VMD+OptiX: Bringing Interactive Molecular Ray Tracing from Remote GPU Clusters to your VR Headset

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/
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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
Goal: A Computational Microscope
Study the molecular machines in living cells
Ribosome: target for antibiotics
Poliovirus
Goal: Intuitive interactive viz. in crowded molecular complexes

Results from 64 M atom, 1 μs sim!

Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers
Immersive Viz. w/ VMD

- VMD began as a CAVE app (1993)
- Use of immersive viz by molecular scientists limited due to cost, complexity, lack of local availability, convenience
- Commoditization of HMDs excellent opportunity to overcome cost/availability
- This leaves many challenges still to solve:
  - Incorporate support for remote visualization
  - UIs, multi-user collaboration/interaction
  - Rendering perf for large molecular systems
  - Accommodating limitations idiosyncrasies of commercial HMDs

VMD running in a CAVE w/ VR Juggler
Lighting Comparison

- Two lights, no shadows
- Two lights, hard shadows, 1 shadow ray per light
- Ambient occlusion + two lights, 144 AO rays/hit
Computational Biology’s Insatiable Demand for Processing Power

Number of atoms


- Lysozyme
- ApoA1
- ATP Synthase
- Ribosome
- STMV
- HIV capsid
VMD 1.9.3 + OptiX 3.8 + CUDA 7.0
~1.5x Performance Increase

- OptiX GPU-native “Trbvh” acceleration structure builder yields substantial perf increase vs. CPU builders running on Opteron 6276 CPUs

- New optimizations in VMD TachyonL-OptiX RT engine:
  - CUDA C++ Template specialization of RT kernels
    - Combinatorial expansion of ray-gen and shading kernels at compile-time: stereo on/off, AO on/off, depth-of-field on/off, reflections on/off, etc…
    - Optimal kernels selected from expansions at runtime
  - Streamlined OptiX context and state management
  - Optimization of GPU-specific RT intersection routines, memory layout

VMD/OptiX GPU Ray Tracing of chromatophore w/ lipids.
VMD Molecular Structure Data and Global State

Scene Graph

Graphical Representations
- DrawMolecule
- Non-Molecular Geometry

User Interface Subsystem
- Tcl/Python Scripting
- Mouse + Windows
- VR Input “Tools”

Display Subsystem
- VMDDisplayList
- DisplayDevice
- OpenGLDisplayDevice
- FileRenderer
- Windowed OpenGL GPU
- OpenGL Pbuffer GPU
- Tachyon CPU RT
- TachyonL-OptiX GPU RT
- Batch + Interactive

Scene Graph

Graphical Representations

User Interface Subsystem

Display Subsystem
VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API

Scene Graph

RT Progressive Subframe
- rtContextLaunchProgressive2D()
- Check for User Interface Inputs, Update OptiX Variables
- rtBufferGetProgressiveUpdateReady()
- rtContextStopProgressive()

TrBvh RT Acceleration Structure

Draw Output Framebuffer

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VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node

VMD Scene

Scene Data Replicated, Image Space Parallel Decomposition onto GPUs

TrBvh RT Acceleration Structure

GPU 0
GPU 1
GPU 2
GPU 3

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VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster

Scene Data Replicated, Image Space + Sample Space Parallel Decomposition onto GPUs

VCA 0:
8 K6000 GPUs

VCA N:
8 K6000 GPUs

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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
Stereoscopic Panorama Ray Tracing w/ OptiX

• Render 360° images and movies for VR headsets such as Oculus Rift, Google Cardboard
• Ray trace panoramic stereo spheremaps or cubemaps for very high-frame-rate display via OpenGL texturing onto simple geometry
• Stereo requires spherical camera projections poorly suited to rasterization
• Benefits from OptiX multi-GPU rendering and load balancing, remote visualization
HMD Ray Tracing Challenges

- HMDs require high frame rates (90Hz or more) and minimum latency between IMU sensor reads and presentation on the display.
- Multi-GPU workstations fast enough to direct-drive HMDs at required frame rates for simple scenes with direct lighting, hard shadows.
- Advanced RT effects such as AO lighting, depth of field require much larger sample counts, impractical for direct-driving HMDs.
- Remote viz. required for many HPC problems due to large data.
- Remote viz. latencies too high for direct-drive of HMD.
- Our two-phase approach: moderate-FPS remote RT combined with local high-FPS view-dependent HMD reprojection w/ OpenGL.
VMD+OptiX
Progressive RT Engine

Omnistereo
Image Stream

HMD Quaternion
+ Input Updates

View-dependent
OpenGL HMD
Reprojection
(up to 150 FPS)

Scene
H.264 Video

15Mbps Internet Link

RT @ Remote VCA GPU Cluster
8 to 30 FPS @ 3072x1536
HMD View-Dependent Reprojection with OpenGL

• Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface
• HMD sees standard perspective frustum view of the textured surface
• Commodity HMD optics require software lens distortion and chromatic aberration correction prior to display, implemented with multi-pass FBO rendering
• Low-latency redraw as HMD head pose changes
VMD can support a variety of HMD lens designs, e.g.
Come See A Live Demo!

• Demo shown by collaborators in Indiana U. booth on and off throughout exhibition
• RT @ NVIDIA VCA cluster in Santa Clara, thousands of miles away
• Work-in-progress:
  – 6DOF controller UI
  – Alternative HMD lens designs
Future Work

- Support for more commodity HMDs as they become generally available
- Support for OSes besides Linux
- Ray tracing engine and optimizations:
  - Multi-node parallel RT and remote viz. on general clusters and supercomputers, e.g. NCSA Blue Waters, ORNL Titan
  - Interactive RT stochastic sampling strategies to improve interactivity
  - Improved omnidirectional cubemap/spheremap sampling approaches
- Tons of work to do on VR user interfaces, multi-user collaborative visualization, …
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Visualization Publications
http://www.ks.uiuc.edu/Research/vmd/


- **Unlocking the Full Potential of the Cray XK7 Accelerator.** M. D. Klein and J. E. Stone. Cray Users Group, Lugano Switzerland, May 2014.

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


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


- **An Efficient Library for Parallel Ray Tracing and Animation.** John E. Stone, Master's Thesis, University of Missouri-Rolla, Department of Computer Science, April 1998

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