Preparing and Analyzing Large Molecular Simulations with VMD

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VMD Tutorials Home Page

- http://www.ks.uiuc.edu/Training/Tutorials/
  - Main VMD tutorial
  - VMD images and movies tutorial
  - QwikMD simulation preparation and analysis plugin
  - Structure check
  - VMD quantum chemistry visualization tutorial
  - Visualization and analysis of CPMD data with VMD
  - Parameterizing small molecules using ffTK
Overview

• Introduction
• Data model
• Visualization
• Scripting and analytical features
• Trajectory analysis and visualization
• High fidelity ray tracing
• Plugins and user-extensibility
• Large system analysis and visualization
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

Structure

Parameterization

Analysis

Preparation with QwikMD

Refinement with MDFF

MD/Cell Simulation

Parallel Analysis

Remote Visualization

X-ray, cryo-EM, cryo-ET, NMR
VMD – “Visual Molecular Dynamics”

- Unique capabilities:
  - Trajectories are fundamental to VMD
  - Support for very large systems, now reaching billions of particles
  - Extensive GPU acceleration
  - Parallel analysis/visualization with MPI

- Visualization and analysis of:
  - Molecular dynamics simulations
  - “Particle” systems and whole cells
  - Cryo-EM densities, volumetric data
  - Quantum chemistry calculations
  - Sequence information

MD Simulations  
Cell-Scale Simulation  
Integrate w/ Cryo-EM/ET
VMD Serves Many Communities

- **VMD user statistics:**
  - 103,000 unique registered users; 17,000 (16%) are NIH funded researchers
  - 25,000 citations, over 3,000 citations per year
- Supports key data types, file formats, and databases
- **User extensible** to support new tools, data types, **custom analyses**

![System Size](image.png)
Goal: A Computational Microscope
Study the molecular machines in living cells

Ribosome: target for antibiotics

Poliovirus
VMD is a Tool for Accessing Information about the Cell
VMD Interoperates with Mainstream Research Tools

- Provides tools for simulation preparation, visualization, and analysis
- Interpret and process multi-modal structural information
- Connects with key software tools to enable state-of-the-art simulations
- Openness, extensibility, and interoperability are VMD hallmarks
- Uses advanced algorithms and hardware technologies to address data size challenges posed by cutting-edge experimental imaging and simulation
VMD is a Platform for Developing Research Tools
Over 110 VMD Plugins, Half Developed by Users

- VMD user-extensible scripting w/ Tcl/Tk, Python
- User-developed plugins:
  - Alanine Scanning
  - Collective Variable Analyzer
  - Clustering Tool
  - Carbon Nanostructure Builder
  - TorsionPlot
  - RMSD Trajectory Tool
  - Many others…
Selected VMD Plugins: Center Developed, and **User Developed**

### Analysis
- APBSRun
- CatDCD
- Contact Map
- GoFROGGUI
- HeatMapper
- ILSTools
- IRSpecGUI
- MultiSeq
- NAMD Energy
- NAMD Plot
- NetworkView
- NMWiz
- ParsePEP
- PBCTools
- PMEtot
- PropKa GUI
- RamaPlot
- RMSD Tool
- RMSD Trajectory Tool
- RMSD Visualizer Tool
- Salt Bridges
- Sequence Viewer
- Symmetry Tool
- Timeline
- TorsionPlot
- VolMap

### Modeling
- AutoIonize
- AutoPSF
- Chirality
- Cionize
- Cispeptide
- CGTools
- Dowser
- fttK
- Inorganic Builder
- MDDF
- Membrane
- Merge Structs
- Molefacture
- Mutator
- Nanotube
- Psfgen
- RESPTool
- RNAView
- Solvate
- SSRestraints
- Topotools

### Visualization
- Clipping Plane Tool
- Clone Rep
- DemoMaster
- Dipole Watcher
- Intersurf
- Navigate
- NavFly
- MultiMolAnim
- Color Scale Bar
- Remote
- Palette Tool
- ViewChangeRender
- ViewMaster
- Virtual DNA Viewer
- VMD Movie Maker

### Collaboration
- Remote Control

### Data Import and Plotting
- Data Import
- Multiplot
- PDBTool
- MultiText

### Externally Hosted Plugins and Extensions
- Check sidechains
- MultiMSMS
- Interactive Essential Dynamics
- Mead Ionize
- Clustering Tool
- iTrajComp
- Swap RMSD
- Intervor
- SurfVol
- vmdICE

### Simulation
- AlaScan
- AutoIMD
- IMDMenu
- NAMD GUI
- NAMD Server
- QMTool

**75 MolFile I/O Plugins:** structure, trajectory, sequence, and density map

http://www.ks.uiuc.edu/Research/vmd/plugins/
Goal: A Computational Microscope
Study the molecular machines in living cells

All-Atom Molecular Dynamics

- HIV Capsid
- ATP Synthase
- Photosynthetic Chromatophore
- Aquaporin
- Lysozyme
- Ribosome
- STMV

Number of Atoms

10^5, 10^6, 10^7, 10^8

Year


(2 nm)^3, (100 nm)^3
Technology Opportunities and Collaborations

- Supercomputer Centers, Cray, IBM
  - Remote visualization
  - Performance, power profiling and optimization
- NVIDIA
  - GPU computing
  - Ray tracing
  - Remote visualization
  - ARM, Tablets, power profiling and optimization
- Intel
  - x86, Xeon Phi optimization, ray tracing
- Amazon
  - Cloud deployment of VMD/NAMD, related tools
  - Remote visualization
- Universities:
  - G. Fiorin, J. Henin, Toni Giorgino, collective variables
  - T. Ertl, U. Stuttgart: visualization algorithms
  - M. Kuttel, U. Cape Town: visualization and analysis
  - W. Sherman, Indiana U.: VR HMDs, visualization

Energy efficiency: ARM+GPU

GPU computing, Ray tracing, Remote viz.

VR HMDs, 6DoF input devices
Making Our Research Tools Easily Accessible

• Cloud based deployment
  – Full virtual machines (known as “AMI” in Amazon terminology)
  – Amazon AWS EC2 GPU-accelerated instances:
    http://www.ks.uiuc.edu/Research/cloud/

• Docker “container” images available in NVIDIA NGC registry
  – Users obtain Docker images via registry, download and run on the laptop, workstation, cloud, or supercomputer of their choosing
  – https://ngc.nvidia.com/registry/


VMD Data Model
VMD “Molecule”

• Collection of self-consistent molecular information
  – Atomic structure, time-varying atomic coordinates, velocities, …
  – Volumetric data
  – Graphics objects

• Key missing information required for visualization is auto-generated heuristically – “guessed”, if not provided in input files
  – Bond topology

• Limitations:
  – Fixed atom count per-timestep, requires use of “dummy atoms” for so-called “open system” simulations
  – VMD doesn’t store or use MD force field parameters, various other data that are typically specific to particular simulation tools, force fields, etc.
Overcoming the Biomolecular Orientation of VMD

• VMD molecular data structures are optimized for biomolecules
  – Expects atom/residue names that (roughly) follow RCSB Protein Databank conventions
  – Significant up-front structure analysis enables increased interactivity later
  – Cost of this is decreased generality in various cases:
    • Fixed atom count per timestep
    • Unrecognized atom naming conventions can inhibit use of some of the high-level atom selections

• Nanodevice and materials science data can be displayed in VMD
  – Assign per-atom name/type fields after loading
  – Enable VMD to better recognize structural elements
  – Example: xyz or LAMMPS dump files lack some expected fields, so it helps to use special features of LAMMPS plugin to assign them
Atomic Structure

- Per-Atom attributes:
  - Name
  - Type
  - Residue ID, Unique residue ID, Residue Name, Residue Type
  - Bond list
  - Atomic number
  - Alternate location identifier
  - Insertion code
  - Chain
  - Segment name
  - Atom/Residue classification (protein, nucleic, hydrogen, water, “other”)
Other, Optional Per-Atom Fields

• Optional per-atom attributes:
  – Mass
  – Charge
  – Radius
  – Occupancy
  – B-factor
  – Fields primarily used by simulation preparation tools:
    • Bond Orders
    • Angles, Dihedrals, Impropers, Cross-Term Maps
Time-Varying Trajectory Data

- Atomic coordinates
- Atomic velocities
- PBC unit cell
- QM, QM/MM molecular orbital data
- User-defined time-varying scalar quantities:
  - user, user2, user3, user4
VMD LAMMPS Molfile Plugin

https://sites.google.com/site/akohlmey/software/lammps-plugin

- Reads LAMMPS text mode trajectory “dump” files
- Map LAMMPS per-atom fields to VMD molfile API:
  - LAMMPSREMAPFIELDS environment variable allows user to control mapping of per-atom fields to VMD molfile API
  - List of mappings of LAMMPS fields into VMD fields, e.g. “VMD=LAMMPS”
  - Example to map LAMMPS forces into VMD velocity fields:
    set env(LAMMPSREMAPFIELDS) “vx=fx,vy fy,vz=fz”
- Adapt LAMMPS trajectories with varying atom counts to VMD
  - LAMMPSMAXATOMS environment variable sets peak atom count for VMD, adding “dummy” atoms as placeholders:
    Dummy atoms initialized with properties: name = @, type = X, resname = @@@, segid = @@@, chain = @, mass =0, charge=0, radius=0, element=X.
  - LAMMPSDUMMYPOS sets default atomic coords for dummy atoms that don't exist for a given frame:
    set env(LAMMPSDUMMYPOS) {0.0 0.0 -10.0}
Exporting Molecular Data

• VMD can be used to prepare MD simulations in conjunction with plugins and user scripting
• Need to watch out for assumptions made by heuristics, structure building tools
• Example: bond topology may need to be modified or deleted for some force fields
• Use the most appropriate structure manipulation tools for the MD package in use, e.g. for LAMMPS, the best choice in VMD is the “topotools” plugin
VMD Visualization Concepts
VMD Approach to Visualization

- Molecular scene is composed of “graphical representations”
- Each representation encapsulates a group of selected atoms, a drawing style, coloring style, and other parameters
- Representations are independent of each other, can be toggled on/off easily, allowing molecular scenes to be built-up incrementally
- VMD atom selection language is shared with its analytical and scripting interfaces
Selection, Filtering

- Most viz tools allow interactive visual picking, menu-driven selections of structure components to display or operate on.
- VMD also extensively uses a text-based selection language (think google):
  - “water within 10 of protein and z > 0”
  - Allows selection on user-defined fields
  - Promotes synergy between interactive and scripting interfaces
  - Works very well when dealing with huge time-varying structures
Structure Visualization

Molecular representations provide different levels of abstraction, atomic detail vs. higher level organizational information

- Atoms, VdW spheres, bonds, ball-stick, …
- Coarse-grained “beads”
- Ribbons, secondary structure, “cartoon” reps, RNA/DNA
- Molecular surfaces
- Molecular orbitals (quantum chemistry)
Computed Properties

- Smoothing of thermal noise
- Secondary structure
- Hydrogen bonds, salt bridges
- Forces, energies, stress, strain
- Time averaging of electrostatic fields, occupancy maps
- Quality-of-fit cross correlation with cryo-EM density maps
- Normal modes, principal component analysis, essential dynamics
- Cluster simulation trajectory timesteps by structural similarity

Chemoreceptor trimer-of-dimers analysis with Bendix plugin in VMD
Display of Computed Properties on Structures

Per-residue solvent-accessible surface area of Ubiquitin

PME electrostatic potential contour for a helicase on a volumetric slice plane
CheA kinase PCA: first principal component porcupine plot
Molecular Visualization Challenges

• Geometrically complex scenes
• Often show a mix of structural and spatial properties
• Time varying!
• Spatial relationships important to see clearly: depth cueing, shadows, AO helpful
Satellite Tobacco Mosaic Virus
Exportin Cse1p

Nanopore
VMD Shading Comparison: EF-Tu

- Outline Shader
- “Goodsell” Shader
- Glossy Shader
- Ambient Occlusion, Shadowing
VMD Scripting
VMD Scripting

• Built-in Tcl interpreter is standard in all builds
• Custom builds can contain Python interpreter too
• Collection of simple VMD scripts:
  http://www.ks.uiuc.edu/Research/vmd/script_library/
Atom Selections

set ionsel [atomselect top “ions”]
set watsel [atomselect top “water”]
set solute [atomselect top “not water and not ions”]

set numions [$ionsel num]
set coords [$solute get {x y z}]

Built-in “Measure” Analysis Routines

• Provide high-performance routines for common analysis functions
• Operate on atom selections, sometimes over a frame range

  set com [measure center $sel weight mass]
  set avpos [measure avpos $sel first 0 last 999 step 1]
  set c [measure contacts 1.0 $sel1 $sel2]

  set txmat [measure fit $sel1 $sel2]
  $sel2 move $txmat
# Print RMSD between two selections between the first timestep and each # later timestep for the given molecule id (default: top)

proc print_rmsd_trajectory {{mol top}} {
    set reference  [atomselect $mol "protein" frame 0]  # use frame 0 for the reference
    set compare    [atomselect $mol "protein"]          # the frame being compared
    set numsteps   [molinfo $mol get numframes]         # query number of trajectory frames
    for {set frame 0} {$frame < $numsteps} {incr frame} {
        $compare frame $frame
        set transmat [measure fit $compare $reference]   # compute the transformation
        $compare move $transmat                        # align comparison to reference
        set rmsd [measure rmsd $compare $reference]     # compute the RMSD
        puts "RMSD of $frame is $rmsd"                  # print the RMSD
    }
}
Trajectory Analysis and Visualization
Visualization of MD Trajectories

- Allow researchers study trajectories by analyzing force profiles, energies, structural changes, etc.
- Visualization selections, graphics, structure properties, colors can all be recomputed for each trajectory timestep!
Folding Dynamics of Villin Headpiece Unveiled

6.9μs folding simulation of 30K atoms: 380GB trajectory


Key Folding Intermediates
Time-Averaged Volumetric Properties

• Compute density, distance, occupancy, potential maps for a frame or averaged over a trajectory

• Example: display binding sites for diffusively bound ions as probability density isosurfaces

`tRNA magnesium ion occupancy: VMD volmap plugin`
Petascale Computing - A Key Instrument for Life Science
MDFF Solves Structures from X-ray Crystallography and Cryo-EM

Electron microscopy

FEI microscope

Electron density of protein in action at low resolution

X-ray crystallography

APS at Argonne

Ideal protein structure at high resolution
Acetyl – CoA Synthase
Evaluating Quality-of-Fit for Structures Solved by Hybrid Fitting Methods

Compute Pearson correlation to evaluate quality-of-fit between a reference cryo-EM density map and a simulated density map from an all-atom structure.

MDFF Cross Correlation Timeline

Regions with poor fit

Regions with good fit
### Rabbit Hemorrhagic Disease Virus (RHDV)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Traj. frames</strong></td>
<td>10,000</td>
</tr>
<tr>
<td><strong>Structure component selections</strong></td>
<td>720</td>
</tr>
<tr>
<td><strong>Single-node XK7 (projected)</strong></td>
<td>336 hours (14 days)</td>
</tr>
<tr>
<td><strong>128-node XK7</strong></td>
<td>3.2 hours</td>
</tr>
<tr>
<td></td>
<td>105x speedup</td>
</tr>
<tr>
<td><strong>2048-node XK7</strong></td>
<td>19.5 minutes</td>
</tr>
<tr>
<td></td>
<td>1035x speedup</td>
</tr>
</tbody>
</table>

Calculation of 7M CCs would take **5 years** using serial CPU algorithm!

VMD Tesla V100 Cross Correlation Performance
Rabbit Hemorrhagic Disease Virus: 702K atoms, 6.5Å resolution
Volta GPU architecture almost 2x faster than previous gen Pascal:

<table>
<thead>
<tr>
<th>Application and Hardware platform</th>
<th>Runtime, Speedup vs. Chimera, VMD+GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chimera Xeon E5-2687W (2 socket) [1]</td>
<td>15.860s, 1x</td>
</tr>
<tr>
<td>VMD-CUDA IBM Power8 + 1x Tesla K40 [2]</td>
<td>0.488s, 32x, 0.9x</td>
</tr>
<tr>
<td>VMD-CUDA Intel Xeon E5-2687W + 1x Quadro K6000 [1,2]</td>
<td>0.458s, 35x, 1.0x</td>
</tr>
<tr>
<td>VMD-CUDA Intel Xeon E5-2698v3 + 1x Tesla P100</td>
<td>0.090s, 176x, 5.1x</td>
</tr>
<tr>
<td>VMD-CUDA IBM Power8 “Minsky” + 1x Tesla P100</td>
<td>0.080s, 198x, 5.7x</td>
</tr>
<tr>
<td>VMD-CUDA Intel Xeon E5-2697Av4 + 1x Tesla V100</td>
<td>0.050s, 317x, 9.2x</td>
</tr>
<tr>
<td>VMD-CUDA IBM Power9 “Newell” + 1x Tesla V100</td>
<td>0.049s, 323x, 9.3x</td>
</tr>
</tbody>
</table>


Clustering Analysis of Molecular Dynamics Trajectories

High Fidelity Ray Tracing of Molecular Scenes
Ray Tracing in VMD

- Support for ray tracing of VMD molecular scenes began in 1995
- Tachyon parallel RT engine interfaced with VMD (1999)
- Tachyon embedded as an internal VMD rendering engine (2002)
- Built-in support for large scale parallel rendering (2012)
- Refactoring of VMD to allow fully interactive ray tracing as an alternative to OpenGL (2014)
Interactive Ray Tracing, Lighting Comparison: STMV Capsid

Two lights, no shadows (e.g. as used by OpenGL)

Ambient occlusion lighting and shadows w/ RT
Diverse Shading and Lighting Approaches

Decrystallization: Interactive Ray Tracing w/ Ambient Occlusion Lighting, Depth of Field Focal Blur

Myoglobin
Geometrically Complex Scenes

Ray tracing techniques well matched to molecular viz. needs:

• Curved geometry, e.g. spheres, cylinders, toroidal patches, easily supported
• Greatly reduced memory footprint vs. polygonalization
• Runtime scales only moderately with increasing geometric complexity
• Occlusion culling is “free”, RT acceleration algorithms do this and much more
Benefits of Advanced Lighting and Shading Techniques

• Exploit visual intuition
• Spend computer time in exchange for scientists’ time, make images that are more easily interpreted
High Fidelity Interactive Visualization

• VMD interactive ray tracing
  – Interactive ray tracing on GPUs with progressive refinement of image and lighting quality
  – Fully interactive rendering of large structures with advanced lighting features, and WYSIWYG “What you see is what you get” final image output
VMD Atomic Detail Visualization of Cellular Architecture with Instancing

- VMD 1.9.4 supports instancing of graphical representations associated with molecules
- Exploit **VBO caching** in OpenGL to eliminate host-GPU geometry transfers
- **OptiX instancing** of geometry buffers to minimize GPU memory footprint for cell-scale scenes w/ atomic structures
Capsid acts as an osmotic regulator

Results from 64 M atom, 1 μs sim

Chloride ions permeate through the hexameric center
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


Ongoing VR Work

- OpenXR – cross platform muti-vendor HMD support
- Ray tracing engine and optimizations:
  - AI denoising for better average quality
  - Interactive RT stochastic sampling strategies to improve interactivity
  - Improved omnidirectional cubemap/spheremap sampling approaches
  - AI multi-view warping to allow rapid in-between view generation amid multiple HMD head locations
  - H.265 for high-res omnidirectional video streaming
  - Multi-node parallel RT and remote viz. on general clusters and supercomputers, e.g. NCSA Blue Waters, ORNL Titan
- Tons of work to do on VR user interfaces, multi-user collaborative visualization, …
VMD Planetarium Dome Master Camera

- RT-based dome projection -- rasterization poorly suited to non-planar projections
- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, and so on
- Both mono and stereoscopic
- No further post-processing required
VMD Plugins and Support for User-Extensibility
QwikMD: Guided MD Simulation and Training

Smooths initial learning curve (non-expert users)

Speed up tedious simulation preparation tasks (expert users)

Reproducibility: detailed log of all steps

Interactive preparation, simulation, and analysis

Carbon Nanostructure Builder
http://www.ks.uiuc.edu/Research/vmd/plugins/nanotube/

• Build single-wall carbon / boron nitride nanotubes, graphene-like sheets or stacks
Parametrization with the Force Field Toolkit (FFTK)

A plugin enabling the simulation of drug-like small molecules by lowering force field development barriers

A graphical interface organized to follow the standardized CGenFF workflow

Leverages VMD’s powerful graphics capabilities to visualize parameter-related data within the context of molecular structure

Future Plans:
- Support free-for-academics QM software, ORCA (Neese, Max Planck)
- Parametrization tools for additional MM force fields
  - AMBER force field (Gumbart, Georgia Tech.)
  - Drude polarizable force fields (Roux, U. Chicago; MacKerell, U. Maryland)

*NEW in VMD 1.9.3*
Import data from the CGenFF Program webserver to assign initial parameters by analogy

Extensive training material available from the Center’s website

Documentation Website
Workshop Tutorial
Screencast Demos

Interactively explore energy profiles
Example VMD Visualization and Analysis Plugins

**Bendix**
Dahl ACE, Chavent M and Sansom MSP  

**Normal Mode Wizard**
Bakan A, Meireles LM, Bahar I  
Large System Analysis and Visualization
All-Atom Molecular Dynamics Today

- HIV Capsid
- ATP Synthase
- Aquaporin
- Lysozyme
- STMV
- Photosynthetic Chromatophore

Number of Atoms

- $(2 \text{ nm})^3$
- $(100 \text{ nm})^3$

Year

HIV-1 Data: ~1.2 TB/day @ 4096 XK7 nodes
NAMD simulations can generate up to 10TB of output per day on 20% of Summit
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/ Tesla K20X GPUs

Parallel VMD currently available on:
ORNL Summit and Titan, NCSA Blue Waters, IU Big Red II, CSCS Piz Daint, many similar systems
Remote Visualization and Analysis

In-development: VMD w/ built-in remote visualization

- Access large data located anywhere in the world
- Enable capabilities not possible with conventional laptops or workstations
- VMD session available to any device, browser

Clusters, Supercomputers

Workstations, Servers, Cloud

Chemical Visualization of Human Pathogens: the Retroviral Capsids.

Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.

Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering.
VMD “QuickSurf” Representation, Ray Tracing

All-atom HIV capsid simulations w/ up to 64M atoms on Blue Waters
HIV-1 Parallel HD Movie Rendering on Blue Waters Cray XE6/XK7

New VMD TachyonL-OptiX on XK7 vs. Tachyon on XE6: K20X GPUs yield up to twelve times geom+ray tracing speedup

<table>
<thead>
<tr>
<th>Ray Tracer Version</th>
<th>Node Type and Count</th>
<th>Script Load</th>
<th>State Load</th>
<th>Geometry + Ray Tracing</th>
<th>Total Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>New TachyonL-OptiX</td>
<td>64 XK7 Tesla K20X GPUs</td>
<td>2 s</td>
<td>39 s</td>
<td>435 s</td>
<td>476 s</td>
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<tr>
<td>New TachyonL-OptiX</td>
<td>128 XK7 Tesla K20X GPUs</td>
<td>3 s</td>
<td>62 s</td>
<td>230 s</td>
<td>295 s</td>
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<tr>
<td>TachyonL-OptiX [1]</td>
<td>64 XK7 Tesla K20X GPUs</td>
<td>2 s</td>
<td>38 s</td>
<td>655 s</td>
<td>695 s</td>
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<tr>
<td>TachyonL-OptiX [1]</td>
<td>128 XK7 Tesla K20X GPUs</td>
<td>4 s</td>
<td>74 s</td>
<td>331 s</td>
<td>410 s</td>
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<td>TachyonL-OptiX [1]</td>
<td>256 XK7 Tesla K20X GPUs</td>
<td>7 s</td>
<td>110 s</td>
<td>171 s</td>
<td>288 s</td>
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<tr>
<td>Tachyon [1]</td>
<td>256 XE6 CPUs</td>
<td>7 s</td>
<td>160 s</td>
<td>1,374 s</td>
<td>1,541 s</td>
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<tr>
<td>Tachyon [1]</td>
<td>512 XE6 CPUs</td>
<td>13 s</td>
<td>211 s</td>
<td>808 s</td>
<td>1,032 s</td>
</tr>
</tbody>
</table>

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


VMD w/ OptiX 5

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization
- Remote RT on NVIDIA GPU clusters
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- GPU memory sharing via NVLink on Quadro GP100, Tesla P100
- VMD+OptiX 5, NVIDIA NGC container: https://ngc.nvidia.com/registry/
- In-progress:
  - OptiX denoising support: fast turnaround w/ AO, DoF, etc
  - Denoising to enable practical use of path tracing in VMD

GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.


IBM AC922 w/ 6 GPUs

Power Supplies (2x)
- 2200W
- 200VAC, 277VAC, 400VDC input

Nvidia Volta GPU
- 3 per socket
- SXM2 form factor
- 300W
- NVLink 2.0
- Air/Water Cooled

Memory DIMM's (16x)
- 8 DDR4 16 DIMMs per socket
- 8, 16, 32, 64, 128GB DIMMs

Power 9 Processor (2x)
- 16,22C water cooled
- 16, 20C air cooled

BMC Card
- iKVM
- 1 Gb Ethernet
- VGA
- 1 USB 3.0

PCIe slot (4x)
- Gen4 PCIe
- 2, x16 HHHL Adapter
- 1, Shared slot
- 1 x8 HHHL Adapter
IBM AC922 Summit Node

3 GPUs Per CPU Socket

Tesla V100 GPU
Tesla V100 GPU
Tesla V100 GPU

Tesla V100 GPU
Tesla V100 GPU
Tesla V100 GPU

Nvlink 2.0
2x 50GBps:
100GBps

DDDR4 DRAM
120GBps

POWER9 CPU
64GBps

X-Bus

POWER9 CPU

1.6TB SSD
“Burst Buffer”

InfiniBand
12GBps

DDDR4 DRAM
120GBps

InfiniBand
12GBps
VMD Off-Screen Rendering w/ EGL

- Containers+Cloud+Workstations with recent NVIDIA drivers
- VMD on HPC systems w/ latest GPUs:
  - Cray XC50, CSCS Piz Daint
  - ORNL Summit in progress now
  - IBM OpenPOWER, drivers 375.66 and later support both GLX and EGL
OpenGL: GLX vs. EGL

Viz Application (user)

OpenGL

GLX

X server (root)

Viz Application (user)

OpenGL

EGL

Driver

GPU

Driver

GPU
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.
### VMD EGL Performance on Amazon EC2 Cloud

<table>
<thead>
<tr>
<th>MPI Ranks</th>
<th>EC2 “G2.8xlarge” GPU Instances</th>
<th>HIV-1 movie rendering time (sec), (I/O %) 3840x2160 resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>626s (10% I/O)</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>347s (19% I/O)</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>221s (31% I/O)</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>141s (46% I/O)</td>
</tr>
<tr>
<td>16</td>
<td>4</td>
<td>107s (64% I/O)</td>
</tr>
<tr>
<td>32</td>
<td>8</td>
<td>90s (76% I/O)</td>
</tr>
</tbody>
</table>

**Performance at 32 nodes reaches ~48 FPS**


64M atom HIV-1 capsid simulation rendered via EGL
VMD OptiX/EGL NGC Container

- https://ngc.nvidia.com/registry/
- CUDA-accelerated viz+analysis
- EGL off-screen rendering – no windowing system needed
- OptiX high-fidelity GPU ray tracing engine built in
- All dependencies included
- Easy to deploy on a wide range of GPU accelerated platforms

Preparation, Visualization, Analysis of All-Atom Cell-Scale Simulations

- Parallel analysis, visualization w/ MPI
- Support for large memory (TB), up to 2 billion atoms per “molecule” now
- Interactive rasterization w/ Vulkan, EGL
- Interactive ray tracing on CPUs and GPUs

• 200 nm spherical envelope
• Membrane with ~50% occupancy by proteins
• 63M atoms in envelope model

---


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
### VMD Tesla P100 Performance for $C_{60}$ Molecular Orbitals, 516x519x507 grid

<table>
<thead>
<tr>
<th>Hardware platform</th>
<th>Runtime,</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBM Power8 (2 socket) (ORNL ‘crest’) [1]</td>
<td>8.03s,</td>
<td>0.4x</td>
</tr>
<tr>
<td>Intel Xeon E5-2660v3 (2 socket) [1]</td>
<td>7.14s,</td>
<td>0.5x</td>
</tr>
<tr>
<td>IBM Power8 (ORNL ‘crest’) + 1x Tesla K40 [1]</td>
<td>3.49s,</td>
<td>1.0x</td>
</tr>
<tr>
<td>Intel Xeon E5-2698v3 + 1x Tesla P100</td>
<td>1.35s,</td>
<td>2.5x</td>
</tr>
<tr>
<td>IBM Power8 “Minsky” + 1x Tesla P100</td>
<td>1.09s,</td>
<td>3.3x</td>
</tr>
<tr>
<td>IBM Power8 (ORNL ‘crest’) + 4x Tesla K40 [1]</td>
<td>0.91s,</td>
<td>3.8x</td>
</tr>
<tr>
<td>Intel Xeon E5-2698v3 + 4x Tesla P100</td>
<td>0.37s,</td>
<td>9.4x</td>
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<tr>
<td>IBM Power8 “Minsky” + 4x Tesla P100</td>
<td>0.30s,</td>
<td>11.6x</td>
</tr>
</tbody>
</table>

VMD Tesla V100 Performance for C<sub>60</sub> Molecular Orbitals, 516x519x507 grid

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<tr>
<td>IBM Power8 (ORNL ‘crest’) + 1x Tesla K40 [1]</td>
<td>3.49s,</td>
<td>1.0x</td>
</tr>
<tr>
<td>Intel Xeon E5-2697Av4 + 1x Tesla V100</td>
<td>0.610s,</td>
<td>5.7x</td>
</tr>
<tr>
<td>Intel Xeon E5-2697Av4 + 2x Tesla V100</td>
<td>0.294s,</td>
<td>11.8x</td>
</tr>
<tr>
<td>IBM Power9 “Newell” + 1x Tesla V100</td>
<td>0.394s,</td>
<td>8.8x</td>
</tr>
<tr>
<td>IBM Power9 “Newell” + 2x Tesla V100</td>
<td>0.207s,</td>
<td>16.8x</td>
</tr>
<tr>
<td>IBM Power9 “Newell” + 3x Tesla V100</td>
<td>0.151s,</td>
<td>23.1x</td>
</tr>
<tr>
<td>IBM Power9 “Newell” + 4x Tesla V100</td>
<td>0.130s,</td>
<td>26.8x</td>
</tr>
<tr>
<td>IBM Power9 “Newell” + 6x Tesla V100</td>
<td>0.156s,</td>
<td>22.3x</td>
</tr>
</tbody>
</table>

Acknowledgements

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“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