Interactive High-Fidelity Biomolecular and Cellular Visualization with RTX Ray Tracing APIs

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

15:00-15:50, Room 230B, San Jose Convention Center
San Jose, CA, Wednesday March 20th, 2019
VMD – “Visual Molecular Dynamics”

- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
  - Sequence information
- User extensible scripting and plugins
- Over 100,000 users, 28,000 citations
- http://www.ks.uiuc.edu/Research/vmd/
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 64M atom, 1 μs sim!

Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers
High Fidelity Ray Tracing with OptiX

- Advanced rendering techniques save scientists time, produce images that are easier to interpret
- Ambient Occlusion, Depth of Field, high quality transparency, instancing, ....

- **Interactive RT** on laptop, desk, cloud, and **remote supercomputers**
- Interactivity is critically important for scientists that need to obtain results without becoming a graphics expert

- Large-scale parallel rendering: in situ or post hoc visualization tasks
- **Stereoscopic panorama and full-dome projections**
- **Omnidirectional VR**: YouTube, HMDs
Lighting Comparison, STMV Capsid

Two lights, no shadows

Ambient occlusion + two lights, 144 AO rays/hit
VMD w/ OptiX 6

- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization
- Remote ray tracing with NvPipe video streaming
- Stereoscopic panoramic and full-dome projections
- Omnidirectional VR for YouTube, VR HMDs
- VMD+OptiX NGC container: https://ngc.nvidia.com/registry/
- In-progress:
  - Denoising: faster turnaround w/ AO, DoF, etc

Interactive Ray Tracing of Tomograms

- High resolution cellular tomograms, billions of voxels
- Even isosurface or lattice site graphical representations involve ~100M geometric primitives
- >= 24GB GPUs allow interactive RT of large cellular tomograms

VMD “QuickSurf” Representation, Ray Tracing

All-atom HIV capsid simulations w/ 64M atoms on Blue Waters
VMD/OpiX RTX Acceleration
What is RTX Acceleration Doing?

• Hardware acceleration (Turing RT cores) of:
  – BVH AS traversal
  – Ray-triangle intersection

• BVH AS can embed triangle geometry
  – Triangle geometry buffer can then be ephemeral
Secondary Benefits and RTX Performance Observations

- Traversal and intersection work performed by RT cores vacates GPU SMs and makes them available for other RT work
- RTX hardware traversal performance approaches GPU memory bandwidth limits
- Future RTX hardware could end up being bandwidth bound in some cases
- Start adapting geometric data representations for minimum footprint, e.g. by using compressed or quantized data representations such as Octohedron Normal Vector encoding (replace 3x 32-bit floats with a single 32-bit int)
Ray Tracing Gems

- Ch. 4, “A Planetarium Dome Master Camera”
- Ch. 27, “Interactive Ray Tracing Techniques for High-Fidelity Scientific Visualization”
- Tons of great material and code samples!

- See Eric Haines RTG GTC talk:
  - Room 230B (Concourse Level) on Thursday 2-3 PM

- RTG book signings on Thursday, 3-4pm @ GTC book seller
VMDDisplayList

DisplayDevice

Graphical Representations
- DrawMolecule
- Non-Molecular Geometry

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

Scene Graph

Display Subsystem
- OpenGLDisplayDevice
- FileRenderer

Scene Graph

VMD Molecular Structure Data and Global State
VMD Scene w/ OptiX Classic APIs

Scene Graph

TrBvh RT Acceleration Structure

OptiX Classic Scene Construction

Incoming VMD Geom

All Geometry

Alloc Geom Buffers

Assign Closest-Hit Material Shaders

...
VMD Scene w/ OptiX RTX APIs

Scene Graph

OptiX RTX Scene Construction

Incoming VMD Geom

- General Geometry
- Alloc Geom Buffers
- Assign Closest-Hit Material Shaders
- Triangle Meshes
- Alloc Tri Buffers
- Assign Closest-Hit Material Shaders
  ...

TrBvh RT Acceleration Structure
VMD OptiX RT performance on Quadro RTX 6000

<table>
<thead>
<tr>
<th></th>
<th>Chromatophore @ 4Kx4K</th>
<th>Chrom Cell, 512x DoF @ 1080p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quadro GV100</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2x Quadro GV100</td>
<td>1.97</td>
<td>1.95</td>
</tr>
<tr>
<td>Quadro RTX 6000</td>
<td>8.02</td>
<td>8.18</td>
</tr>
</tbody>
</table>
VMD Planetarium Dome Master Camera

- Fully interactive RT with ambient occlusion, shadows, depth of field, reflections, ...
- Both mono and stereoscopic
- No post-processing required

Ray Tracing Gems Ch. 4
Planetarium Dome Master Projections
NSF CADENS Dome Show w/ NCSA AVL
Birth of Planet Earth Fulldome Show

- Premieres March 28, Zeiss Großplanetarium, Berlin, Germany
- First public showing on March 30, Das Planetarium am Insulaner, Berlin, Germany
- Joint project with:
  - Spitz Creative Media
  - NCSA Advanced Visualization Lab
  - Thomas Lucas Productions, Inc.
  - Tellus Science Museum
- NSF Support: CADENS award ACI-1445176
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
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, …


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, path tracing require **large sample counts**, difficult for direct-driving HMDs today.
- 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.
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 proxy geometry
- Stereo requires spherical camera projections poorly suited to rasterization
- Benefits from OptiX multi-GPU rendering and load balancing, remote visualization
A) Monoscopic circular projection. Eye at center of projection (COP).

B) Left eye stereo circular projection. Eye offset from COP by half of interocular distance.

C) Stereo eye separation smoothly decreased to zero at zenith and nadir points on the polar axis to prevent incorrect stereo when HMD sees the poles.
Satellite Tobacco Mosaic Virus: Capsid, Interior RNA, and Ions
Ambient Occlusion Lighting, Depth-of-Field Focal Blur, …
HIV-1 Capsid, Capsid Hexamer Detail, and Ions
Range-Limited Ambient Occlusion Lighting, VR “Headlight”, …
**Progressive Ray Tracing Engine**
Ray tracing loop runs continuously in new thread

Decodes H.264 video stream from remote VCA GPU cluster

**Omnistereo Image Stream**

**HMD Display Loop**
HMD loop runs in main VMD application thread at max OpenGL draw rate

View-dependent stereo reprojection for current HMD head pose

HMD distortion correction

**Camera + Scene**

**Remote VCA GPU Cluster**
Ray tracing runs continuously, streams H.264 video to VMD client

**15Mbps Internet Link**

**VMD**
## 2016: Remote Omnidirectional Stereoscopic RT Performance @ 3072x1536 w/ 2-subframes

<table>
<thead>
<tr>
<th>Scene</th>
<th>Per-subframe samples AA : AO (AO per-hit)</th>
<th>RT update rate (FPS)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>STMV shadows</strong></td>
<td>1:0</td>
<td>22.2, 18.1, 10.3</td>
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<td>2:0</td>
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<td>4:0</td>
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<tr>
<td><strong>STMV Shadows+AO</strong></td>
<td>1:1</td>
<td>18.2, 16.1, 12.4</td>
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<td>1:2</td>
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<td></td>
<td>1:4</td>
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<tr>
<td><strong>STMV Shadows+AO+DoF</strong></td>
<td>1:1</td>
<td>16.1, 11.1, 8.5</td>
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<tr>
<td><strong>HIV-1 Shadows</strong></td>
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<td>20.1, 18.1, 10.2</td>
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<td><strong>HIV-1 Shadows+AO</strong></td>
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<td>17.4, 12.2, 8.1</td>
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## 2019: Local RTX Omnidirectional Stereoscopic RT Performance @ 3072x1536 w/ 1-subframe

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<td>STMV Shadows+AO</td>
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<td>STMV Shadows+AO+DoF</td>
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<td>HIV-1 Shadows+AO</td>
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<td>72.0, 61.0, 37.5, 23.1</td>
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HMD View-Dependent Reprojection with OpenGL

• Texture map panoramic image onto reprojection geometry that matches the original RT image formation surface (sphere for equirectangular, cube for cube map)
• 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
• Enables low-latency, high-frame-rate redraw as HMD head pose changes (150Hz or more)
Ongoing Ray Traced VR Work

• OpenXR – cross platform multi-vendor HMD support

• VMD RTX 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, …
Next Generation: Simulating a Proto-Cell

- ORNL Summit: NVLink-connected Tesla V100 GPUs enable next-gen visualizations
- 200nm diameter
- ~1 billion atoms w/ solvent
- ~1400 proteins in membrane
NVIDIA DGX-2
16x 32GB Tesla V100 GPUs w/ 300GB/s NVLink, fully switched
512GB HBM2 RAM w/ 2.4TB/s Bisection Bandwidth, 2 PFLOPS
RT Opportunities and Challenges Posed by Future DGX-2-Like Node/System Designs

- 512GB of fast HBM2 RAM w/ 2.4TB/sec bisection bandwidth!!!
- CPUs “oversubscribed” by GPUs
- GPU RT must dis-involve CPUs to greatest possible extent
- Fully-switched NVLink-connected memory systems permit fine-grained multi-GPU RT algorithms via direct peer memory load/stores
- Throughput oriented GPU RT work scheduling can hide both local and remote memory latencies gracefully
- Application control of the distribution of scene geometry among GPUs, replication or distribution of RT acceleration structures
- Permit both “capacity” oriented distributed memory RT approaches and “performance” focused RT approaches heavy on data replication.
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Making Our Research Tools Easily Accessible

- 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/
  - https://ngc.nvidia.com/registry/hpc-vmd

- 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/


VMD / NAMD / LM, NGC Containers

VMD

VMD is designed for modeling, visualization, and analysis of biomolecular systems such as proteins, nucleic acids, lipid membranes, carbohydrate structures, etc. VMD provides a wide variety of graphical representations for visualizing and coloring molecular structures: molecular surfaces, space-filling CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, secondary structure cartoons, and others.

VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VMD can act as a graphical front end for an external MD program by rendering the trajectory and providing additional analysis functions.
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

Acknowledgements

• Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
• NVIDIA CUDA and OptiX teams
• Funding:
  – NIH support: P41GM104601
  – DOE INCITE, ORNL Titan: DE-AC05-00OR22725
  – NSF Blue Waters:
    NSF OCI 07-25070, PRAC “The Computational Microscope”,
    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
Related Publications
http://www.ks.uiuc.edu/Research/gpu/


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


• **Chemical Visualization of Human Pathogens: the Retroviral Capsids.** Juan R. Perilla, Boon Chong Goh, John E. Stone, and Klaus Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.


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


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