Visualizing the Atomic Detail Dynamics of Biomolecular Complexes in Our Compute-Rich but I/O-Constrained Future

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http://www.ks.uiuc.edu/Research/vmd/
Session: Visualization and HPC
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VMD – “Visual Molecular Dynamics”

- 100,000 active users worldwide
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/

Cell-Scale Modeling

MD Simulation
Goal: A Computational Microscope

Study the molecular machines in living cells
What Drives Increasing Molecular Dynamics System Size and Timescale?

• Working to gain insight into structure and dynamics of molecular basis of disease

• Many health-relevant biomolecular complexes are large, and key processes often occur at long timescales, presenting many computational challenges…

• New hybrid modeling approaches that combine the best structure information from multiple modalities of experimental imaging, physics, e.g. from MD force fields:
  – “Computational Microscopy”

• Parallel computing provides the resources required to keep pace with advances in structure determination and modeling
NAMD simulations can generate up to 10TB of output per day on 20% of Summit
Molecular Dynamics Trajectory Analysis

- MD simulations sample femtosecond timescales
- Millions of timesteps stored per trajectory
- Dynamics of biomolecular complexes are main interest, but solvent often accounts for half or more of the simulation content

Skip I/O for regions of bulk solvent where possible [1]

- Modern MD tools, e.g., VMD, NAMD, LAMMPS, HOOMD, employ extensive embedded scripting (Python, Tcl, etc) to permit simulation preparation, custom simulation protocols, analysis, and visualization
- Unified collective variables module allows identical analytical computations to be performed within LAMMPS, NAMD, and VMD, during pre-simulation modeling, in-situ, and post-hoc [2]


Petascale Molecular Dynamics I/O and Storage Challenges

- NAMD simulations can produce up to 10TB/day @ 1024 nodes (~20%) of ORNL Summit, more as ongoing performance optimizations raise NAMD performance further
- Petascale science campaigns require months of simulation runs
- Long-term storage of large-fractional petabytes impractical
- Historical “download output files for analysis and visualization” approach is a non-starter at this scale
- Demands visualization and analysis operate on the data in-place on the HPC system, whether post-hoc, in-transit, or in-situ
- Analyses must identify salient features of structure, dynamics, cull data that don’t contribute to biomolecular processes of interest
VMD Petascale Visualization and Analysis

- Combination of growing system sizes and timescales of simulation trajectories poses a major data size challenge for molecular visualization and analysis
- Parallel I/O rates up to **275 GB/sec** on 8192 Cray XE6 nodes – can read in **231 TB in 15 minutes**!
- Analyze/visualize large trajectories **too large to transfer off-site**:
  - User-defined parallel analysis operations, data types
  - Parallel rendering, movie making
- Supports GPU-accelerated compute nodes for both visualization and analysis tasks:
  - GPU accelerated trajectory analysis w/ CUDA
  - OpenGL and GPU ray tracing for visualization and movie rendering

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

Parallel VMD currently available on:
ORNL Summit and Titan, NCSA Blue Waters, IU Big Red II, CSCS Piz Daint, many similar systems
VMD EGL Rendering: Supports full VMD GLSL shading features
Vulkan support coming soon...

Swine Flu A/H1N1 neuraminidase bound to Tamiflu

64M atom HIV-1 capsid simulation

High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL.
J. E. Stone, P. Messmer, R. Sisneros, and K. Schulten. High Performance Data Analysis
Next Generation: Simulating a Proto-Cell

- Emulate aspects of the *Mycoplasma mycoides* bacterium
- 200nm diameter
- ~1 billion atoms w/ solvent
- ~1400 proteins in membrane

Cryo-ET image of ultra-small bacteria
(scale bar 100nm)
Proto-Cell Data Challenges

- 1B-atom proto-cell requires nodes with more than TB RAM to build complete model...
- 1B-atom proto-cell binary structure file: 63GB
- Trajectory frame atomic coordinates: 12GB, 1.2TB/ns of simulation (1 frame per 10ps)
- Routine modeling and visualization tasks are a big challenge at this scale
  - Models contain thousands of atomic-detail components that must work together in harmony
  - Exploit persistent memory technologies to enable “instant on” operation on massive cell-scale models – eliminate several minutes of startup during analysis/visualization of known structure
  - Sparse output of results at multiple timescales will help ameliorate visualization and analysis I/O
  - Data quantization, compression, APIs like ZFP
Clustering Analysis of Molecular Dynamics Trajectories: Requires I/O+Memory for All-Pairs of Trajectory Frames

Use of Node-Local Burst Buffers and Non-Volatile Memory DIMMs

- Perform viz+analysis in-transit in node-local SSDs, persistent memory NVDIMMs
- ORNL Summit I/O:
  - Parallel FS: 2.5 TB/s
  - Node-local PCIe “burst buffer” SSDs: 10+ TB/sec, 7PB capacity
- Plenty of capacity for full-detail MD trajectories, could enable ~100x increase in temporal resolution in cases where it would be valuable to the science
- Enable all-pairs trajectory clustering analyses and resulting visualizations
- Future systems with NVDIMMs (3D Xpoint, phase change memory) could eventually provide bandwidths approaching DRAM
- Use NVDIMMs w/ mmap(), APIs like PMDK to perform formerly-out-of-core calculations using persistent memory:
  - https://github.com/pmem/pmdk
- Imagine future Summit-like machines w/ NVLink-connected GPUs w/ access to high-bandwidth persistent memory on each node
Trade FLOPS for Reduced I/O

ORNLSummit compute node:
- 6x Tesla V100 GPUs, 2x POWER9 CPUs
- GPUs Peak: ~46 DP TFLOPS, ~96 SP TFLOPS
- Peak IB rate per node: ~23GB/sec
- Ratio of FLOPS vs. I/O:
  ~2,000 DP FLOPS/byte, ~4000 SP FLOPS/byte
  ~16K FLOPS per FP word

Unconventional approach: Recompute to avoid I/O
Computing+Visualizing Molecular Orbitals

- Movies of simulation trajectories provides insight into results
- QM, and hybrid (QM/MM) MO visualizations historically done from huge “cube” files, impractical
- Store QM wavefunctions + Gaussian basis set, only 10s of KB per stored timestep compared to 100s of MB
- Recompute MO grid on-the-fly from QM basis set, huge decrease in RAM+I/O in exchange for heavy FP arithmetic

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VMD C\textsubscript{60} MO Viz. Perf, 516x519x507 Grid: @ .13s/frame, avoids 3.8GB/s I/O per-node

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<th>Hardware platform</th>
<th>Runtime,</th>
<th>Speedup</th>
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Omnidirectional Stereoscopic Ray Tracing

- Ray trace 360° images and movies for Desk and VR HMDs: Oculus, Vive, Cardboard
- Stereo spheremaps or cubemaps allow very high-frame-rate interactive OpenGL display
- AO lighting, depth of field, shadows, transparency, curved geometry, …
- Summit 6x Tesla V100 GPU nodes:
  - Render many omni-stereo viewpoints, no acceleration structure rebuilds, tens of frames/sec per-node!
  - OptiX multi-GPU rendering, NVLink compositing and data distribution, etc…
  - Future: AI for warping between views


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    ACI-1238993, ACI-1440026
“When I was a young man, my goal was to look with mathematical and computational means at the inside of cells, one atom at a time, to decipher how living systems work. That is what I strived for and I never deflected from this goal.” – Klaus Schulten