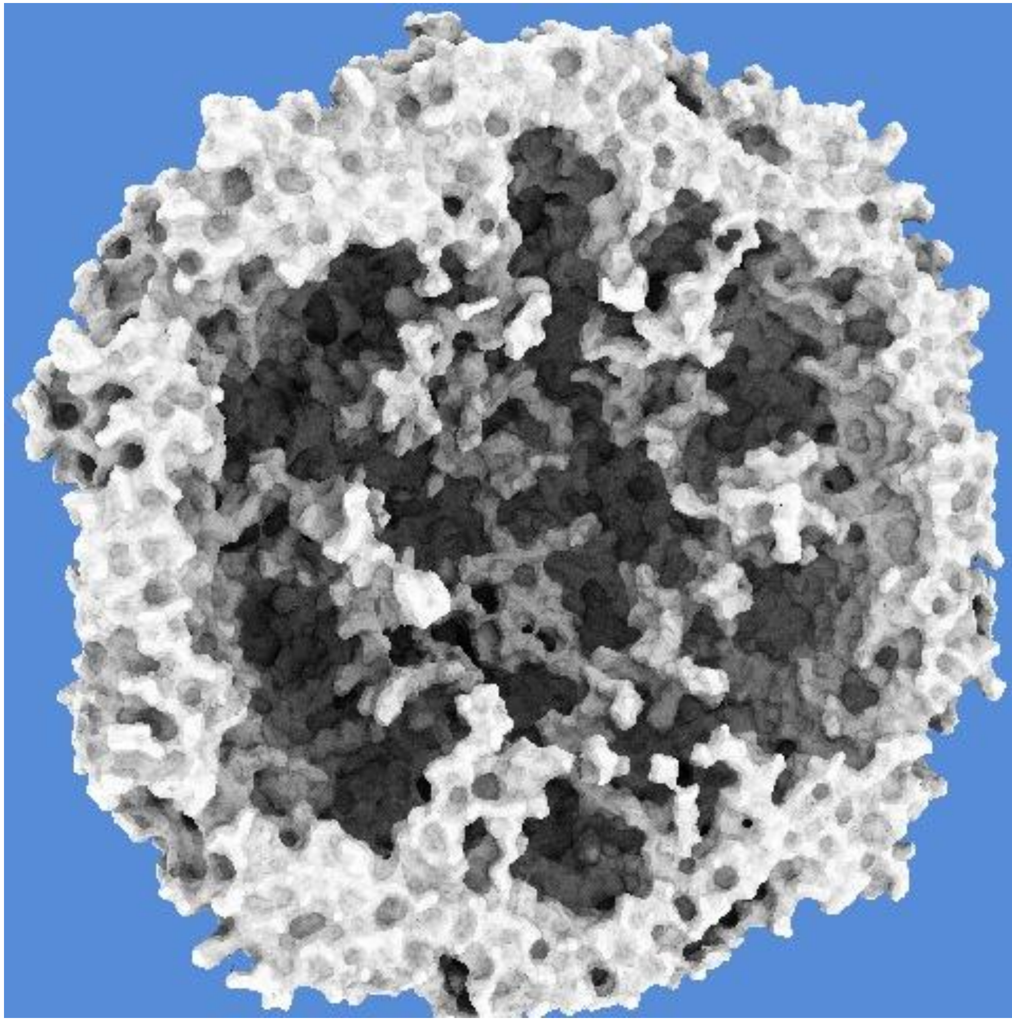
All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

Ray Tracing Molecular Graphics

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

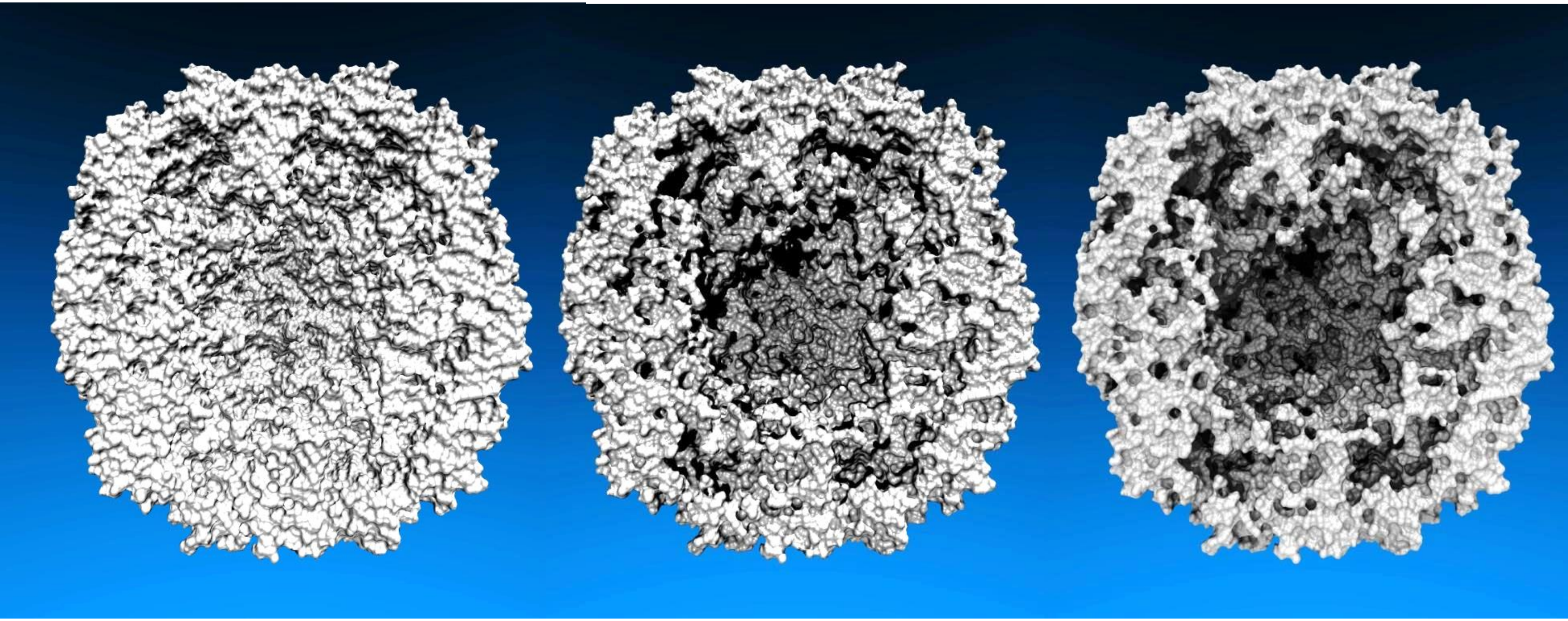


Standard OpenGL rasterization



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

Lighting Comparison

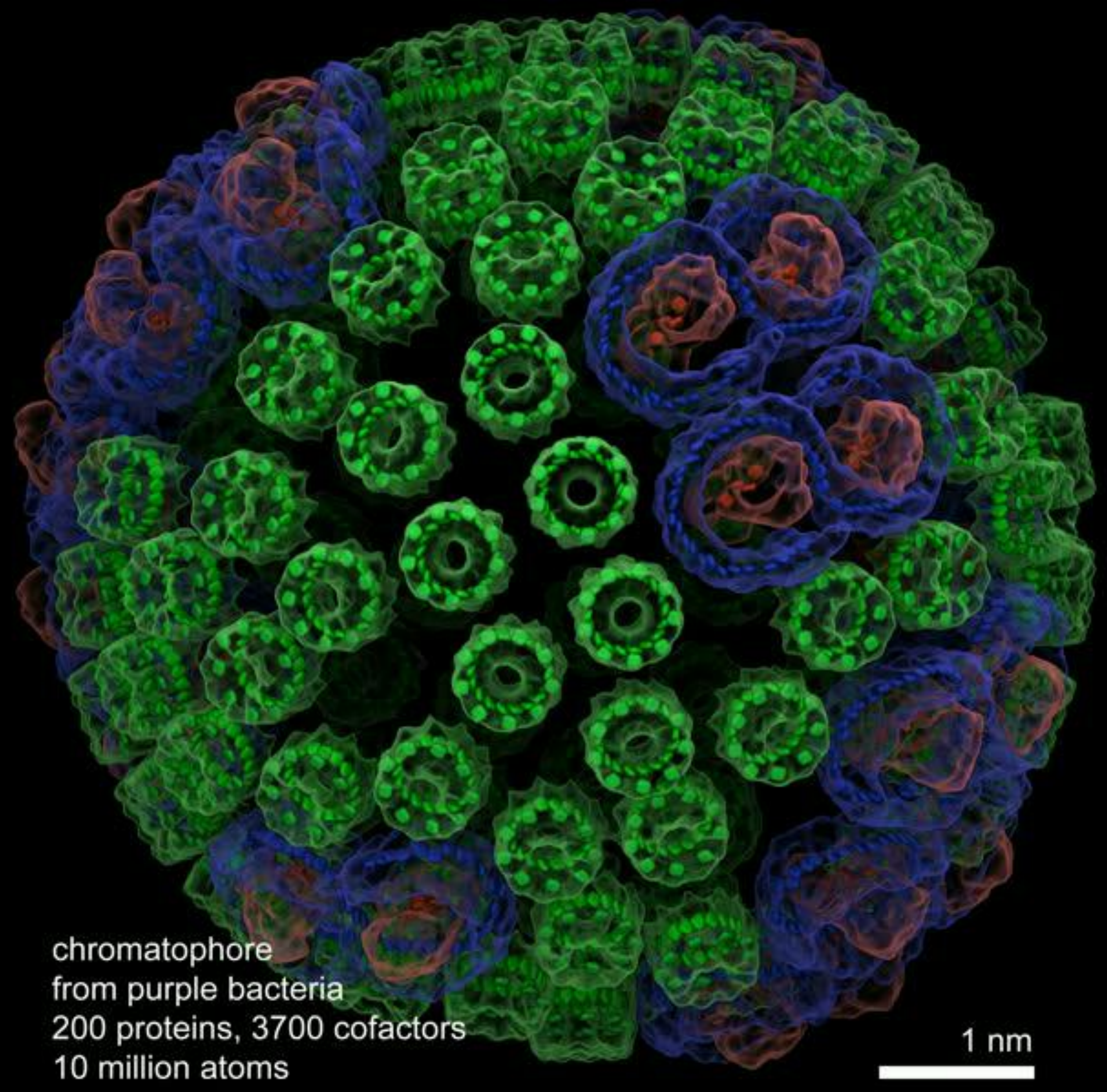


Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

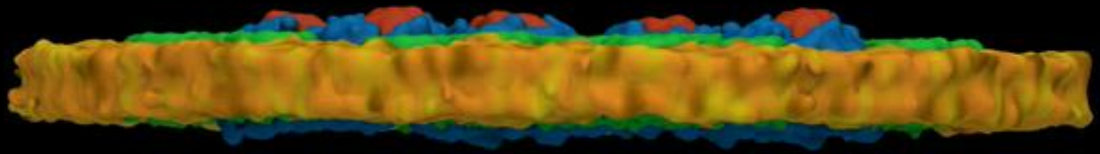
Ambient occlusion + two lights, 144 AO rays/hit

BW VMD/Tachyon Movie Generation



chromatophore
from purple bacteria
200 proteins, 3700 cofactors
10 million atoms

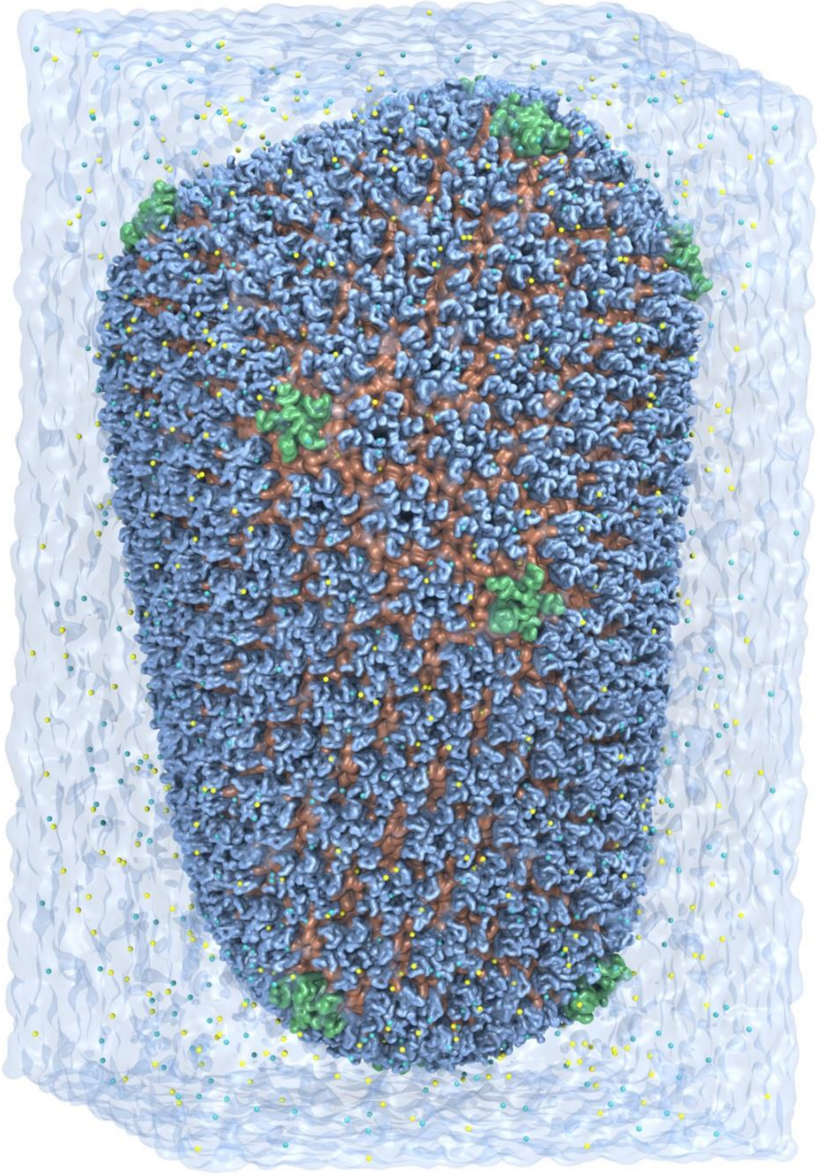
BW VMD/Tachyon Movie Generation



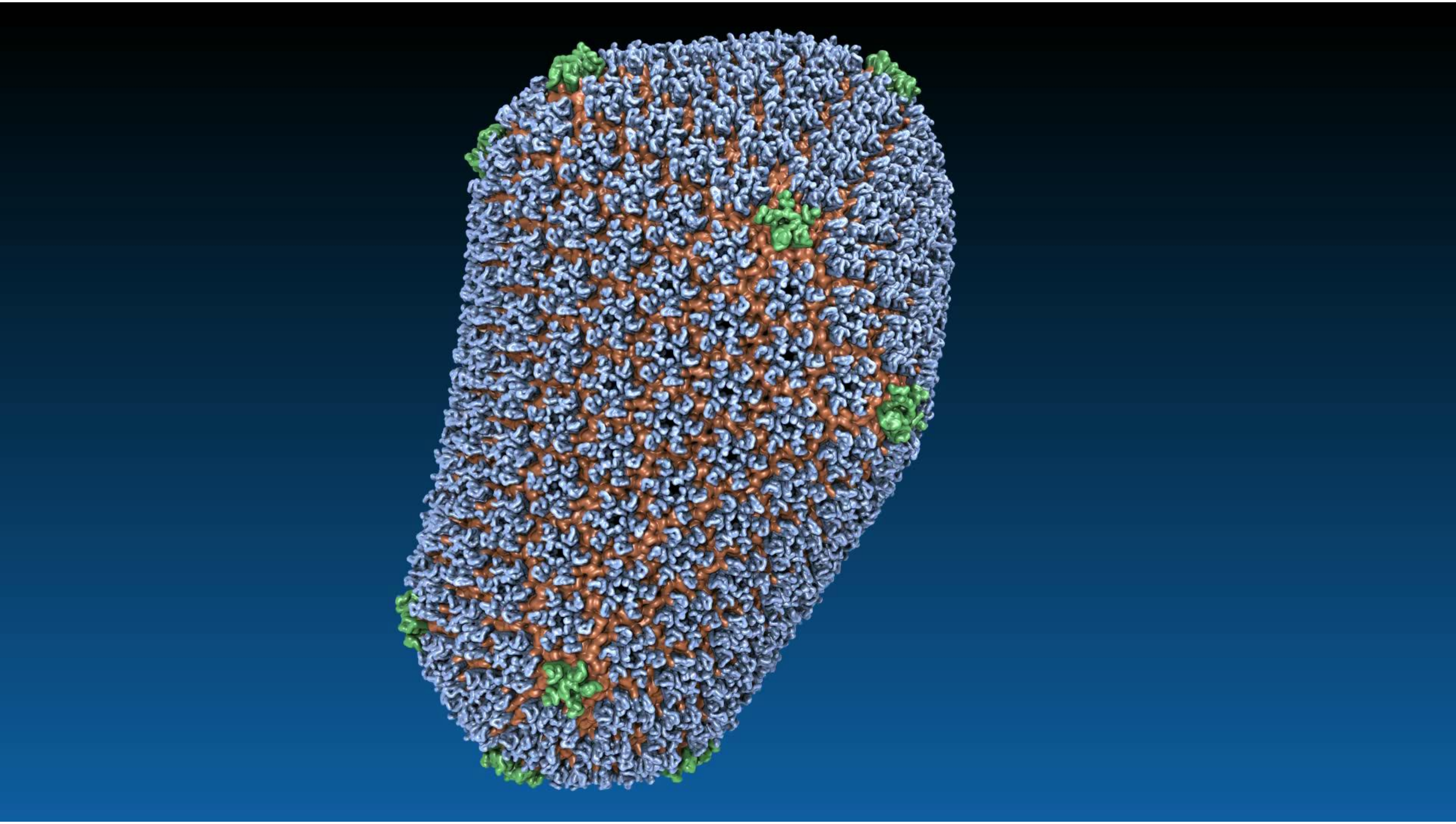
20 M atom chromatophore patch

GPU Ray Tracing of HIV-1 on Blue Waters

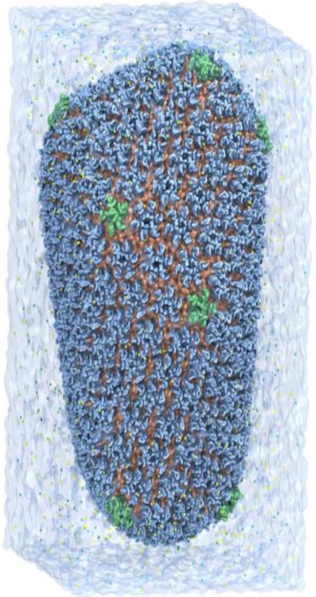
- **Ambient occlusion lighting**, shadows, transparency, antialiasing, depth cueing, **144 rays/pixel minimum**
- 64 million atom virus simulation
- 1000+ movie frames
- Surface generation and ray tracing stages each use >= 75% of GPU memory



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)

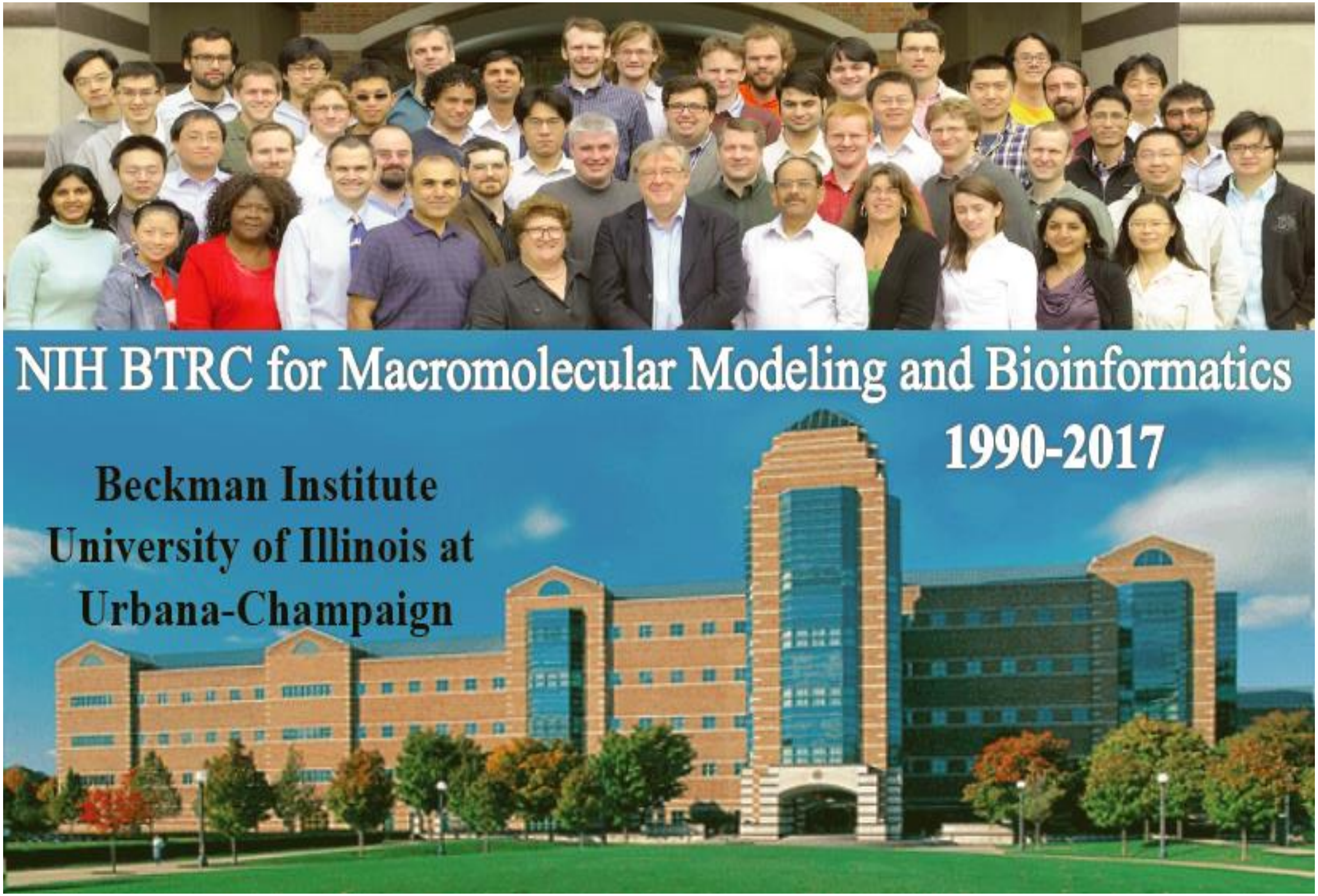
Cray XK7: 1x Opteron 62xx CPU (16-cores) + NVIDIA Tesla K20X

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
- NCSA Blue Waters Team
- NVIDIA CUDA Center of Excellence, University of Illinois at Urbana-Champaign
- Many of the staff at NVIDIA and Cray
- Funding:
  - NSF OCI 07-25070
  - NSF PRAC “The Computational Microscope”
  - NIH support: 9P41GM104601, 5R01GM098243-02


NIH BTRC for Macromolecular Modeling and Bioinformatics
1990-2017
Beckman Institute
University of Illinois at
Urbana-Champaign

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**.**

GPU Computing Publications
http://www.ks.uiuc.edu/Research/gpu/

- **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.

GPU Computing Publications
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.

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.