Molecular Modeling, Visualization, and Analysis in VMD

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

MMBioS – Computational Biophysics Virtual Workshop 2021
June 30th, 2021
VMD – “Visual Molecular Dynamics”

- 125,000 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](image1.png)

![MD Simulation](image2.png)

![Structure](image3.png)

X-ray, cryo-EM, cryo-ET, NMR

Parameterization

Refinement with MDFF

Preparation with QwikMD

Analysis

MD/Cell Simulation

Parallel Analysis

Remote Visualization
VMD Hands-On Tutorials

- [http://www.ks.uiuc.edu/Training/Tutorials/#vmd](http://www.ks.uiuc.edu/Training/Tutorials/#vmd)
  - Main VMD tutorial
  - QwikMD simulation preparation and analysis plugin
  - VMD images and movies tutorial
  - Structure check
  - VMD quantum chemistry visualization tutorial
  - Visualization and analysis of CPMD data with VMD
  - Parameterizing small molecules using ffTK
VMD: Building A Next Generation Modeling Platform

- Provide tools for simulation preparation, visualization, and analysis
  - Reach cell-scale modeling w/ all-atom MD, coarse grained, Lattice Microbes
  - Improved performance, visual fidelity, exploit advanced technologies (GPUs, VR HMDs)
- Enable hybrid modeling and computational electron microscopy
  - Load, filter, process, interpret, visualize multi-modal structural information
- Connect key software tools to enable state-of-the-art simulations
  - Support new data types, file formats, software interfaces
- Openness, extensibility, and interoperability are VMD hallmarks
  - Reusable algorithms made available in NAMD, for other tools
QwikMD: Guided MD Simulation and Training

Smoothes 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

### Selected VMD Plugins: Center Developed, and User Developed

#### Analysis
- APBSRun
- CatDCD
- Contact Map
- GofRGUI
- HeatMapper
- ILSTools
- IRSpecGUI
- MultiSeq
- NAMD Energy
- NAMD Plot
- NetworkView
- NMWiz
- ParseFEP
- PBCTools
- PMEpot
- 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
- ffTK
- Inorganic Builder
- MDFF
- Membrane
- Merge Structs
- Molefacture
- Mutator
- Nanotube
- Psfgen
- RESPTool

#### 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

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

#### 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

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

[http://www.ks.uiuc.edu/Research/vmd/plugins/]
Parallel MDFF Cross Correlation Analysis on Cray XK7

Rabbit Hemorrhagic Disease Virus (RHDV)

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

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

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
High Fidelity Ray Tracing

- 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 laptops, desk, cloud, and remote supercomputers
- **Large-scale MPI parallel rendering:** in situ or post hoc visualization tasks
- Stereoscopic panorama and full-dome projections
- **Omnidirectional VR:** YouTube, HMDs
- Built-in ray tracing engines:
  - **Tachyon:** cross-platform RT
  - **NVIDIA OptiX:** GPU RTX-accelerated
  - **Intel OSPRay:** CPU x86-optimized

VMD/OptiX all-atom Chromatophore
Lighting Comparison, STMV Capsid

Two lights, no shadows

Ambient occlusion + two lights, 144 AO rays/hit
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
Faraday Discussions
Volume: 169
Molecular Simulations and Visualization

Atomic structure of the AIDS pathogen's protein coat
PAGE 643

THE FIRST LIGHT
In pursuit of the most distant galaxies
PAGE 56

CROSSING THE BORDERS
International collaboration makes the most impact
PAGE 35

A SITTING TARGET
An indirect hit on "undruggable" KRAS protein
PAGE 307 & 308
VMD “Coming Soon”: VMD 1.9.4 and VMD-Next
VMD 1.9.4, and VMD-Next

- Python 3.x support
- New “molefacture” structure editor plugin
- Improved structure building and analysis tools
- High performance GPU structure+data clustering
- Density map and volume processing features: high performance GPU image segmentation, density map simulation, masking, visualization
- Many new and updated user-contributed plugins
- Deeper integration of interactive ray tracing
  - Seamless interactive RT in main VMD display window
  - Support trajectory playback in interactive RT
  - Enable multi-node interactive RT on HPC systems
- Built-in (basic) interactive remote visualization on HPC clusters and supercomputers

GPU Ray Tracing of HIV-1 Capsid Detail
Density Map Segmentation

VMD GPU-accelerated density map segmentation of GroEL

New VMD MDFF Density Map Tools

- **New** Map Tools tab of MDFF GUI provides wide array of density map manipulation tools including:
  - **New** Rigid Body Fitting
  - **New** Interactive Histogram
  - Trim, Crop, Clamp, Smooth…
  - **Easy Masking routine**

- **New** Density Segmentation
- Add, subtract, multiply maps
- Cross correlation and potential calculations for MDFF
New Density Map Tools - Masking

Easily select and mask density map regions with VMD selection language

TRPV1 structure (3J5P) and cryo-EM density (emd-5778) colored by local resolution obtained by ResMap

High Res (~3 Å)
Med Res (~4 Å)
Low Res (~5 Å)

Clustering Analysis of Molecular Dynamics Trajectories: Requires I/O+Memory for All-Pairs of Trajectory Frames

VMD w/ OptiX RTX Ray Tracing

- 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/
- GPU memory sharing via NVLink
- In-progress:
  - Denoising: faster turnaround w/ AO, DoF, etc


VMD/OptiX GPU Ray Tracing of all-atom Chromatophore w/ lipids.
VMD/OptiX RTX Acceleration
VMD OptiX RT performance on Quadro RTX 6000

<table>
<thead>
<tr>
<th></th>
<th>Chromatophore @ 4Kx4K</th>
<th>Chrom Cell, 512x DoF @ 1080p</th>
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<tbody>
<tr>
<td><strong>Quadro GV100</strong></td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td><strong>2x Quadro GV100</strong></td>
<td>1.97</td>
<td>1.95</td>
</tr>
<tr>
<td><strong>Quadro RTX 6000</strong></td>
<td>8.02</td>
<td>8.18</td>
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VMD Cinematic Molecular Visualization and Rendering: “Birth of Planet Earth” Fulldome Show
https://www.youtube.com/watch?v=NTgAok6n7l4

VMD RTX Performance Gains for “BoPE” Content:
• BoPE production used Quadro M6000 (Maxwell) GPUs
• BoPE w/ OptiX 6.5 on Quadro RTX 6000 up to 15x faster!

Multiscale modeling and cinematic visualization of photosynthetic energy conversion processes from electronic to cell scales.
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


VMD Examples from In-Progress ANARI Renderers

https://www.khronos.org/anari

Tachyon Ray Tracer
OSPRay Path Tracer
OptiX Path Tracer
VMD+Folding@Home w/ NVIDIA Omniverse+Maya

The diagram illustrates the evolution of molecular structures over time, starting from 1990 to 2020. Key structures include:

- **HIV capsid**
- **Protocell**
- **ATP synthase**
- **Aquaporin**
- **Lysozyme**
- **STMV**

Each structure is annotated with the number of atoms it contains, represented on a logarithmic scale from $10^4$ to $10^9$. The year scale spans from 1990 to 2020.
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  – NSF Support: CADENS award ACI-1445176
“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