S5371—VMD: Visualization and Analysis of Biomolecular Complexes with GPU Computing

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

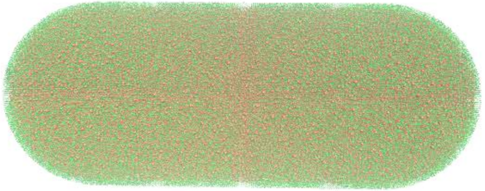
S5371, GPU Technology Conference

9:00-9:50, Room LL21C, San Jose Convention Center,

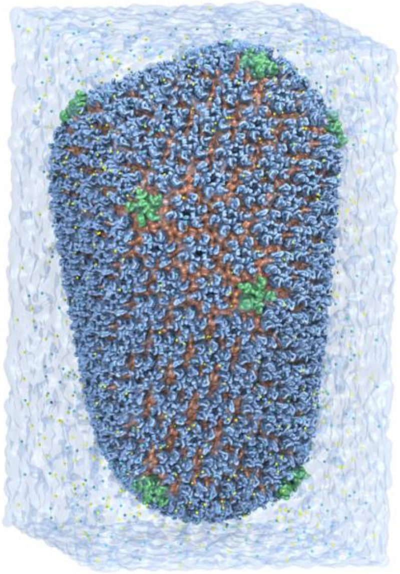
San Jose, CA, Wednesday March 18, 2015

VMD – “Visual Molecular Dynamics”

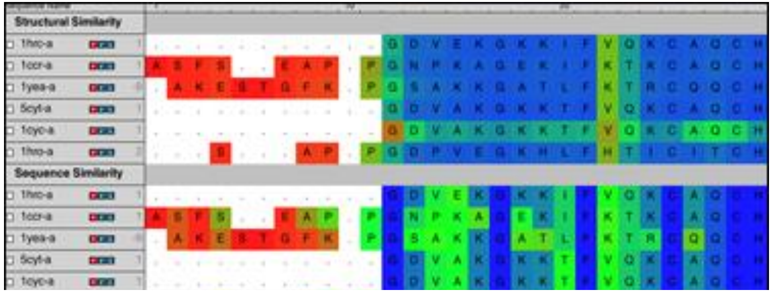
- Visualization and analysis of:
  - molecular dynamics simulations
  - particle systems and whole cells
  - cryoEM densities, volumetric data
  - quantum chemistry calculations
  - sequence information
- User extensible w/ scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Whole Cell Simulation

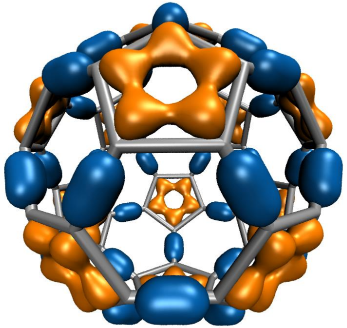


MD Simulations

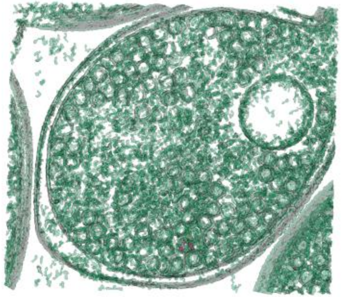


```
Structural Similarity
□ 1hrc-a  1  . . . . . . . . . . . G D V E K G K K I F V Q K C A Q C H
□ 1ccr-a  1  A S F S . . E A P . P G N P K A G E K I F K T K C A Q C H
□ 1yea-a  6  . A K E S T G F K . P G S A K K G A T L F K T R C Q Q C H
□ 5cyt-a  1  . . . . . . . . . . . G D V A K G K K T F V Q K C 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  2  . . . 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  6  . 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
```

Sequence Data



Quantum Chemistry

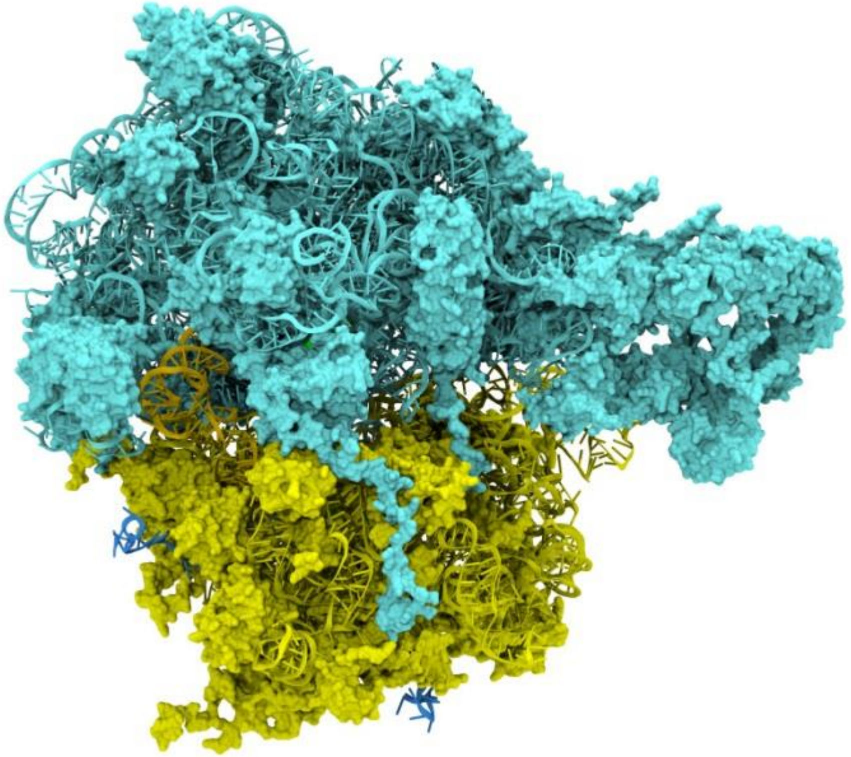


CryoEM, Cellular Tomography

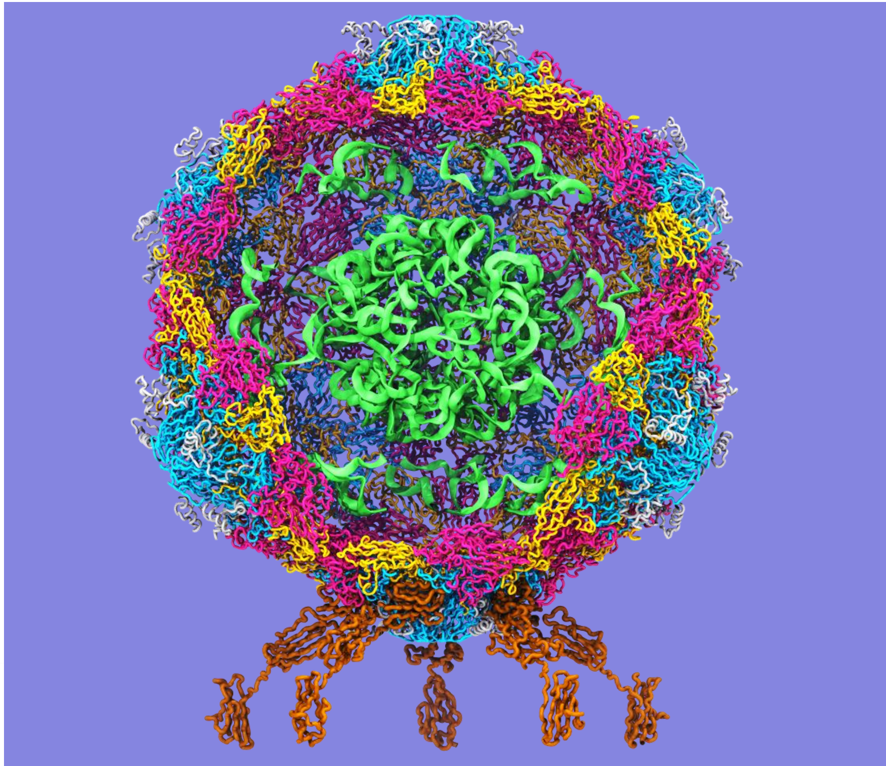
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics

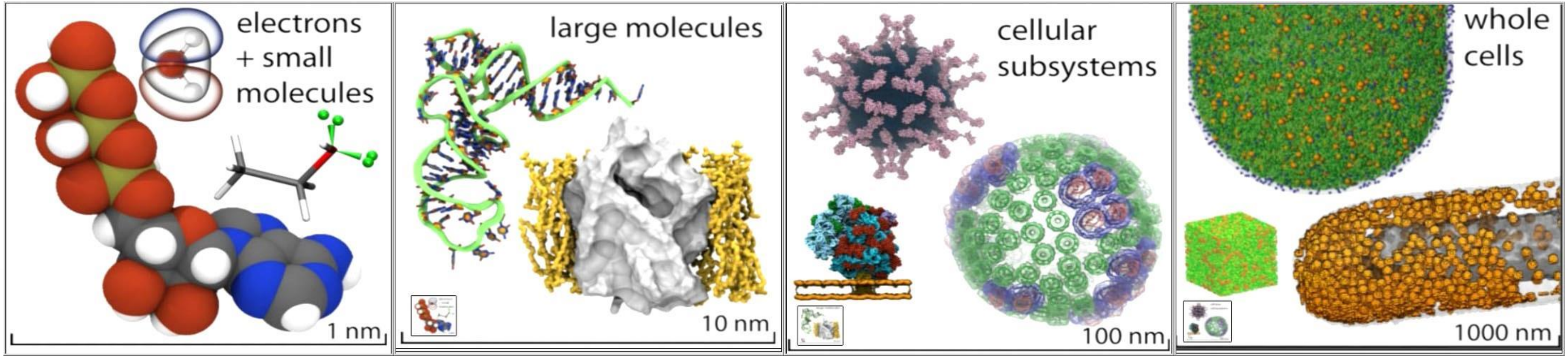


Poliovirus



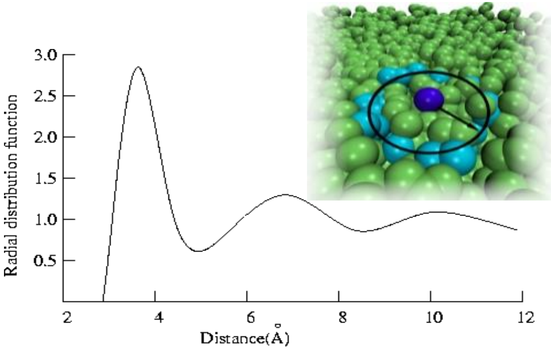
VMD Interoperability Serves Many Communities

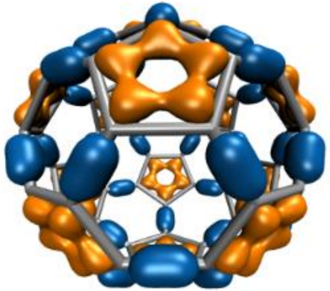
- VMD 1.9.1 user statistics:
  - 100,000 unique registered users from all over the world
- Uniquely interoperable with a broad range of tools: AMBER, CHARMM, CPMD, DL_POLY, GAMESS, GROMACS, HOOMD, LAMMPS, NAMD, and many more …
- Supports key data types, file formats, and databases, e.g. electron microscopy, quantum chemistry, MD trajectories, sequence alignments, super resolution light microscopy
- Incorporates tools for simulation preparation, visualization, and analysis



CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

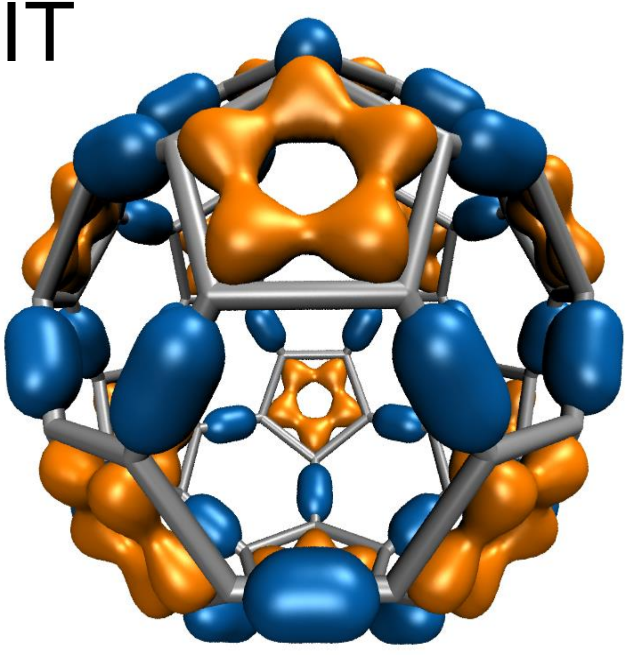
VMD GPU-Accelerated Feature or GPU Kernel	**Exemplary speedup vs. contemporary 4-core CPU**
Molecular orbital display	**30x**
Radial distribution function	**23x**
Molecular surface display	**15x**
Electrostatic field calculation	**11x**
Ray tracing w/ shadows, AO lighting	**7x**
cryoEM cross correlation quality-of-fit	**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





Molecular Orbitals w/ NVRTC JIT

- Visualization of MOs aids in understanding the chemistry of molecular system
- MO spatial distribution is correlated with probability density for an electron(s)
- **Animation** of (classical mechanics) molecular dynamics trajectories provides insight into simulation results
  - To do the same for QM or QM/MM simulations MOs must be computed at **10 FPS** or more
  - **Large GPU speedups (up to 30x vs. 4-core CPU)** over existing tools makes this possible!
- **Run-time code generation** (JIT) and compilation via **CUDA 7.0 NVRTC** enable further optimizations and the **highest performance to date: 1.8x faster than previous best result**



C_{60}

High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs. J. E. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Processing Units (GPGPU-2), ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.

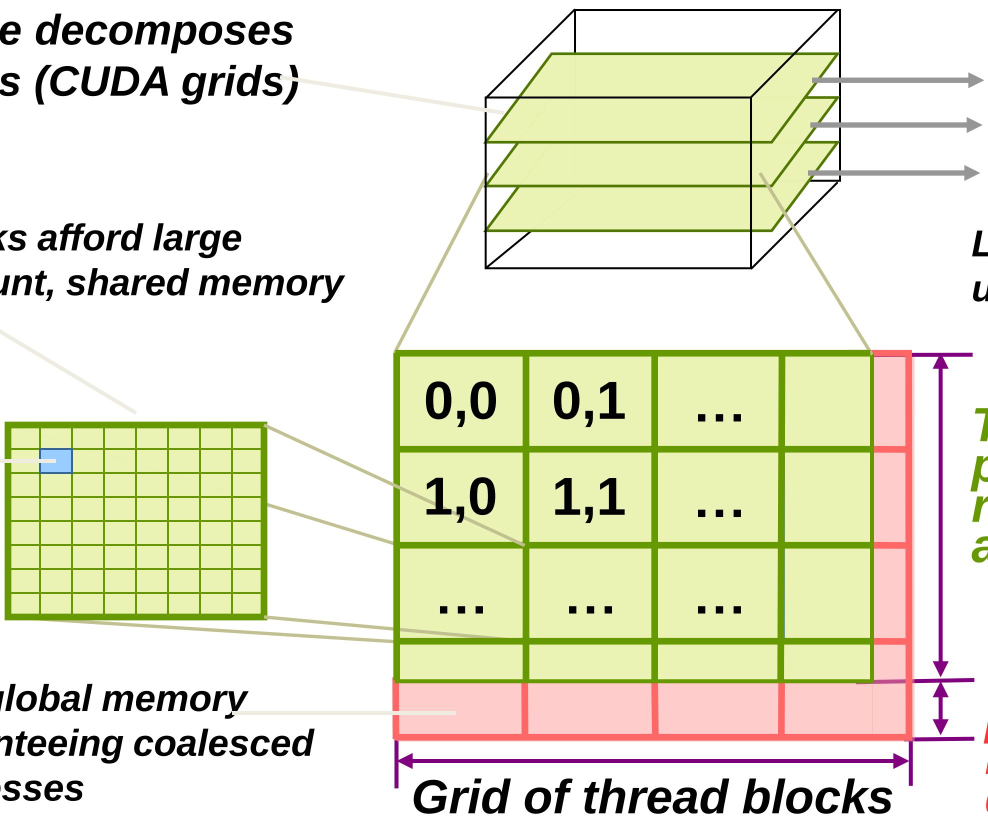
MO GPU Parallel Decomposition

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

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

Each thread computes one MO lattice point.

Padding optimizes global memory performance, guaranteeing coalesced global memory accesses



Lattice computed using multiple GPUs

Threads producing results that are used

Threads producing results that are discarded

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

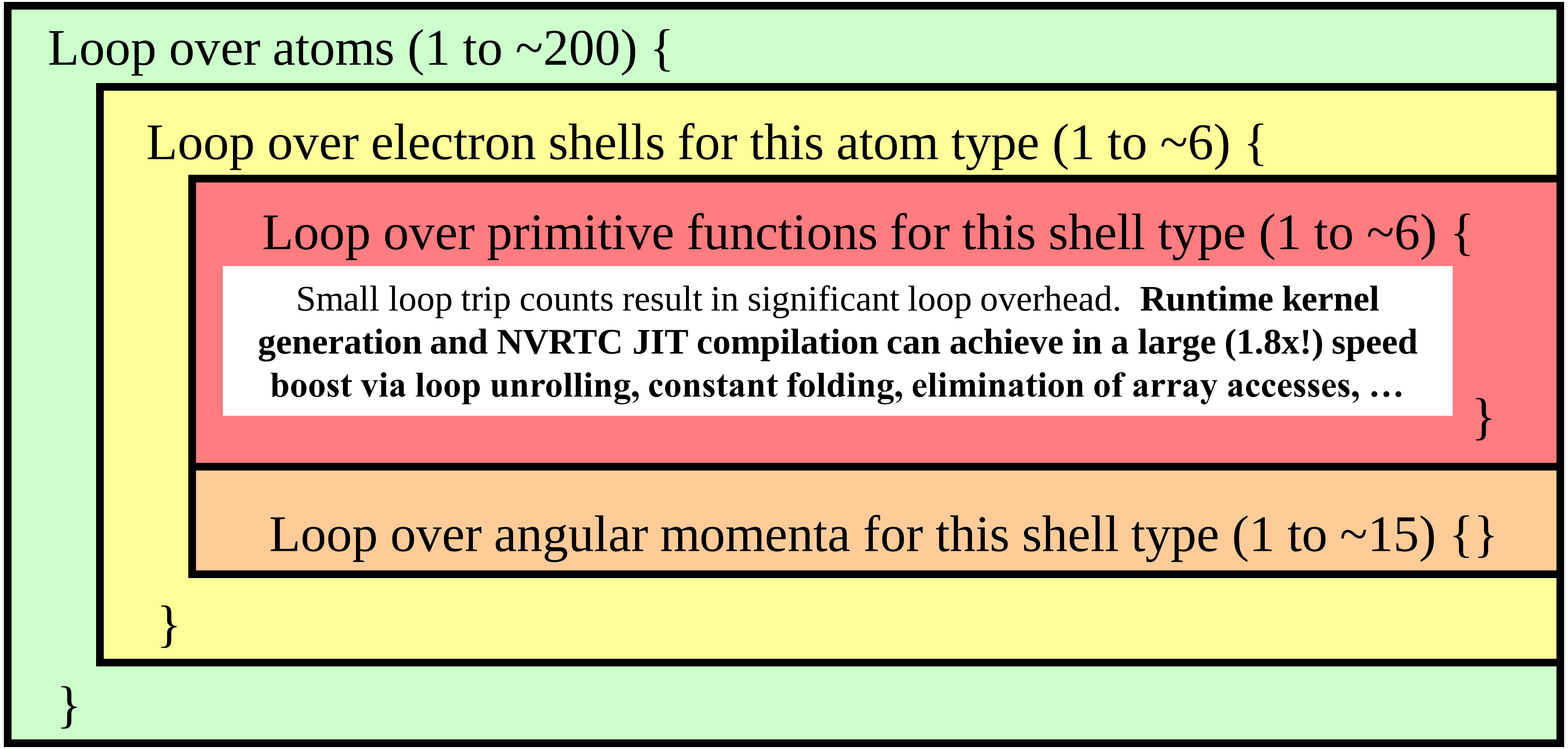
Loop over primitives: largest component of runtime, due to **expf()**

Loop over angular momenta

(unrolled in real code)

MO Kernel Structure, Opportunity for NRTC JIT…

Data-driven execution, but representative loop trip counts in (…)



Loop over atoms (1 to ~200) {

Loop over electron shells for this atom type (1 to ~6) {

Loop over primitive functions for this shell type (1 to ~6) {

Small loop trip counts result in significant loop overhead. **Runtime kernel generation and NVRTC JIT compilation can achieve in a large (1.8x!) speed boost via loop unrolling, constant folding, elimination of array accesses, …**

}

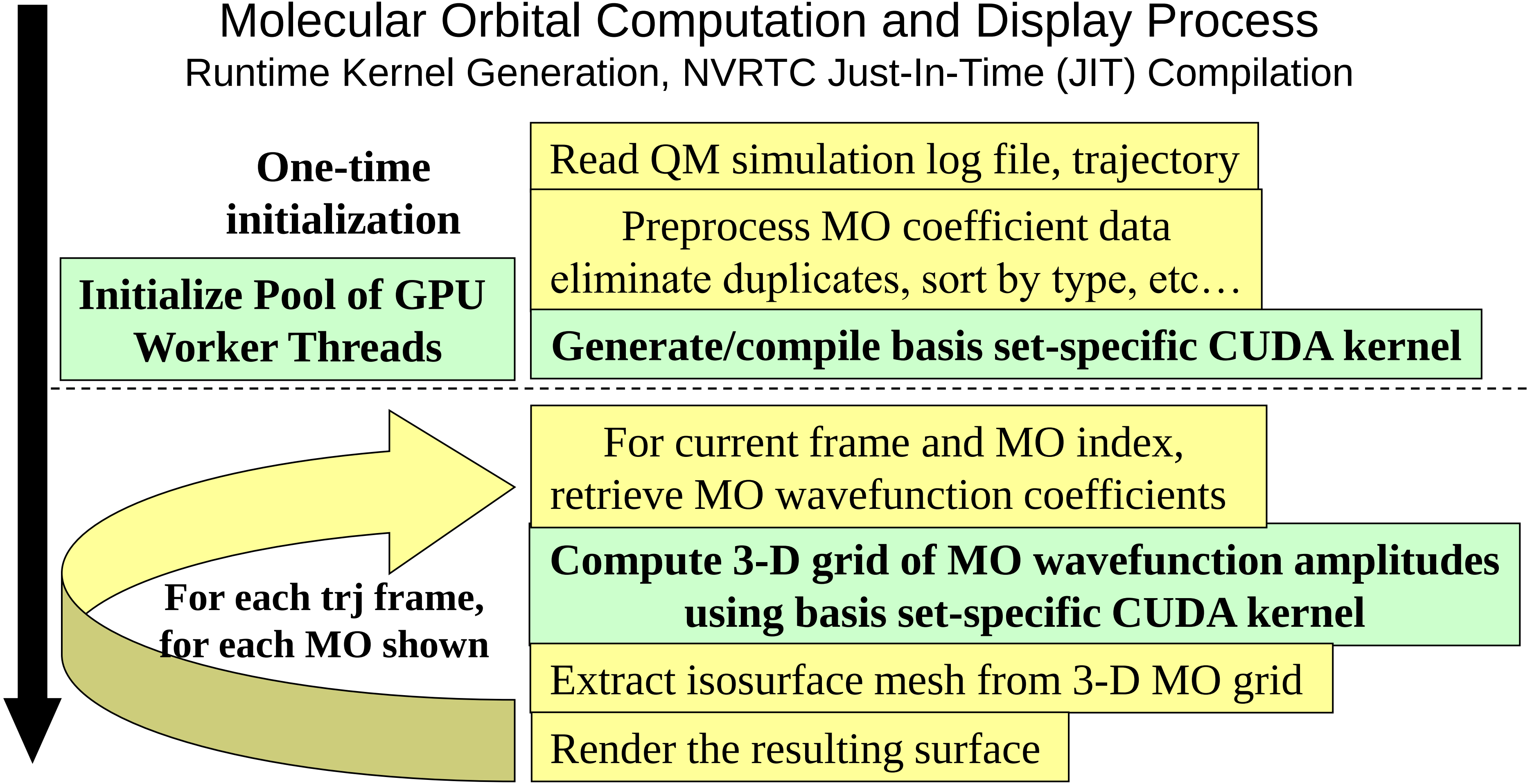
Loop over angular momenta for this shell type (1 to ~15) {}

}

}

Molecular Orbital Computation and Display Process

Runtime Kernel Generation, NVRTC Just-In-Time (JIT) Compilation



One-time initialization

Initialize Pool of GPU Worker Threads

Read QM simulation log file, trajectory

Preprocess MO coefficient data eliminate duplicates, sort by type, etc…

Generate/compile basis set-specific CUDA kernel

For each trj frame, for each MO shown

For current frame and MO index, retrieve MO wavefunction coefficients

Compute 3-D grid of MO wavefunction amplitudes using basis set-specific CUDA kernel

Extract isosurface mesh from 3-D MO grid

Render the resulting surface

```
for (shell=0; shell < maxshell; shell++)  {
  float contracted_gto = 0.0f;


  // Loop over the Gaussian primitives of CGTO
  int maxprim = const_num_prim_per_shell[shell_counter];
  int shell_type = const_shell_symmetry[shell_counter];
  for (prim=0; prim < maxprim;  prim++) {
    float exponent          = const_basis_array[prim_counter      ];
    float contract_coeff = const_basis_array[prim_counter + 1];
    contracted_gto += contract_coeff  * expf(-exponent*dist2);
    prim_counter += 2;
  }
```

General loop-based data-dependent MO CUDA kernel

Runtime-generated data-specific MO CUDA kernel compiled via **CUDA 7.0 NVRTC** JIT…

```
contracted_gto = 1.832937 * expf(-7.868272*dist2);
contracted_gto += 1.405380 * expf(-1.881289*dist2);
contracted_gto += 0.701383 * expf(-0.544249*dist2);
```

1.8x Faster

```
  for (shell=0; shell < maxshell; shell++)  {
   float contracted_gto = 0.0f;

   // Loop over the Gaussian primitives of CGTO
   int maxprim = const_num_prim_per_shell[shell_counter];
   int shell_type = const_shell_symmetry[shell_counter];
   for (prim=0; prim < maxprim;  prim++) {
    float exponent         = const_basis_array[prim_counter      ];
    float contract_coeff = const_basis_array[prim_counter + 1];
    contracted_gto += contract_coeff  * expf(-exponent*dist2);
    prim_counter += 2;
   }

   float tmpshell=0;
   switch (shell_type) {
    case S_SHELL:
     value += const_wave_f[ifunc++] * contracted_gto;
     break;
[…..]
    case D_SHELL:
     tmpshell += const_wave_f[ifunc++] * xdist2;
     tmpshell += const_wave_f[ifunc++] * ydist2;
     tmpshell += const_wave_f[ifunc++] * zdist2;
     tmpshell += const_wave_f[ifunc++] * xdist * ydist;
```

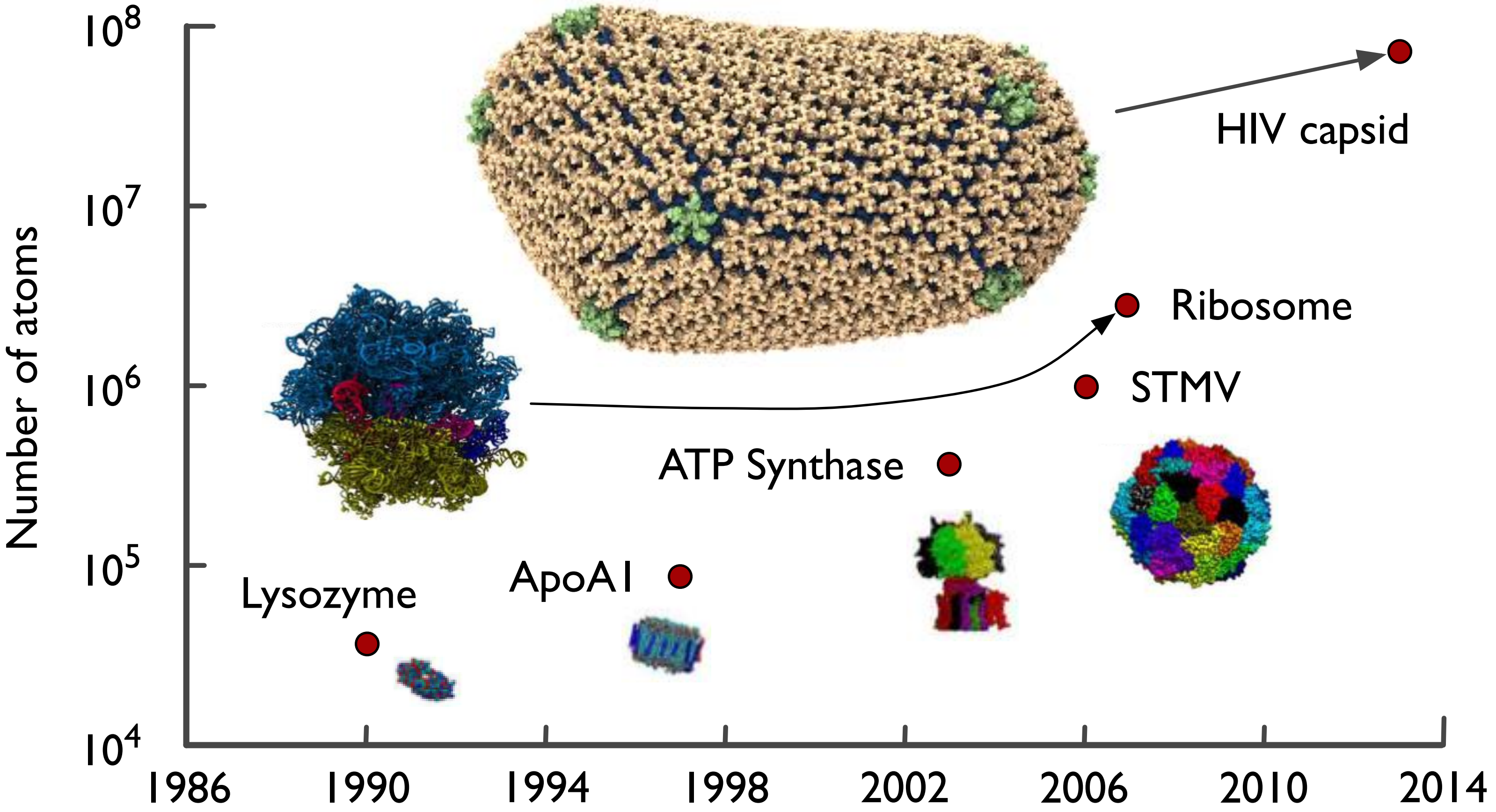
General loop-based data-dependent MO CUDA kernel

Runtime-generated data-specific MO CUDA kernel compiled via **CUDA 7.0 NVRTC** JIT…

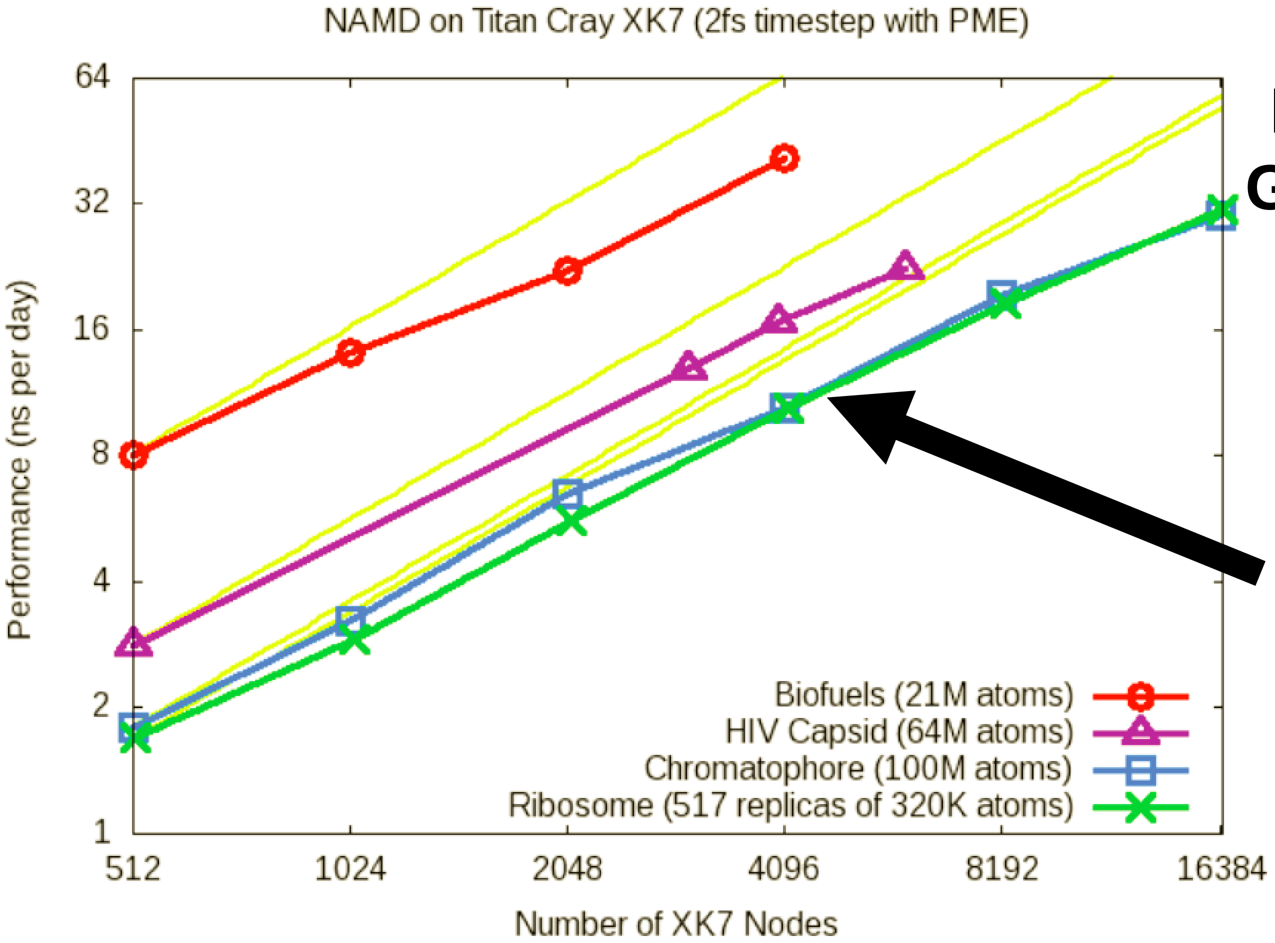
1.8x Faster

```
contracted_gto = 1.832937 * expf(-7.868272*dist2);
contracted_gto += 1.405380 * expf(-1.881289*dist2);
contracted_gto += 0.701383 * expf(-0.544249*dist2);
// P_SHELL
tmpshell = const_wave_f[ifunc++] * xdist;
tmpshell += const_wave_f[ifunc++] * ydist;
tmpshell += const_wave_f[ifunc++] * zdist;
value += tmpshell * contracted_gto;

contracted_gto = 0.187618 * expf(-0.168714*dist2);
// S_SHELL
value += const_wave_f[ifunc++] * contracted_gto;

contracted_gto = 0.217969 * expf(-0.168714*dist2);
// P_SHELL
tmpshell = const_wave_f[ifunc++] * xdist;
tmpshell += const_wave_f[ifunc++] * ydist;
tmpshell += const_wave_f[ifunc++] * zdist;
value += tmpshell * contracted_gto;

contracted_gto = 3.858403 * expf(-0.800000*dist2);
// D_SHELL
tmpshell = const_wave_f[ifunc++] * xdist2;
tmpshell += const_wave_f[ifunc++] * ydist2;
```

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



NAMD Titan XK7 Performance August 2013



NAMD XK7 vs. XE6
GPU Speedup: 2x-4x

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

VMD Petascale Visualization and Analysis

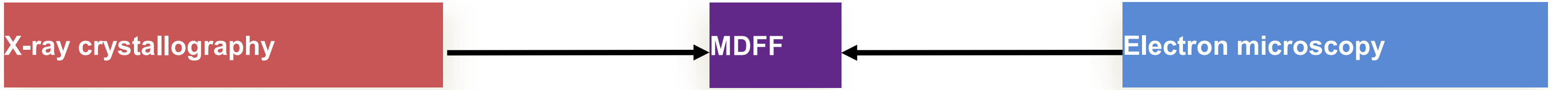
- Analyze/visualize large trajectories too large to transfer off-site:
  - User-defined parallel analysis operations, data types
  - Parallel rendering, movie making
- Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis:
  - **GPU accelerated trajectory analysis w/ CUDA**
  - **OpenGL and GPU ray tracing for visualization and movie rendering**
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 nodes – can read in **231 TB in 15 minutes!**

Parallel VMD currently available on:

ORNL Titan, NCSA Blue Waters, Indiana Big Red II, CSCS Piz Daint, and similar systems

NCSA Blue Waters Hybrid Cray XE6 / XK7
22,640 XE6 dual-Opteron CPU nodes
4,224 XK7 nodes w/ Telsa K20X GPUs

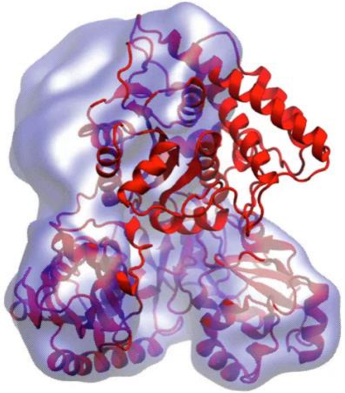
Molecular Dynamics Flexible Fitting (MDFF)


X-ray crystallography

MDFF

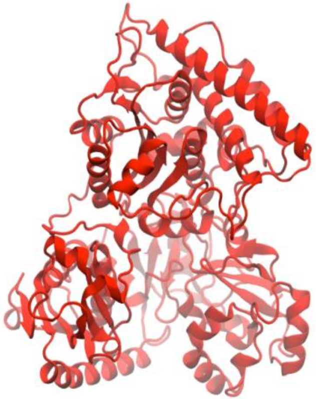
Electron microscopy

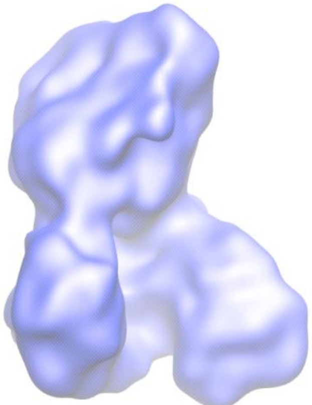
APS at Argonne



FEI microscope

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

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

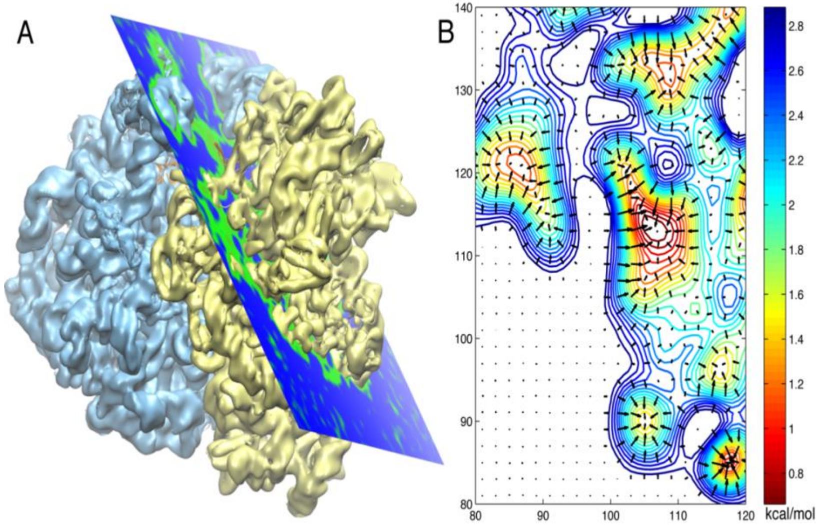
An external potential derived from the EM map is defined on a grid as

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

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

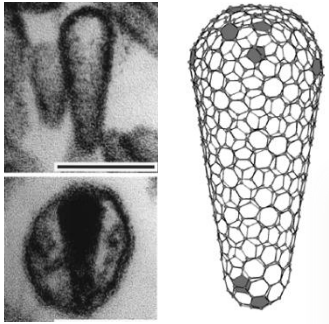
A mass-weighted force is then applied to each atom

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

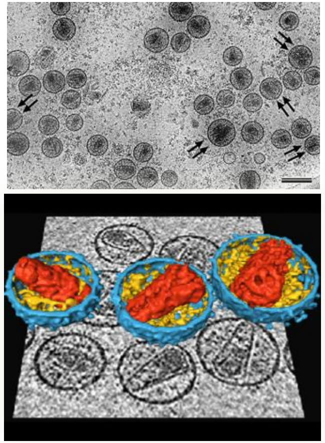


Structural Route to the all-atom HIV-1 Capsid

1st TEM (1999)



1st tomography (2003)

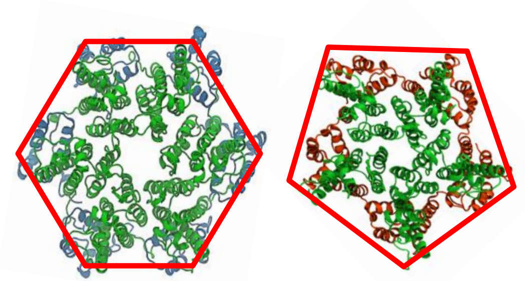


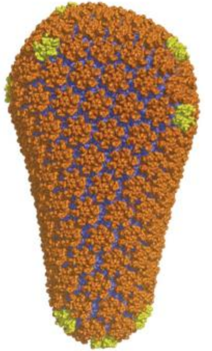
Ganser et al. *Science*, 1999

Briggs et al. *EMBO J*, 2003

Briggs et al. *Structure*, 2006

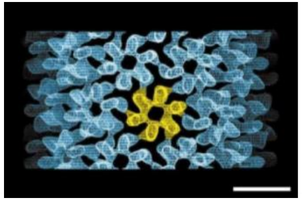
Crystal structures of separated hexamer and pentamer





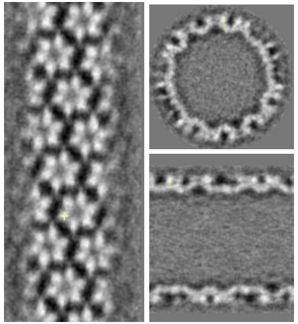
Pornillos et al. , *Cell* 2009, *Nature* 2011

hexameric tubule



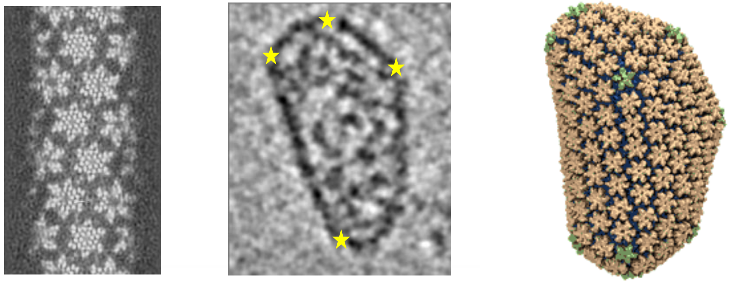
Li et al., *Nature*, 2000

cryo-ET (2006)



Byeon et al., *Cell* 2009

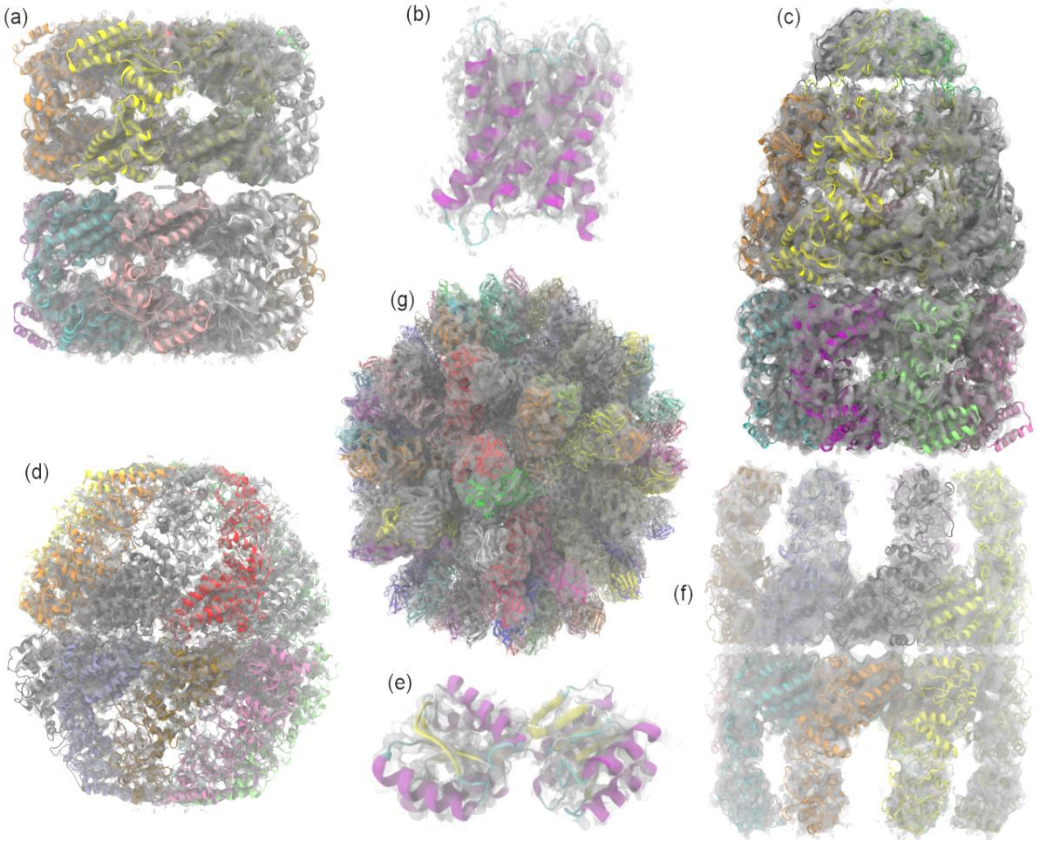
High res. EM of hexameric tubule, tomography of capsid, **all-atom model of capsid by MDFF w/ NAMD & VMD, NSF/NCSA Blue Waters computer at Illinois**



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

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

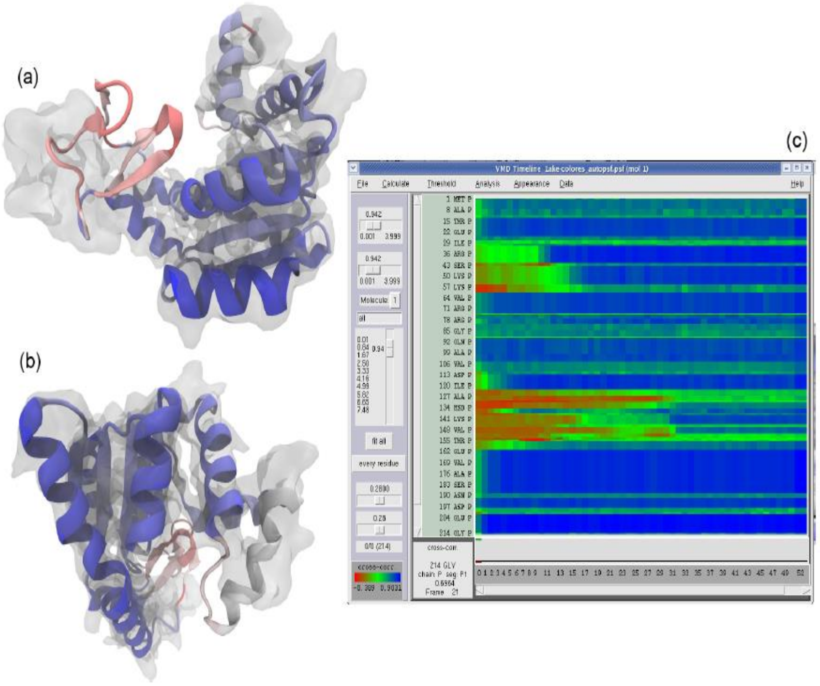
Compute Pearson correlation to evaluate the fit of a reference cryo-EM density map with a **simulated density map** produced from an **all-atom structure**.



GPUs Can Reduce MDFF 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*…

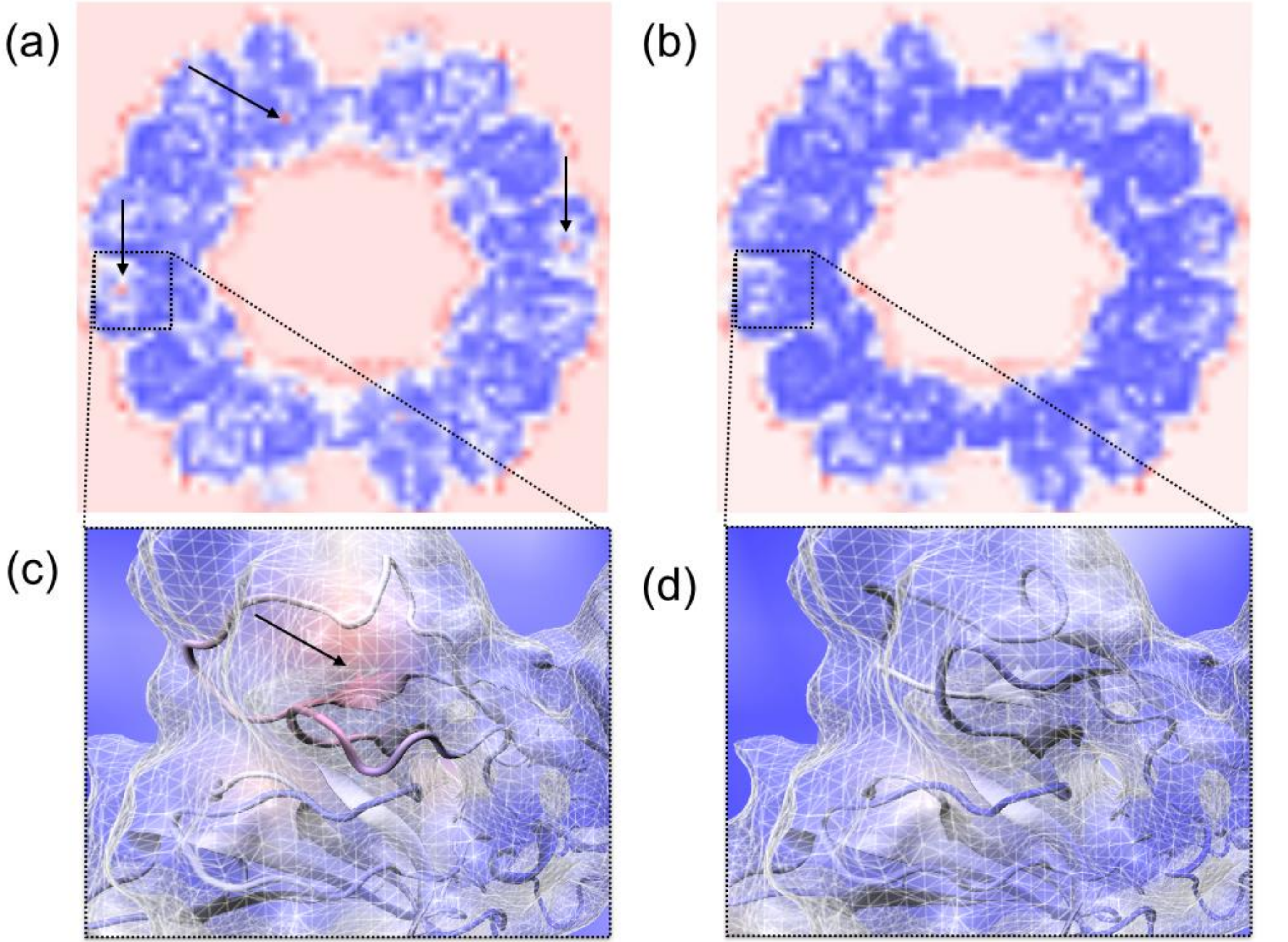
GPU-accelerated petascale supercomputers enable analyses that were previously impractical, allowing detailed study of very large structures such as viruses



GPU-accelerated MDFF Cross Correlation Timeline

Regions with poor fit

Regions with good fit

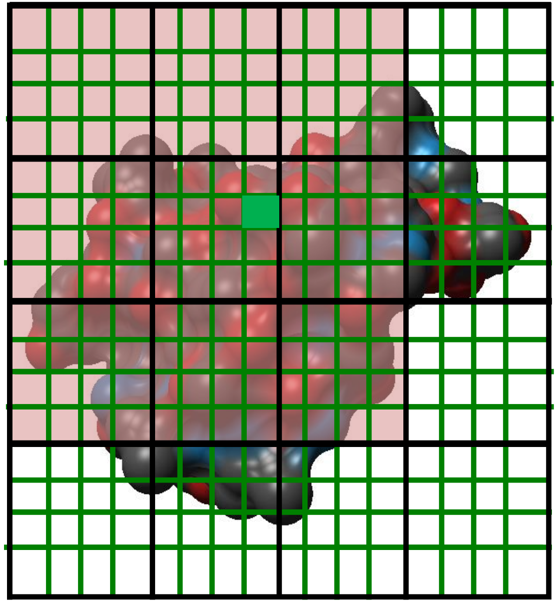

(a)
(b)
(c)
(d)

MDFF Density Map Algorithm

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

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

- Truncated Gaussian and spatial acceleration grid ensure linear time-complexity



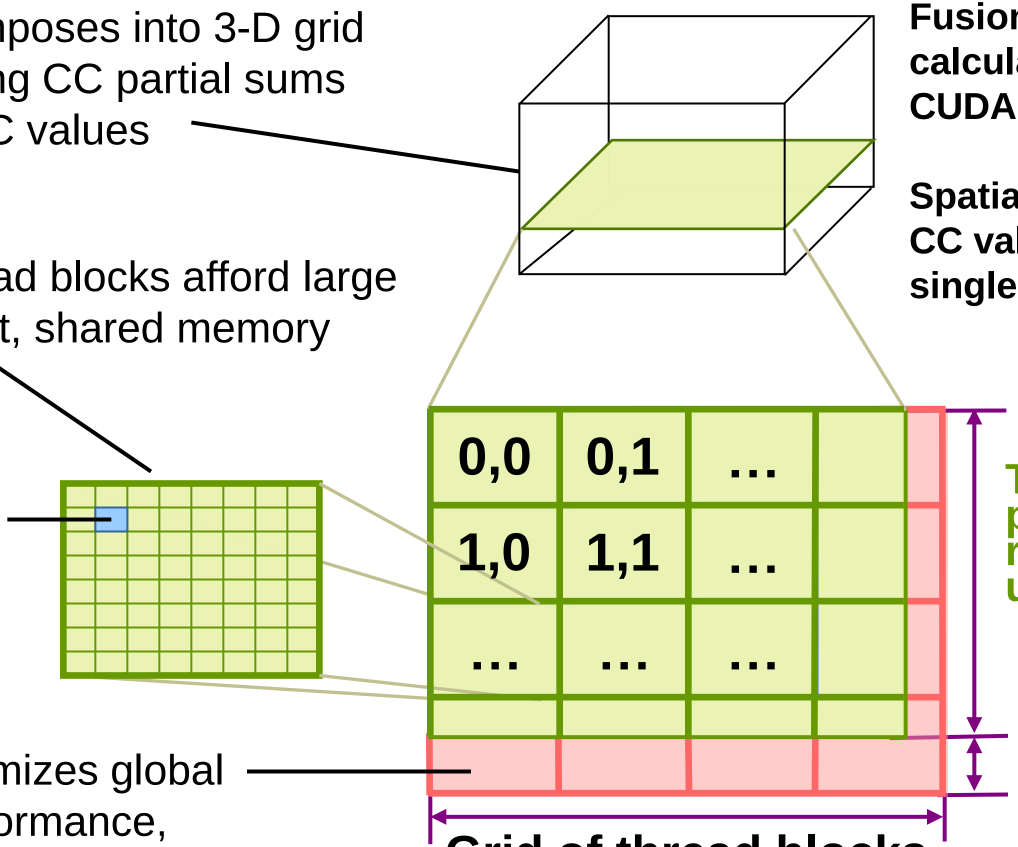
3-D density map lattice point and the neighboring spatial acceleration cells it references

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

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

Grid of thread blocks

Padding optimizes global memory performance, guaranteeing coalesced global memory accesses

Fusion of density and CC calculations into a single CUDA kernel!!!

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

VMD GPU Cross Correlation Performance

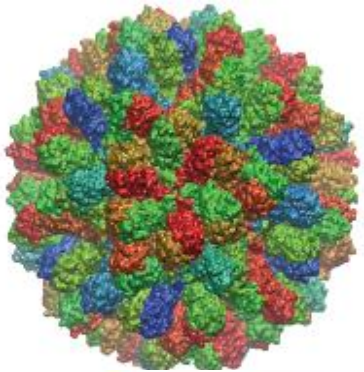
	RHDV	Mm-cpn open	GroEL	Aquaporin
Resolution (Å)	6.5	8	4	3
Atoms	702K	61K	54K	1.6K
VMD-CUDA Quadro K6000	0.458s 34.6x	0.06s 25.7x	0.034s 36.8x	0.007s 55.7x
VMD-CPU-SSE 32-threads, 2x Xeon E5-2687W	0.779s 20.3x	0.085s 18.1x	0.159s 7.9x	0.033s 11.8x
Chimera 1-thread Xeon E5-2687W	15.86s 1.0x	1.54s 1.0x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

GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting. J. E. Stone, R. McGreevy, B. Isralewitz, and K. Schulten. Faraday Discussions 169:265-283, 2014.

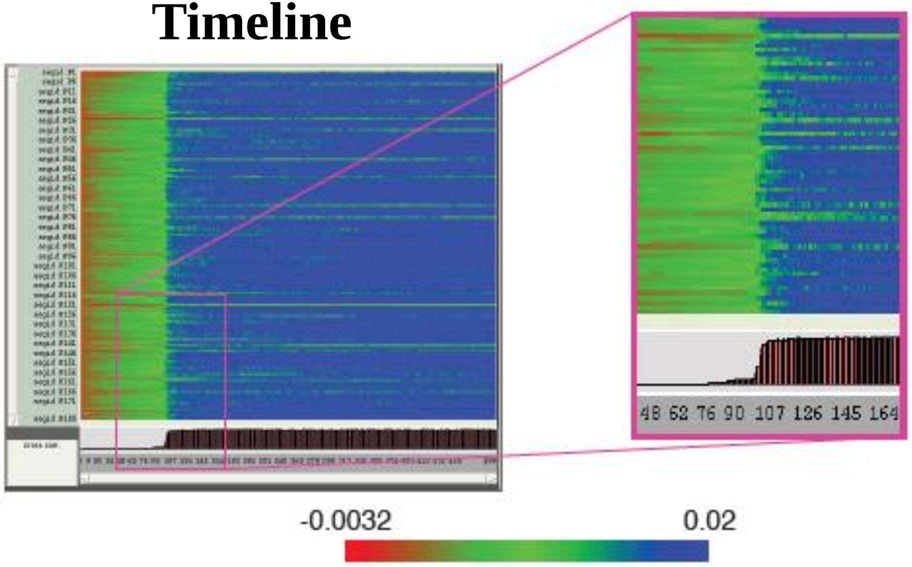
VMD RHDV Cross Correlation Timeline on Cray XK7

	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 CC calculation on a workstation!



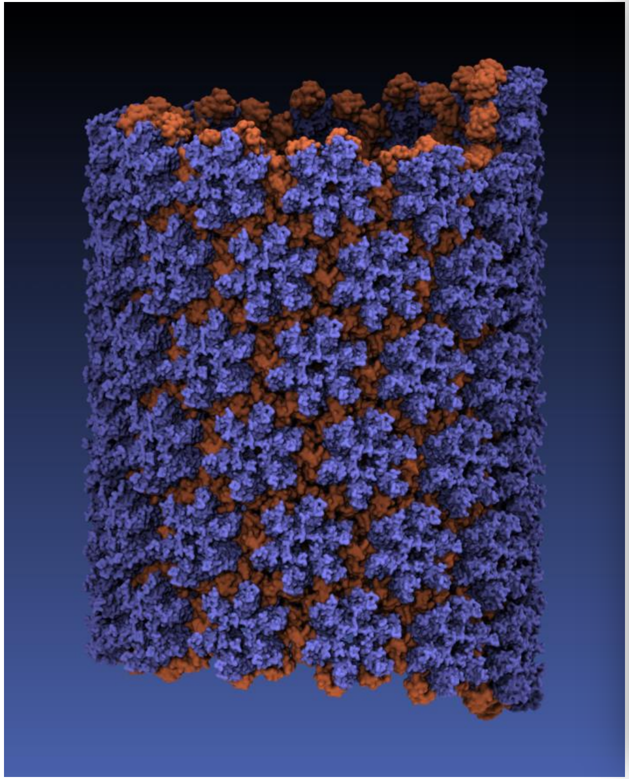
RHDV
Group-relative CC Timeline



Visualization Goals, Challenges

- Increased GPU acceleration for visualization of **petascale molecular dynamics trajectories**
- **Overcome GPU memory capacity limits**, enable high quality visualization of >100M atom systems
- Use GPU to accelerate not only interactive-rate visualizations, but also photorealistic ray tracing with **artifact-free ambient occlusion lighting**, etc.
- Maintain **ease-of-use**, intimate link to VMD analytical features, atom selection language, etc.

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

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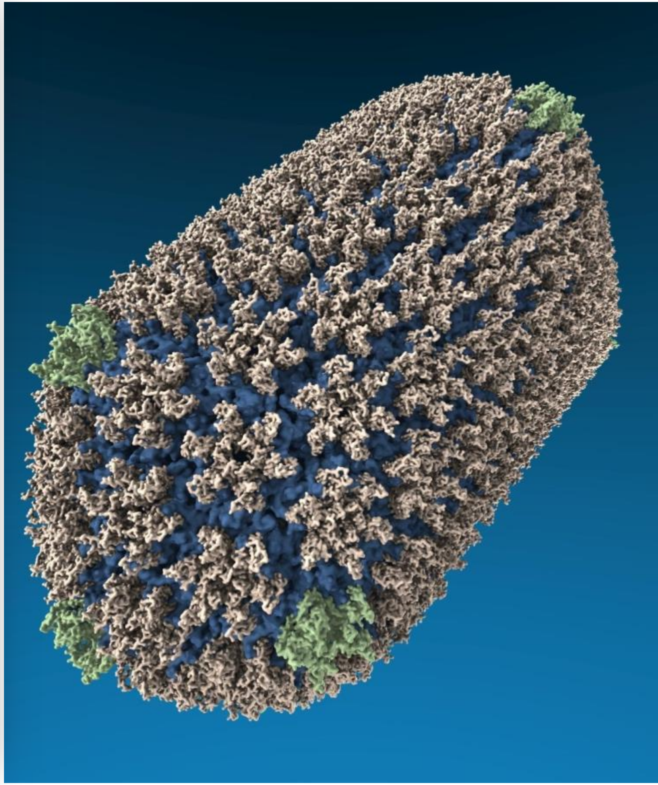
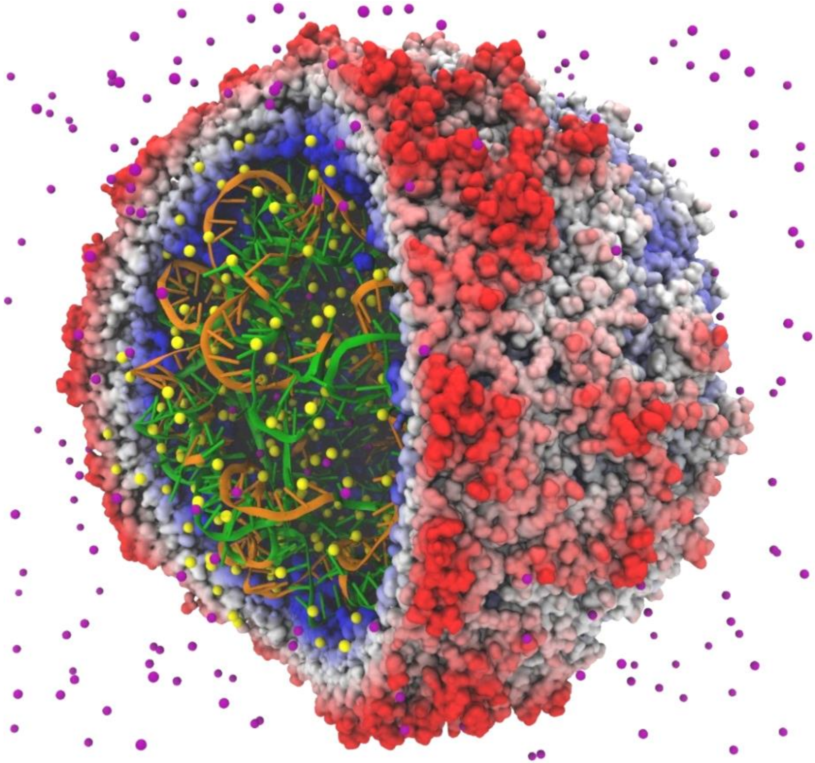


All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters

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

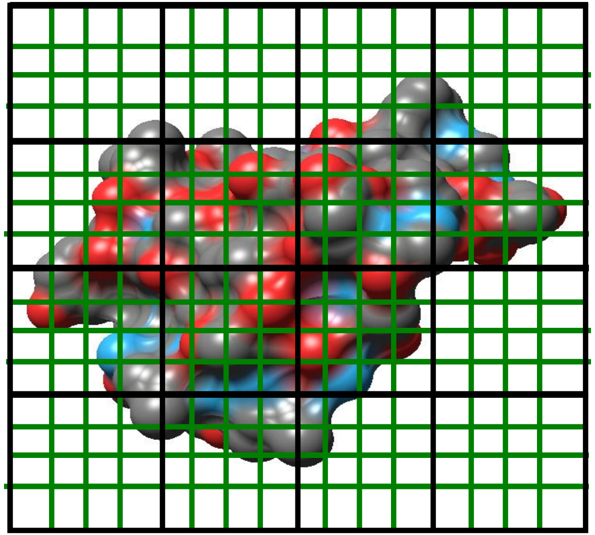
Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories.
M. Krone, J. E. Stone, T. Ertl, K. Schulten. *EuroVis Short Papers*, pp. 67-71, 2012

VMD 1.9.2 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
- **Centralized GPU memory management** among all molecules+representations: enables graceful eviction of surface data for ray tracing, or other GPU-memory-capacity-constrained operations



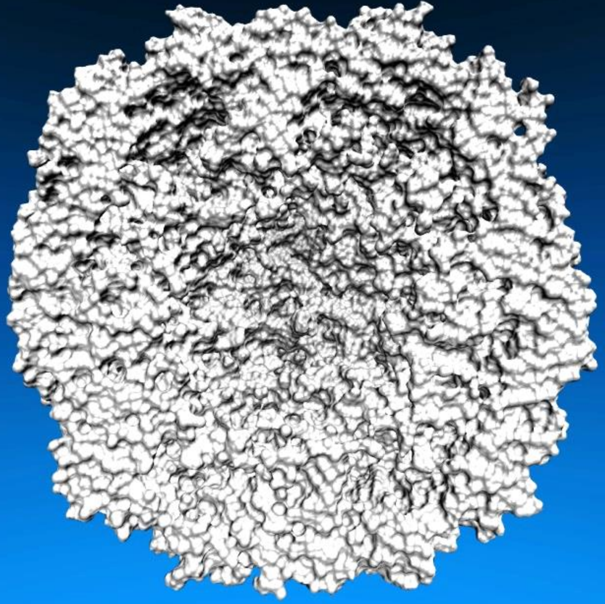
3-D density map lattice, spatial acceleration grid, and extracted surface

VMD GPU-Accelerated Ray Tracing Engine

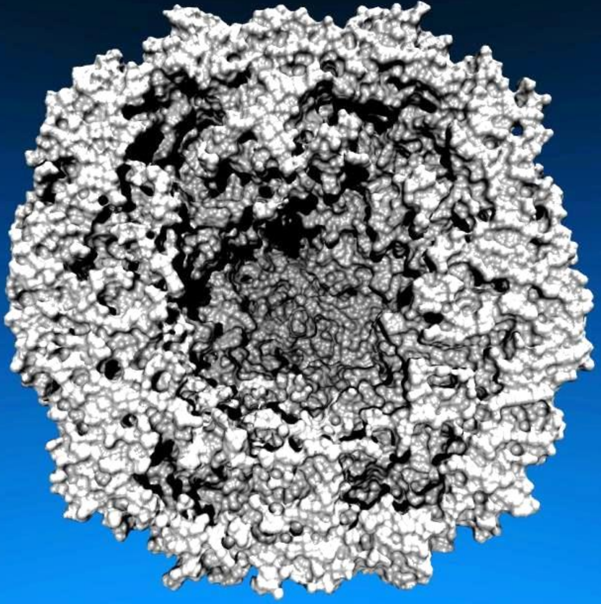
- Complementary to VMD OpenGL GLSL renderer that uses fast, low-cost, interactivity-oriented rendering techniques
- Key ray tracing benefits:
  - Ambient occlusion lighting and hard shadows
  - High quality transparent surfaces
  - Depth of field focal blur and similar optical effects
  - Mirror reflection
  - Single-pass stereoscopic rendering
  - Special cameras: planetarium dome master format

Lighting Comparison, STMV Capsid

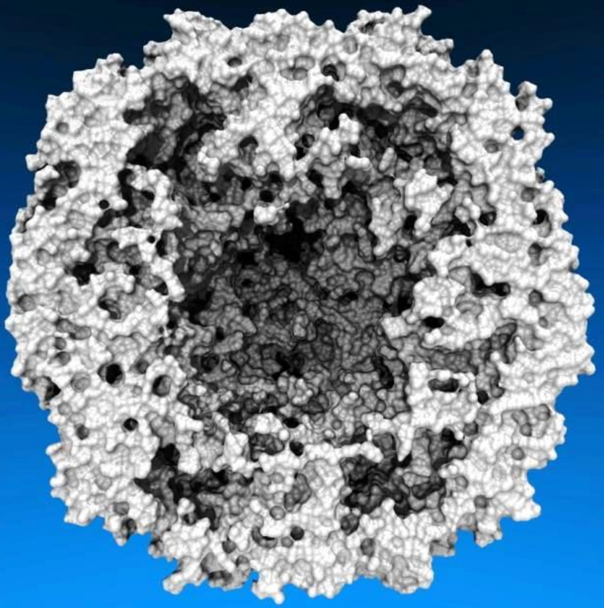
Two lights, no shadows



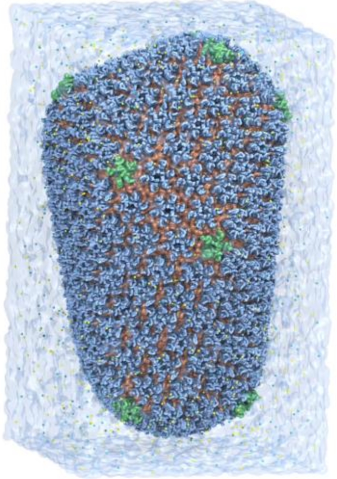
Two lights, hard shadows, 1 shadow ray per light



Ambient occlusion + two lights, 144 AO rays/hit



VMD 1.9.2 HIV-1 Parallel Movie Rendering on Blue Waters Cray XE6/XK7



HIV-1 “HD” 1920x1080 movie rendering:

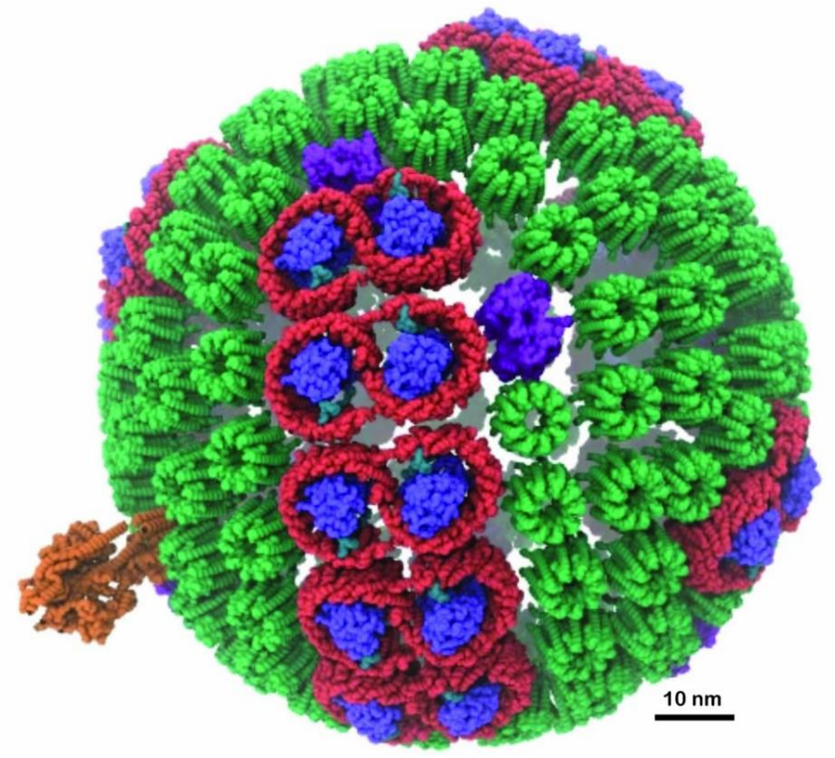
GPUs speed up geom+ray tracing by **up to eight times**

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**

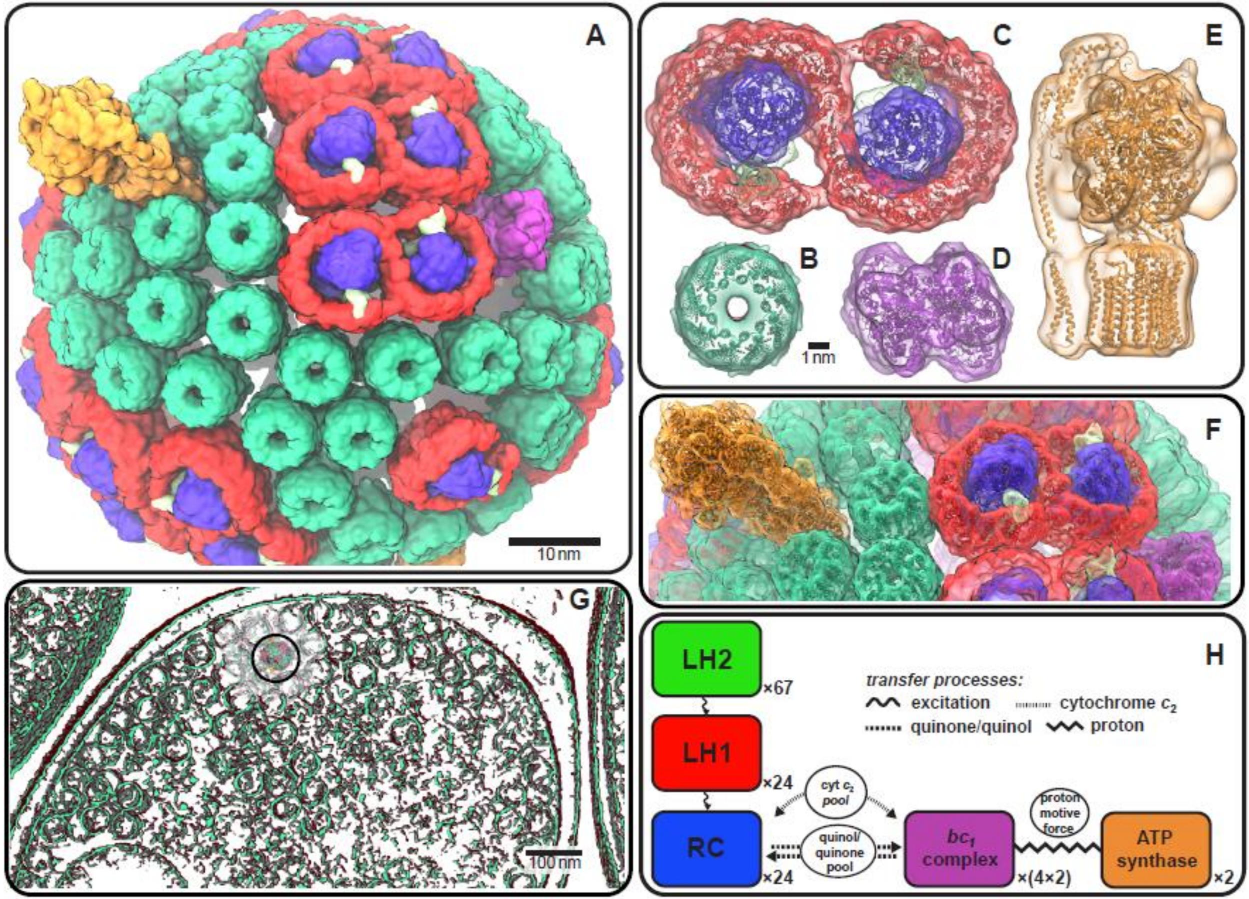
GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms, Stone et al. UltraVis'13: Eighth Workshop on Ultrascale Visualization Proceedings, 2013.

Photosynthetic Chromatophore of Purple Bacteria

- Purple bacteria live in light-starved conditions at the bottom of ponds, with ~1% sunlight
- Chromatophore system
  - 100M atoms, 700 Å^3 volume
  - Contains over 100 proteins, ~3,000 bacteriochlorophylls for collection of photons
  - Energy conversion process synthesizes ATP, which fuels cells…

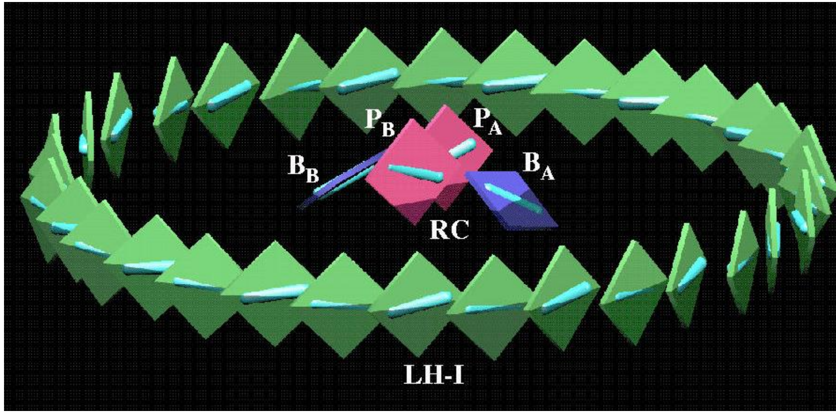


- Movie sums up ~40 papers and 37 years of work by Schulten lab and collaborators
- Driving NAMD and VMD software design:
  - Two decades of simulation, analysis, and visualization of individual chromatophore components w/ NAMD+VMD



Role of Visualization

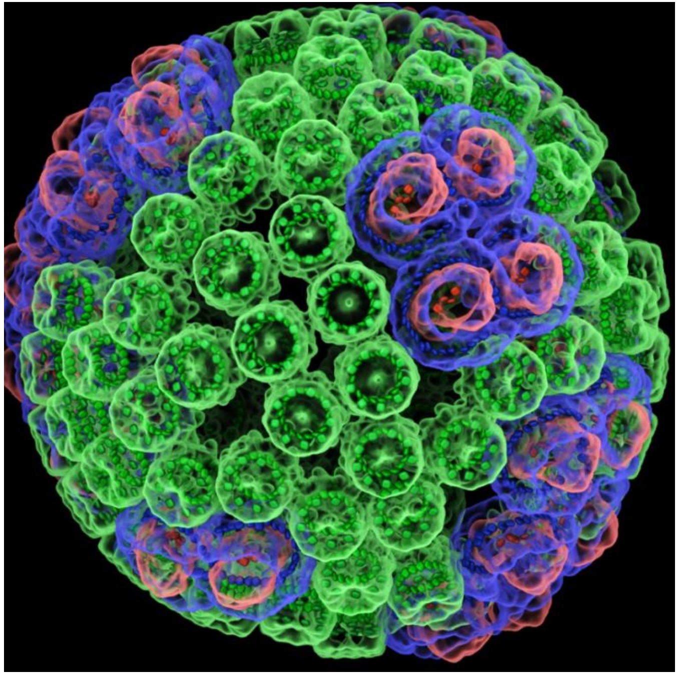
- MD simulation, analysis, visualization provide researchers a so-called ***"Computational Microscope"***
- Visualization is heavily used at every step of structure building, simulation prep and run, analysis, and publication



1998 VMD rendering of LH-I
SGI Onyx2 InfiniteReality w/ IRIS GL

VMD Chromatophore Rendering on Blue Waters

- New representations, GPU-accelerated molecular surface calculations, memory-efficient algorithms for huge complexes
- VMD GPU-accelerated ray tracing engine w/ OptiX+CUDA+MPI+Pthreads
- ***Each revision:*** 7,500 frames render on ~96 Cray XK7 nodes in 290 node-hours, 45GB of images prior to editing

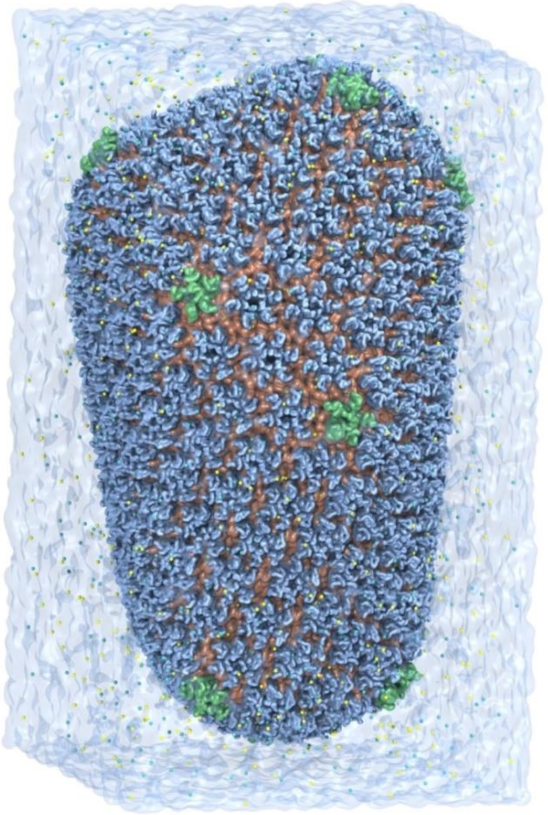


**GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.**

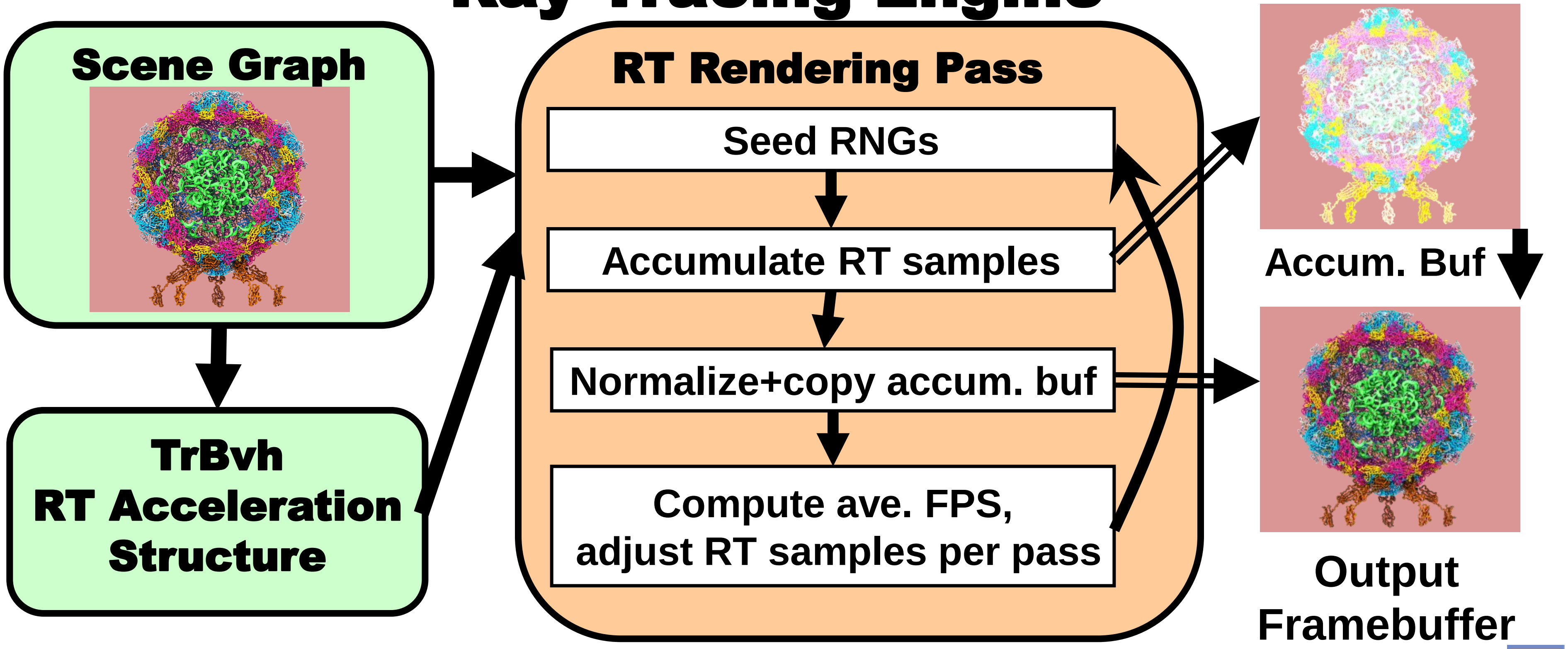
**Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.
M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.
***Winner of the SC'14 Visualization and Data Analytics Showcase**

VMD 1.9.2 Interactive GPU Ray Tracing

- Ray tracing heavily used for VMD publication-quality images/movies
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides –***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers



VMD TachyonL-OptiX Interactive Ray Tracing Engine



Scene Graph

TrBvh
RT Acceleration
Structure

RT Rendering Pass

Seed RNGs

Accumulate RT samples

Normalize+copy accum. buf

Compute ave. FPS,
adjust RT samples per pass

Accum. Buf

Output
Framebuffer

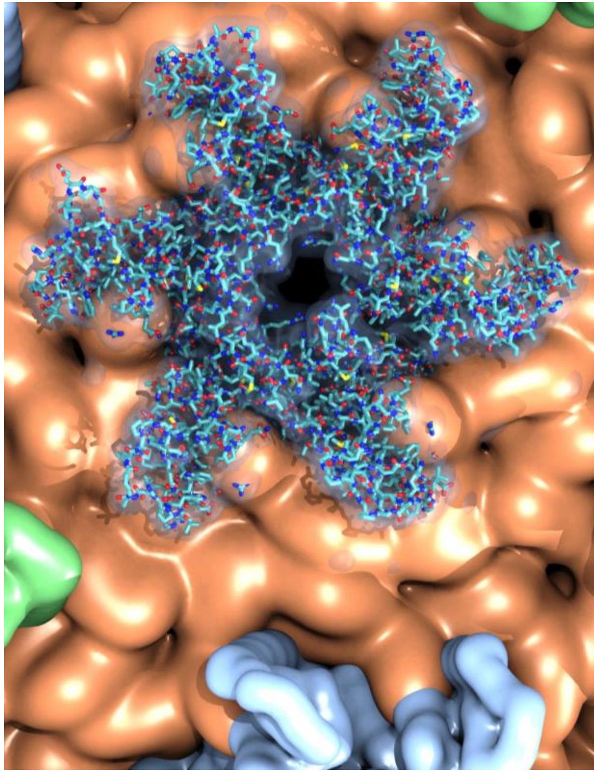
VMD-Next: Coming Soon

- Further integration of interactive ray tracing into VMD
  - Seamless interactive RT in main VMD display window
  - Support trajectory playback in interactive RT
  - Enable multi-node interactive RT on HPC systems

- Improved movie making tools, off-screen OpenGL movie rendering, parallel movie rendering:
  - EGL for parallel graphics w/o X11 server
  - Built-in (basic) interactive remote visualization on HPC clusters and supercomputers

- Improved structure building tools

- Many new and updated user-contributed plugins:



GPU Ray Tracing of HIV-1 Capsid Detail

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

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  SC'14 Visualization and Data Analytics Showcase, 2014.
  ***Winner of the SC'14 Visualization and Data Analytics Showcase**
- **Runtime and Architecture Support for Efficient Data Exchange in Multi-Accelerator Applications.** J. Cabezas, I. Gelado, J. E. Stone, N. Navarro, D. B. Kirk, and W. Hwu. IEEE Transactions on Parallel and Distributed Systems, 2014. **(In press)**
- **Unlocking the Full Potential of the Cray XK7 Accelerator.** M. D. Klein and J. E. Stone. Cray Users Group, Lugano Switzerland, May 2014.
- **GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting.** J. E. Stone, R. McGreevy, B. Isralewitz, and K. Schulten. Faraday Discussions, 169:265-283, 2014.
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- **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.
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