Fighting HIV with GPU-Accelerated Petascale Computing

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Supercomputing 2013 Exhibition
Denver, CO, November 19, 2013
Goal: A Computational Microscope
Study the molecular machines in living cells
Ribosome: target for antibiotics
Poliovirus
NAMD and VMD Use GPUs & Petascale Computing to Meet Computational Biology’s Insatiable Demand for Processing Power
First Simulation of a Virus Capsid (2006)

Satellite Tobacco Mosaic Virus (STMV)

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

$1 \text{ million atoms}$
A huge system for 2006

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

• The STMV project was a turning point
  – Preparing STMV models and placing ions tremendously demanding computational task
  – Existing approaches to visualizing and analyzing the simulation began to break down

• It was already clear in 2006 that the study of viruses relevant to human health would require a long-term investment in better parallel algorithms and extensive use of acceleration technologies in NAMD and VMD

• These difficulties led us to accelerate key modeling tasks with GPUs
VMD Electrostatics: Our First Use of CUDA

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

\[ V_i = \sum_j \frac{q_j}{4\pi \varepsilon_0 |r_j - r_i|} \]

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

*Accelerating Molecular Modeling Applications with Graphics Processors.*
Bringing NAMD to GPU Clusters

2008 NAMD STMV Performance

- **CPU only**
- **with GPU**
- **GPU**

2.4 GHz Opteron + Quadro FX 5600

2008 NCSA “QP” GPU Cluster

Adapting a message-driven parallel application to GPU-accelerated clusters.
Getting Past the “Chicken and the Egg”

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


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

**Fast analysis of molecular dynamics trajectories with graphics processing units-radial distribution function histogramming.** Levine et al., J. Computational Physics, 230:3556-3569, 2011.
All-atom HIV-1 capsid structure solved
Structural Route to the 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)


Hexameric tubules

Li et al., Nature, 2000

Byeon et al., Cell 2009

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

Blue Waters Posed Many Challenges

- Scale NAMD to 100M atoms
  - Read new .js file format
  - Distribute or compress static molecular structure data
  - Parallel atomic data input
  - Use shared memory in a node
  - Parallel load balancing
  - Parallel, asynchronous trajectory and restart file output
  - 2D decomposition of 3D FFT
  - Limit steering force messages
  - Fix minimizer stability issues
- Also build benchmarks…

- Scale NAMD to 300K cores
  - Charm++ shared memory tuning
  - IBM Power7 network layer
  - IBM BlueGene/Q network layer
  - Cray Gemini network layer
  - Cray torus topology information
  - Charm++ replica layers
  - Optimize for physical nodes
  - Adapt trees to avoid throttling
  - Optimize for torus topology
  - Optimize for parallel filesystem

- Optimize for new GPUs…
Twenty Years of NAMD Load Balancing and Communication Optimization Pay off on Blue Waters

Jim Phillips monitors NAMD performance of thousands of cores on 4K workstation
New NAMD+GPUs Will Make Petascale Routine

- 100M-atom simulations need to be commonly available
  - Commodity clusters to the rescue (again)
- GPUs are the future of supercomputing
  - GPU performance growing exponentially
  - GPUs communicate directly via InfiniBand etc.
- **Future NAMD will be GPU-centric**
  - Enabled by Charm++ MPI-interoperability
  - Focus on enabling ~10-100M-atom simulations
  - Benefits extend to smaller simulations
- Rack of 160 GPUs can match 5% of Blue Waters today
  - Dedicated 24/7 to a single simulation
NAMD Cray XK7 Performance August 2013

NAMD on Titan Cray XK7 (2fs timestep with PME)

NAMD XK7 vs. XE6
Speedup: 3x-4x

HIV-1 Simulation Trajectory:
~1.2 TB/day
@ 4096 XK7 nodes
240M atom Influenza Virus Scales to Entire Petascale Machines

(1fs timestep)
Other Projects Using Petascale Computing

From cellular machines to the pharmacy...
From woodchips to gasoline...
From solar energy to cellular fuel...

ribosome
3 M atoms, multiple replicas

second-generation biofuels
> 10 M atoms

photosynthetic chromatophore
100 M atoms
VMD – “Visual Molecular Dynamics”

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

Sequence Data

Quantum Chemistry

Whole Cell Simulation

MD Simulations

CryoEM, Cellular Tomography
# CUDA GPU-Accelerated Trajectory Analysis and Visualization in VMD

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

- **Where to put the data?**
  - Trajectories too large to download
  - **Analyze 231 TB trajectory set in 15 min**, parallel I/O @ **275 GB/sec** on 8,192 nodes

- **Supports GPU-accelerated Cray XK7 nodes for both visualization and analysis tasks**
  - GPU electrostatics, RDF, density quality-of-fit
  - OpenGL Pbuffer off-screen rendering support
  - GPU ray tracing w/ ambient occlusion lighting

- VMD analysis calculations and movie renderings use dynamic load balancing, tested with up to 262,144 CPU cores

- Available on: NCSA Blue Waters, ORNL Titan, Indiana Big Red II

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NCSA Blue Waters
Cray XE6 / XK7 Supercomputer
22,640 XE6 CPU nodes

4,224 XK7 nodes w/ GPUs enable fast VMD analysis and visualization
VMD “QuickSurf” Representation

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

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

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

3-D density map lattice, spatial acceleration grid, and extracted surface
VMD “QuickSurf” Representation, Ray Tracing

All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters
Ray Tracing of VMD Molecular Graphics

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

Standard OpenGL rasterization
VMD w/ new GPU ray tracing engine based on CUDA + OptiX
Lighting Comparison

Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit
GPU Ray Tracing of HIV-1 on Blue Waters

- 64M atom simulation, 1079 movie frames
- **Ambient occlusion lighting**, shadows, transparency, antialiasing, depth cueing, **144 rays/pixel minimum**
- GPU memory capacity hurdles:
  - Regen BVH every simulation timestep, when graphical representations change
  - Surface calc. and ray tracing each use **over 75% of K20X 6GB on-board GPU memory**, even with quantized/compressed colors, surface normals, …
  - Evict non-RT GPU data to host prior to ray tracing
HIV-1 Parallel HD Movie Rendering on Blue Waters Cray XE6/XK7

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

<table>
<thead>
<tr>
<th>Node Type and Count</th>
<th>Script Load Time</th>
<th>State Load Time</th>
<th>Geometry + Ray Tracing</th>
<th>Total Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>256 XE6 CPUs</td>
<td>7 s</td>
<td>160 s</td>
<td>1,374 s</td>
<td>1,541 s</td>
</tr>
<tr>
<td>512 XE6 CPUs</td>
<td>13 s</td>
<td>211 s</td>
<td>808 s</td>
<td>1,032 s</td>
</tr>
<tr>
<td>64 XK7 Tesla K20X GPUs</td>
<td>2 s</td>
<td>38 s</td>
<td>655 s</td>
<td>695 s</td>
</tr>
<tr>
<td>128 XK7 Tesla K20X GPUs</td>
<td>4 s</td>
<td>74 s</td>
<td>331 s</td>
<td>410 s</td>
</tr>
<tr>
<td>256 XK7 Tesla K20X GPUs</td>
<td>7 s</td>
<td>110 s</td>
<td>171 s</td>
<td>288 s</td>
</tr>
</tbody>
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Center Facilities Enable Petascale Biology

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

External Resources, 90% of our Computer Power

Simulation Output
10 Gigabit Network

Petascale Gateway Facility
- Storage
- Compute
- Visualization

High-End Workstations
Immediate On-Demand Computation
Virtual Facilities to Enable Petascale Anywhere

High-end visualization and analysis workstations currently available only in-person in labs like ours must be virtualized and embedded at supercomputer centers.
Optimizing GPU Algorithms for Power Consumption

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

<table>
<thead>
<tr>
<th>Platform</th>
<th>Normalized performance/watt (higher is better)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intel Core i7-3960X</td>
<td>1.00x</td>
</tr>
<tr>
<td>NVIDIA Kayla w/ GeForce 680</td>
<td>1.03x</td>
</tr>
<tr>
<td>NVIDIA Kayla w/ GeForce Titan</td>
<td>1.22x</td>
</tr>
<tr>
<td>NVIDIA Kayla w/ Quadro K4000</td>
<td>1.76x</td>
</tr>
<tr>
<td>NVIDIA Kayla w/ Quadro K2000</td>
<td>2.02x</td>
</tr>
<tr>
<td>NVIDIA Kayla w/ GTX 640</td>
<td>2.51x</td>
</tr>
</tbody>
</table>

Tegra+GPU energy efficiency measurement testbed
Acknowledgements

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  – DOE INCITE
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