VMD 1.8.7 –
Key Features of Recent Release

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

Quick Summary of Features

- Broader platform support

- Updated user interfaces

- Accelerated analysis, rendering, display:
multi-core CPUs, GPUs (CUDA)

- New graphical representations

- Many new rendering features

- New analysis features, atom selection commands

- New and updated VMD plugins

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Updated User Interfaces

- New color scheme

- New rendering controls

- 6DOF input w/ Spacenavigator
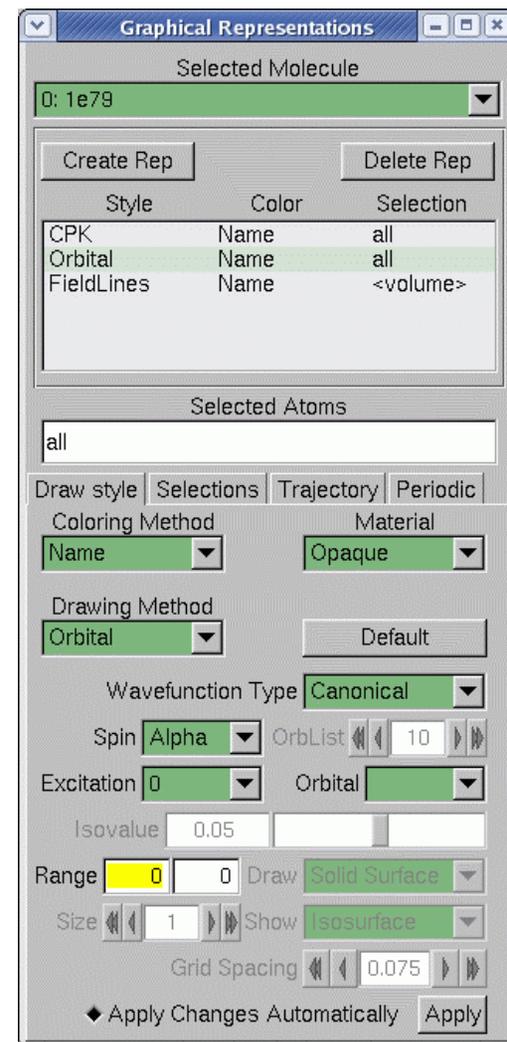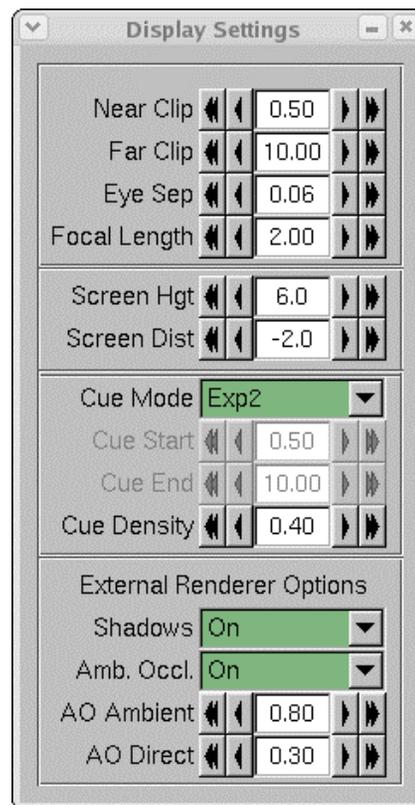
Supported Platforms

- Standard Builds:
  - MacOS X 10.4.x (PowerPC/x86)
  - MacOS X 10.5.x (x86 + CUDA)
  - Linux (32-bit/64-bit x86 + CUDA)
  - Solaris 10 (64-bit Sparc/x86)
  - Windows XP/Vista/7 (32-bit x86 + CUDA)

- Text-mode Analysis Builds:
  - AIX 6.x (64-bit Power)
  - Linux (64-bit PowerPC)
 - Many more platforms via builds from source

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Multi-core Acceleration

- Multi-core CPUs now supported on all VMD platforms, they speed up a broad range of features:
  - "within" distance-based atom selections
  - molecular orbital representation
  - electrostatic map calculations
  - calculation of radial distribution functions
  - implicit ligand sampling
  - distance-based bond search
  - interactive molecular dynamics
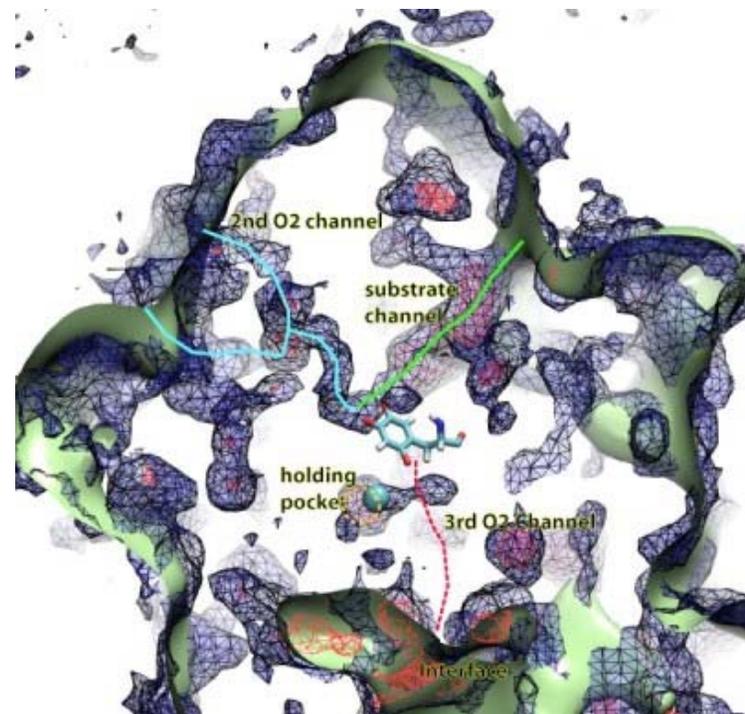 - CAVE/FreeVR virtual reality displays
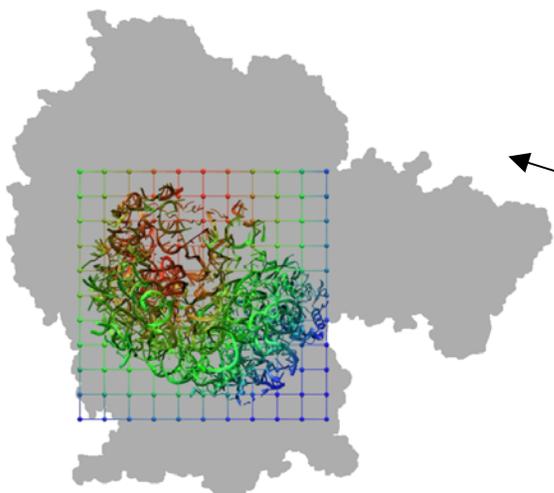
GPU Acceleration (CUDA)
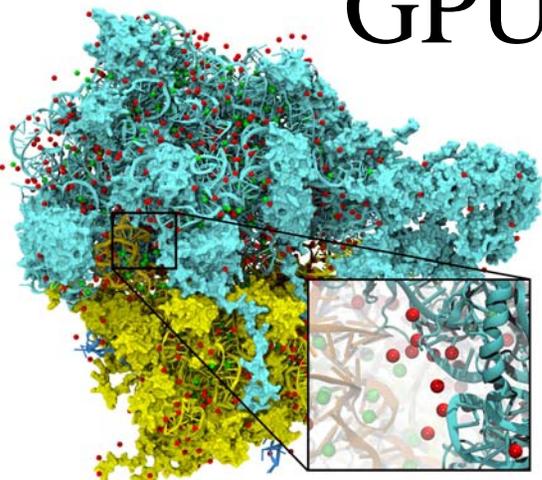
Electrostatic field

calculation, ion placement:

factor of 20x to 44x faster
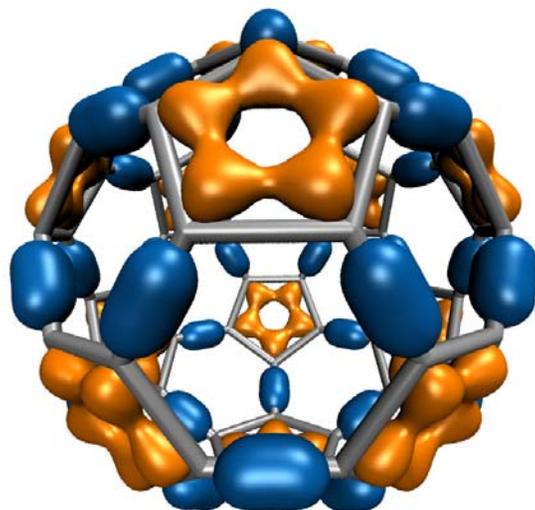
Molecular orbital

calculation and display:
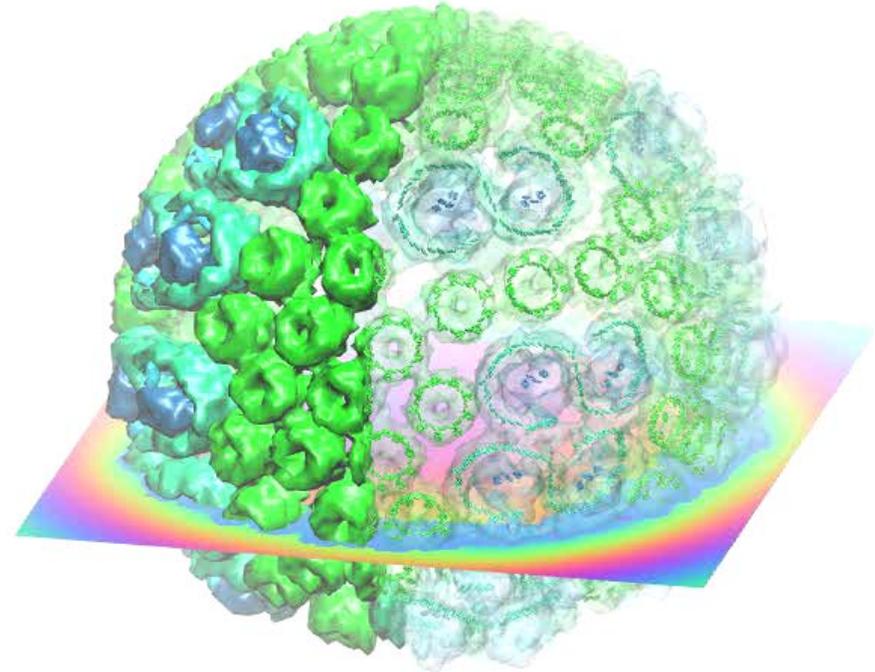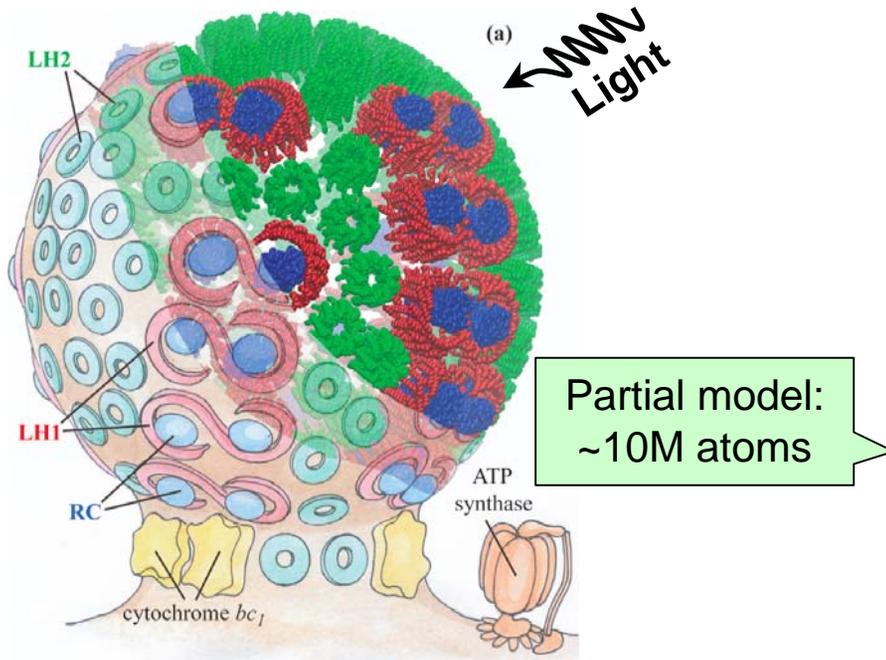
factor of 120x faster

Imaging of gas migration
pathways in proteins with
implicit ligand sampling:

factor of 20x to 30x faster

2nd O2 channel

substrate channel

holding pocket

3rd O2 channel

interface

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Photobiology of Vision and Photosynthesis
Investigations of the chromatophore, a photosynthetic organelle


Electrostatics needed to build full structural model, place ions, study macroscopic properties

Electrostatic field of chromatophore model from multilevel summation method: computed with 3 GPUs (G80) in ~90 seconds, 46x faster than single CPU core

Full chromatophore model will permit structural, chemical and kinetic investigations at a structural systems biology level

# Visualization of Quantum Chemistry Simulations

- New "Orbital" graphical representation

- Plugin interfaces extended for QM information

- New plugin for GAMESS

- Plugins for Gaussian and other QM packages in-development

- Fast: uses SSE, multi-core CPUs, and GPUs for speed
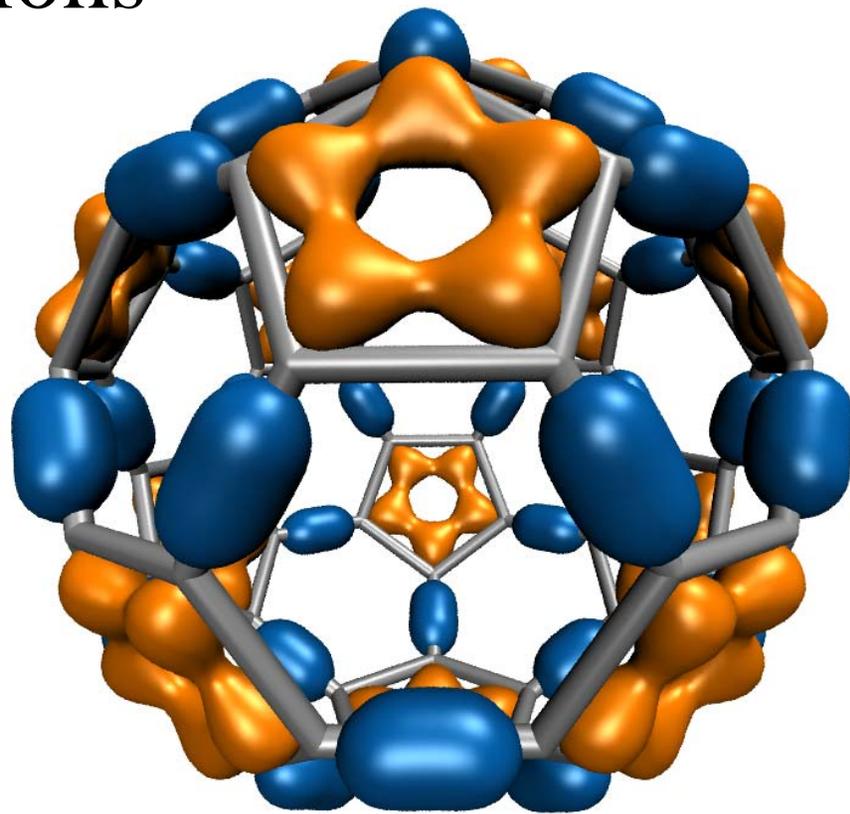
C_{60}

Visualization of Carbohydrates, Multi-branched Structures

- New "PaperChain" and "Twister" graphical representations

- Draw ring structures, colored by "pucker"

- Ribbon-like representations for multi-branched structures

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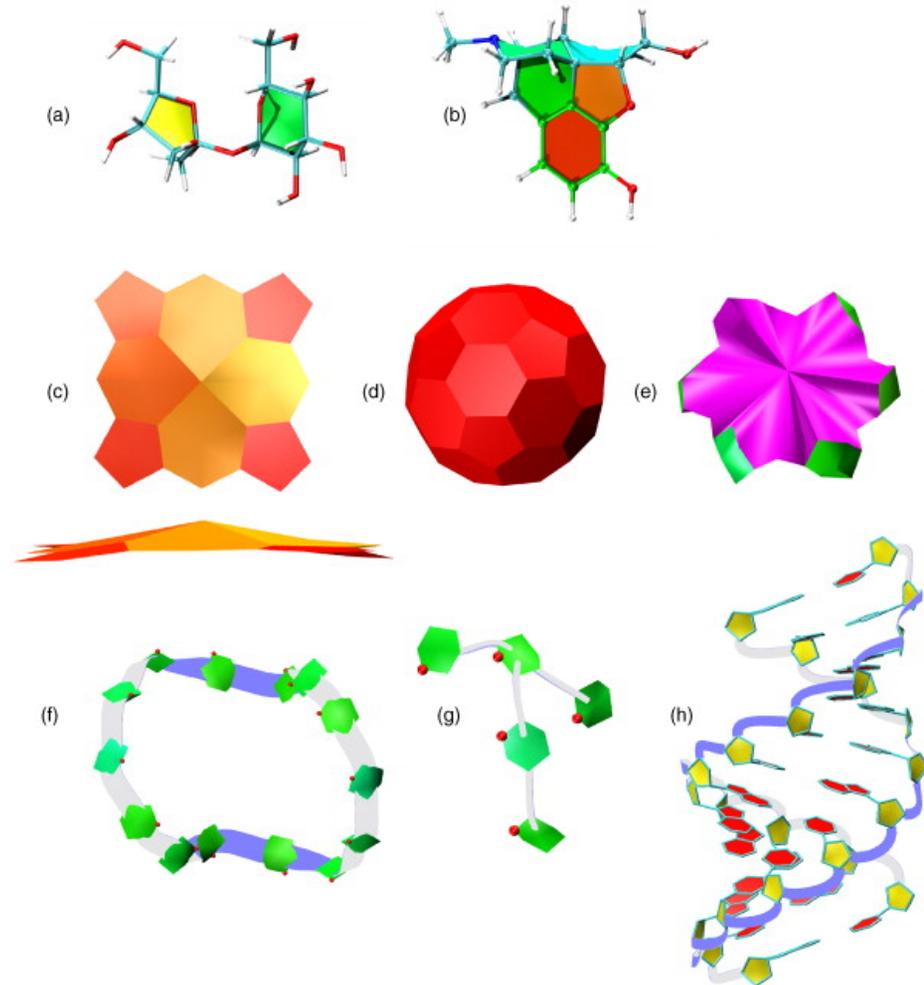
VMD Outline Material Property

- Accentuates the edges of surfaces

- Render CG systems with uniform particle types

- Can be used to emulate David Goodsell's renderings

- Good for grayscale renderings
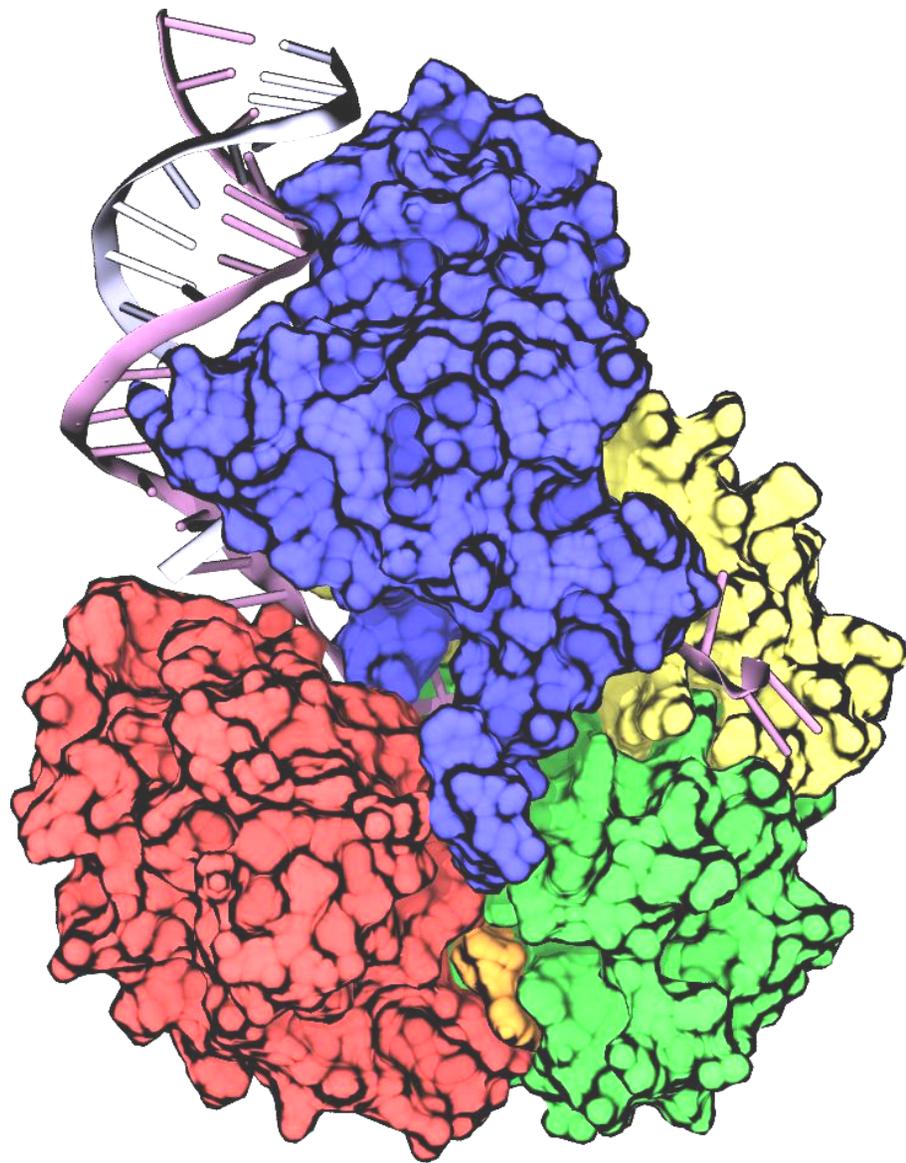
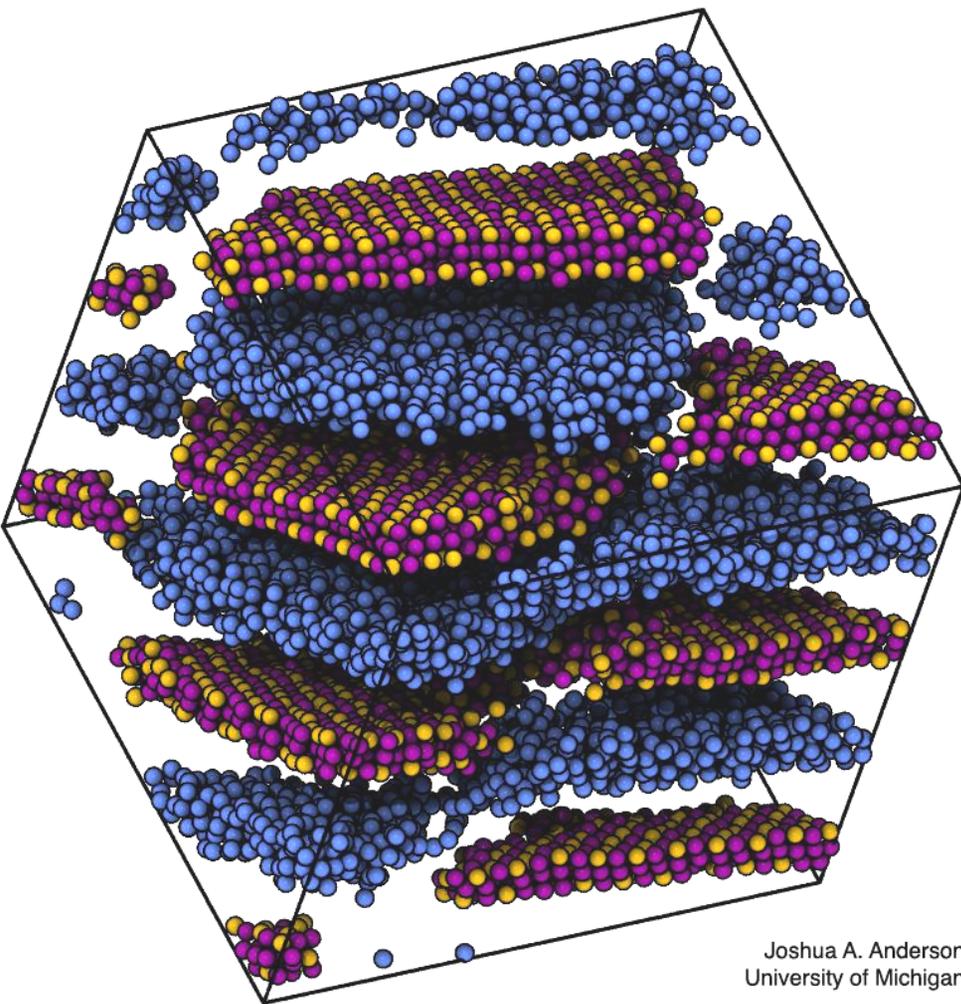- Supported in GLSL mode, Tachyon renderings

Joshua A. Anderson
University of Michigan

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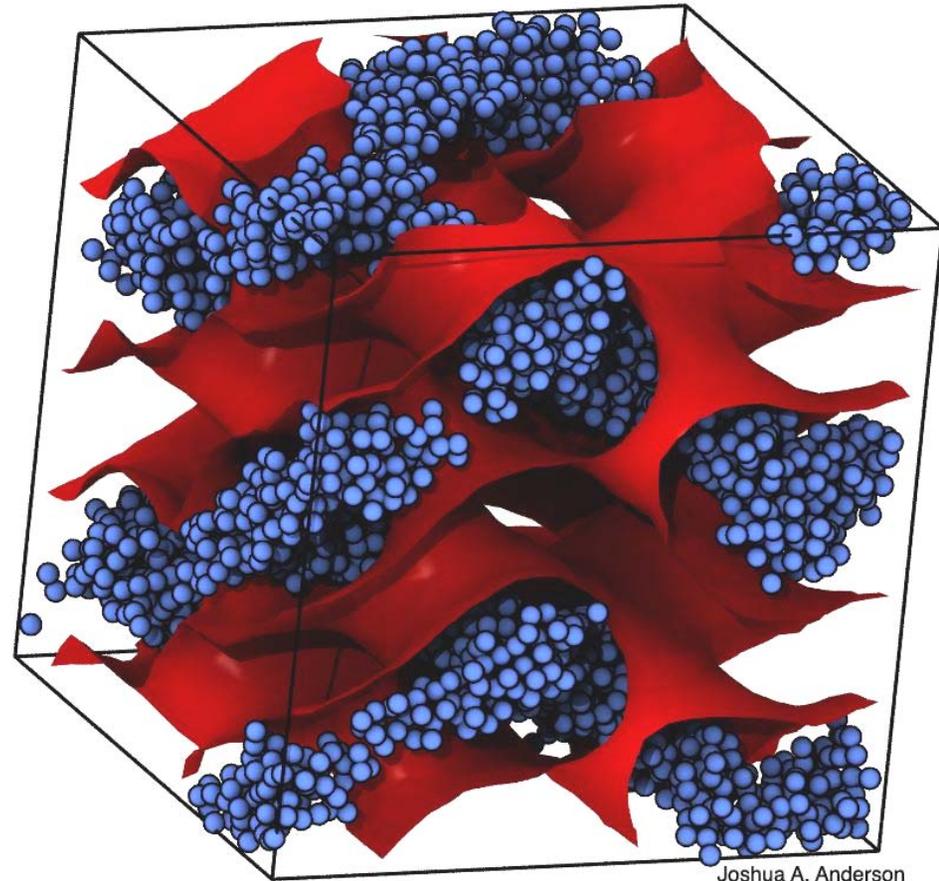
VMD Outline Material Property
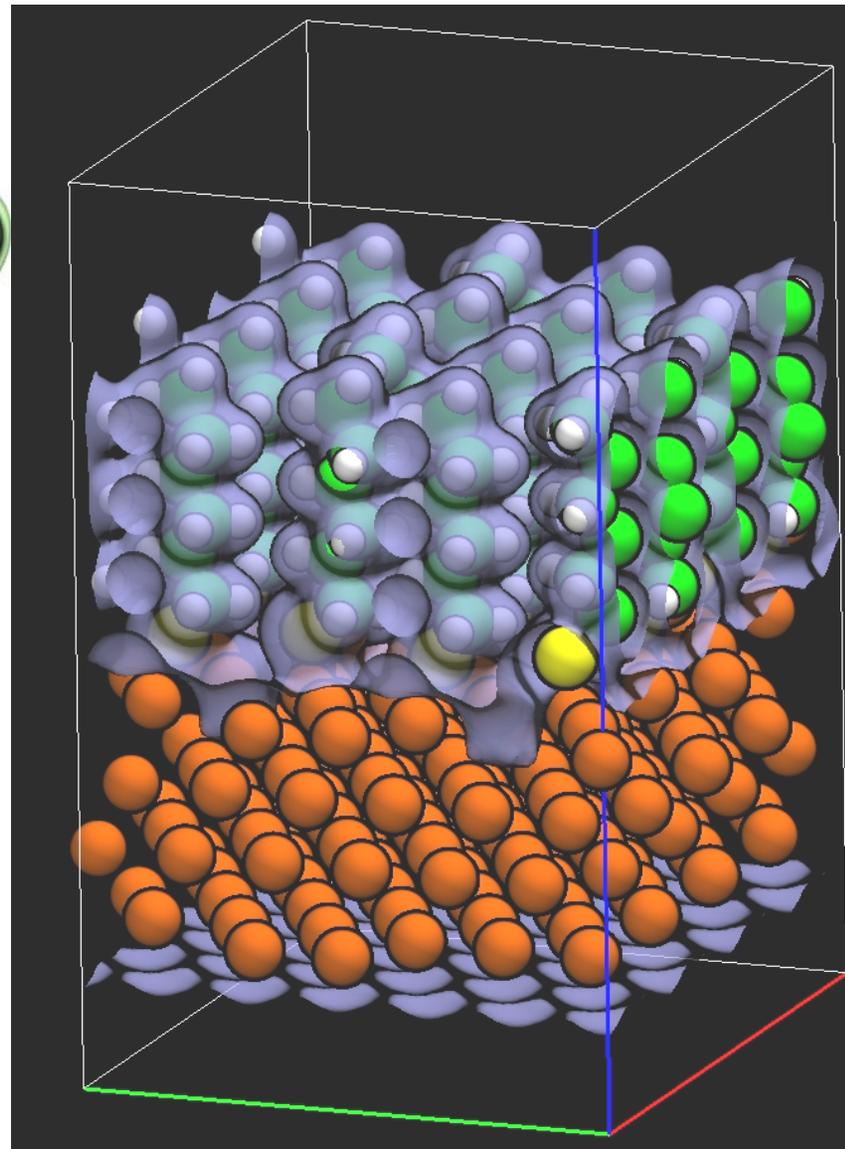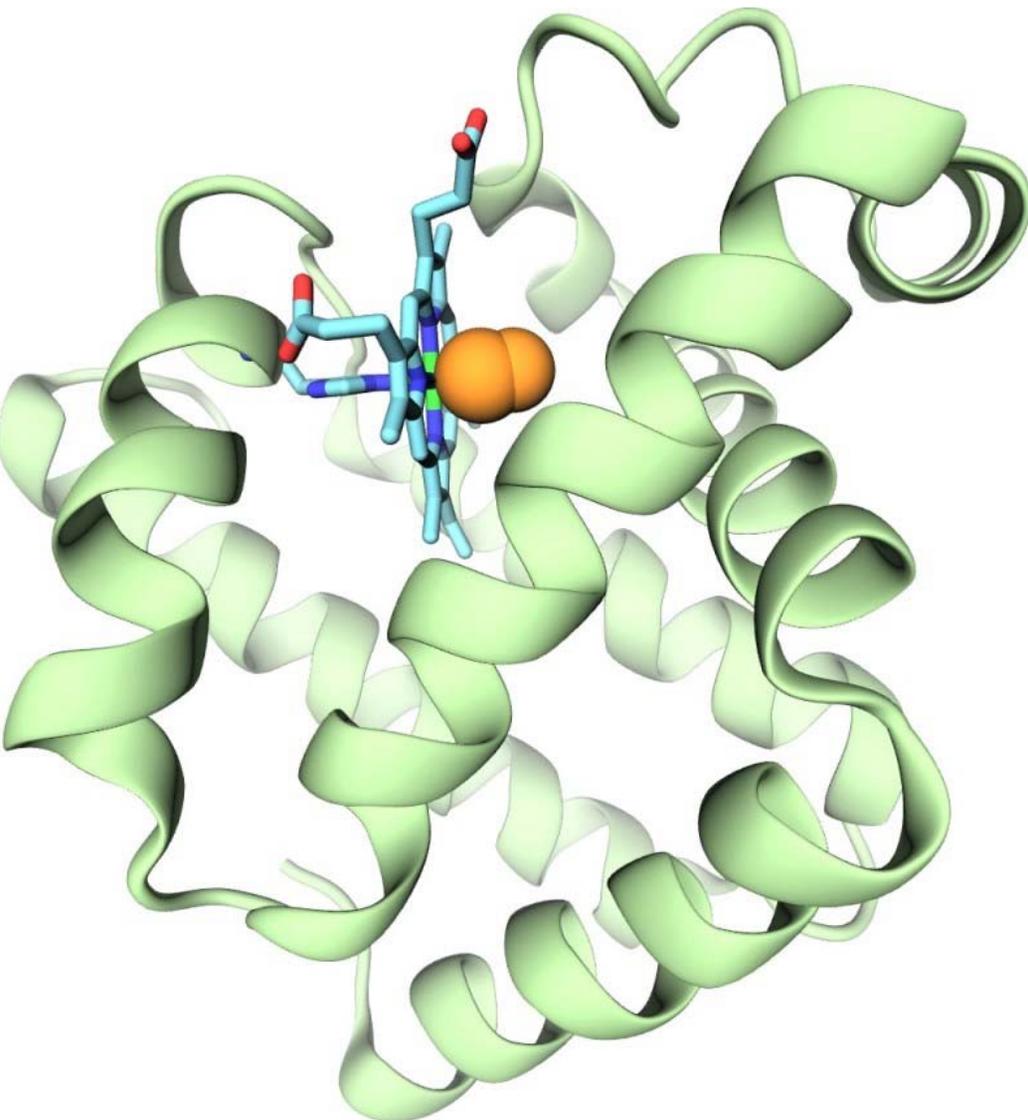
VMD Outline Material Property

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NIH Resource for Macromolecular M
http://www.ks.u

National Center for
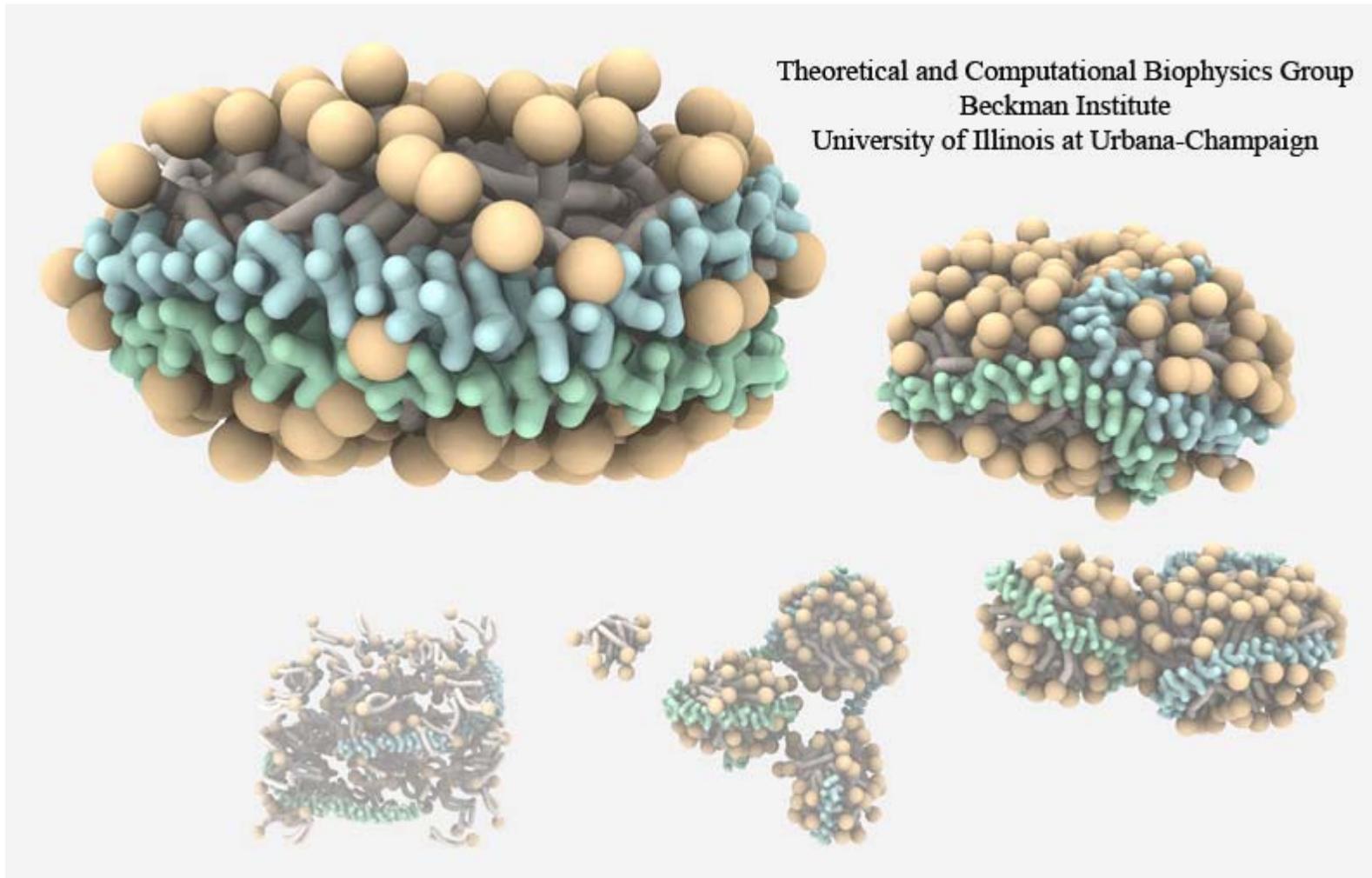Research Resources

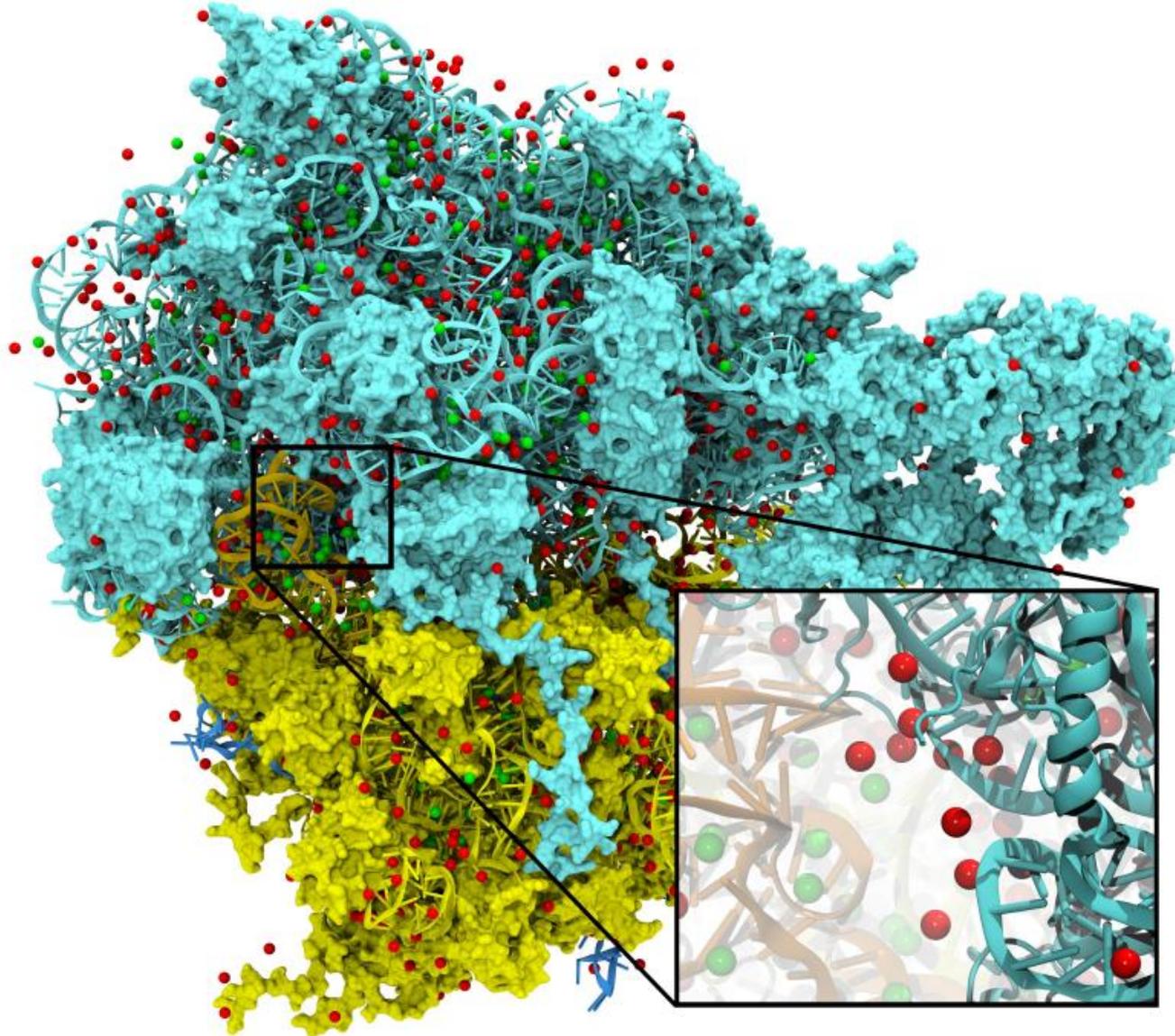# VMD/Tachyon Rendering Advancements: Ambient Occlusion Lighting

- Diffuse omnidirectional lighting

- Creates "soft" shadows

- Enhances shape perception, visibility of pockets and cavities

- Built-in AO GUI controls

- New VMD/Tachyon renders AO over 10 times faster than before

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Ambient Occlusion Rendering Examples

Theoretical and Computational Biophysics Group
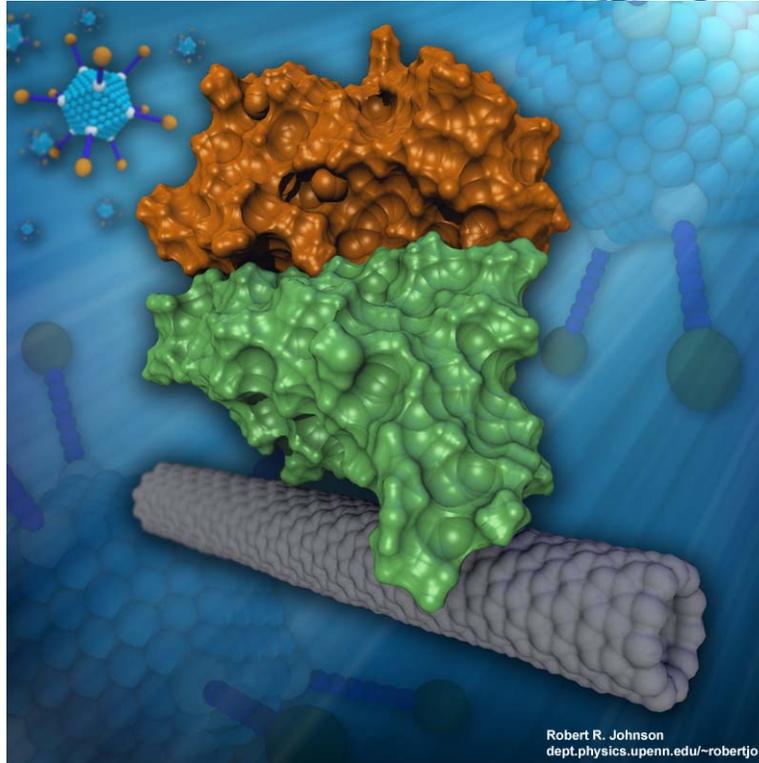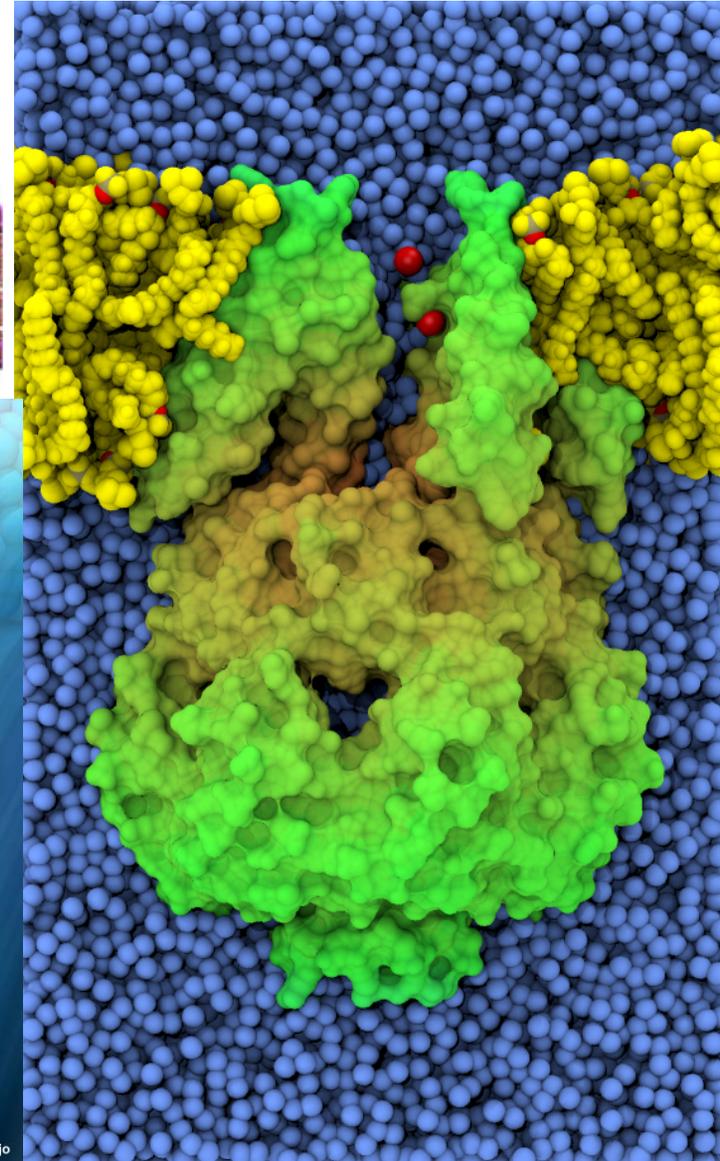Beckman Institute
University of Illinois at Urbana-Champaign
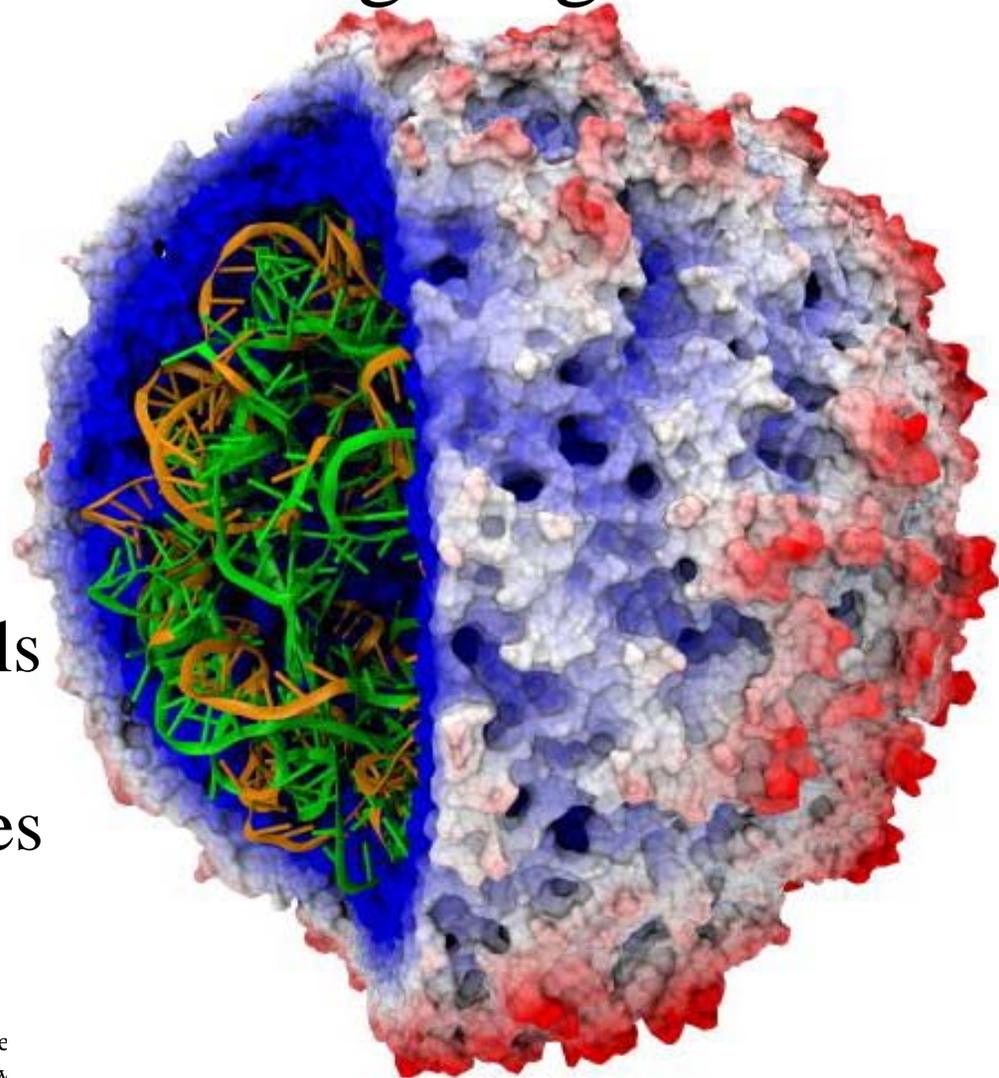
Ambient Occlusion Rendering Examples

Ambient Occlusion Rendering Examples

Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

Robert R. Johnson
dept.physics.upenn.edu/~robertjo
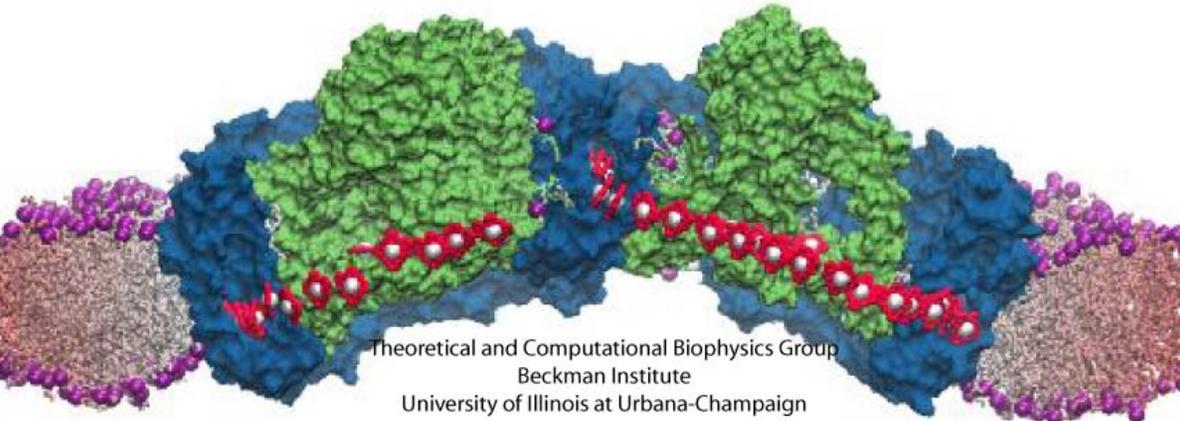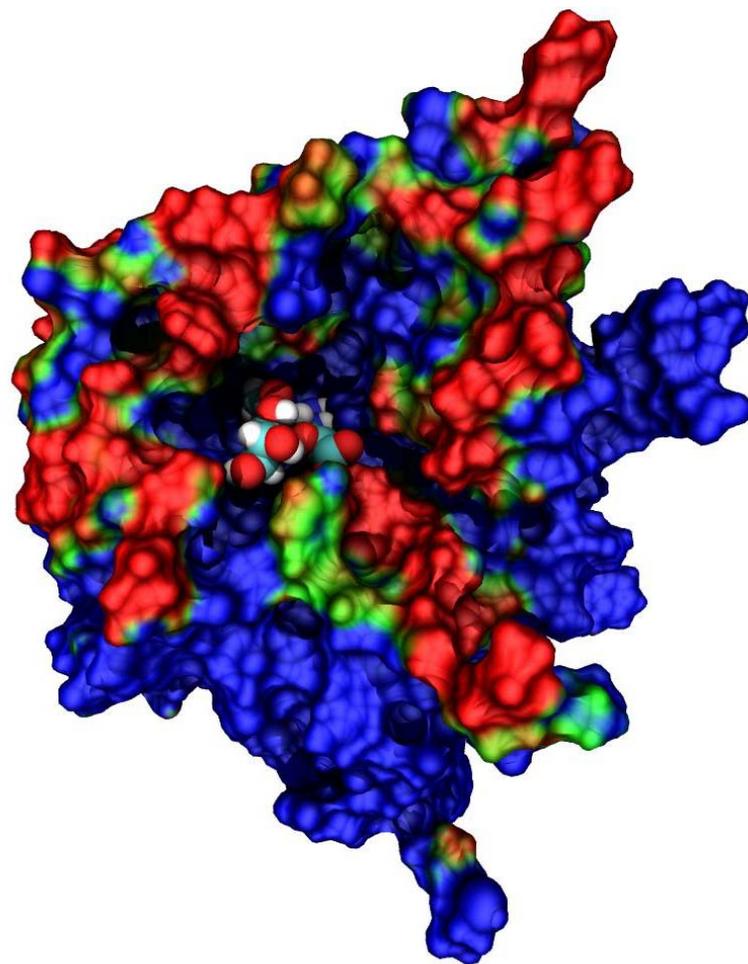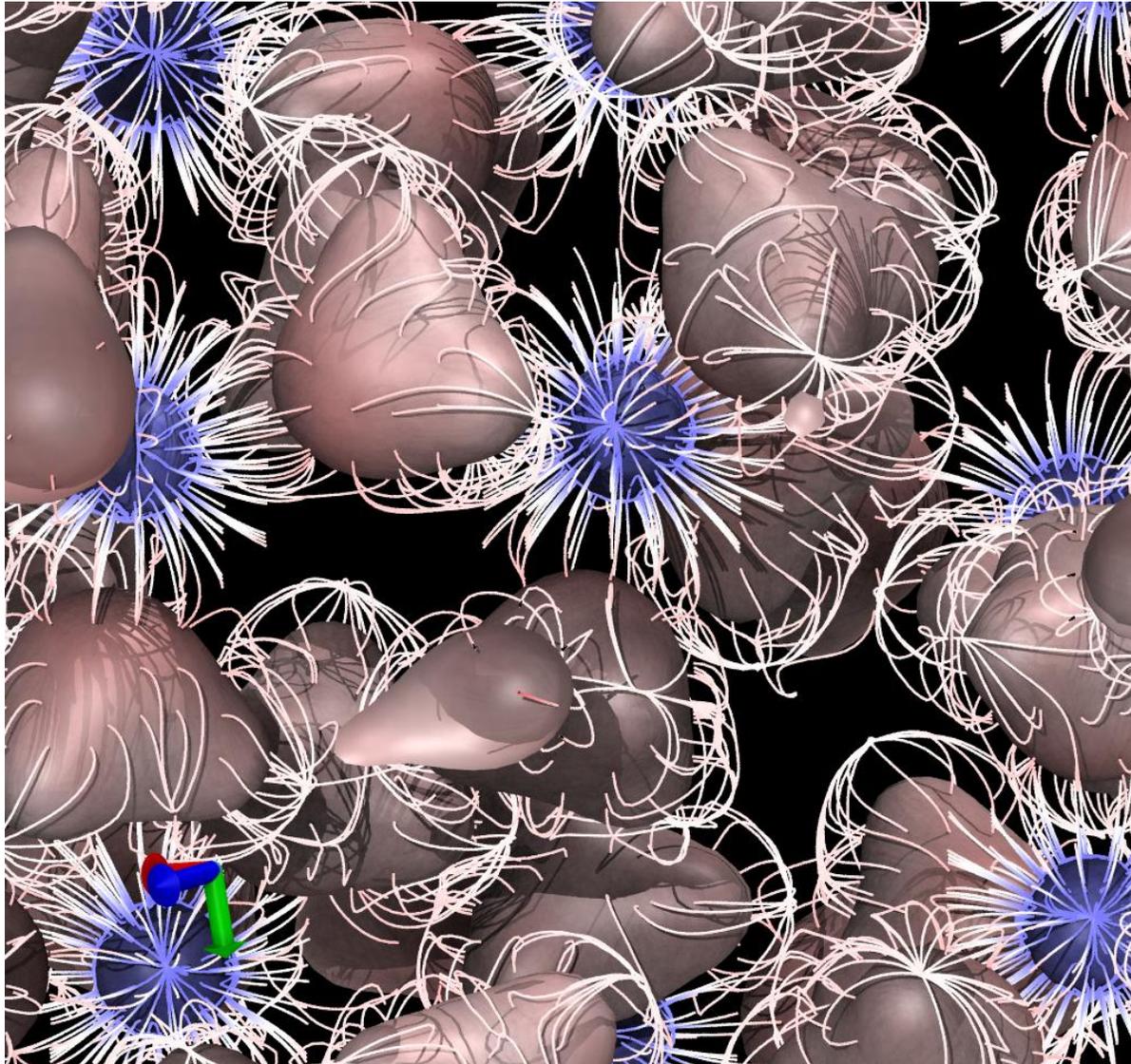
VMD/Tachyon Volumetric Coloring

- Color by potential, density, other volumetric data

- Applies to any representation

- Most commonly used with surfaces, field lines, etc.

- Can now be combined with AO rendering via Tachyon

Volumetric Coloring Example

Beckman Institute, UIUC

Internal Tachyon Renderer

- "TachyonInternal" now available on all platforms

- Directly renders VMD scene to output image file without making intermediate ".dat" files

- Greatly reduced I/O time and disk space usage enables much faster rendering of high quality movies

New/Updated Analysis Features

- New atom selection keywords:
  - "withinbonds" – select atoms connected within N or fewer bonds from candidate selection
  - "ringsize" – find rings structures containing N atoms
  - "maxringsize" – find rings containing up to N atoms

- New atom selection value fields (or queries):
  - "user2", "user3", "user4" – per-atom, per-timestep data fields for use by user scripts
  - "pucker" – return Cremer-Pople pucker for a selected ring structure (size 5 or 6)
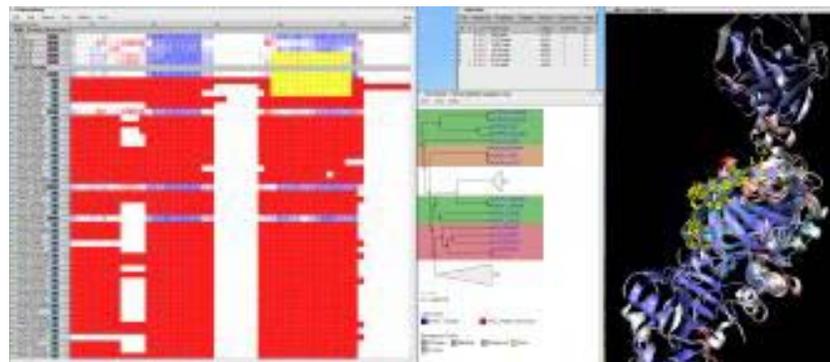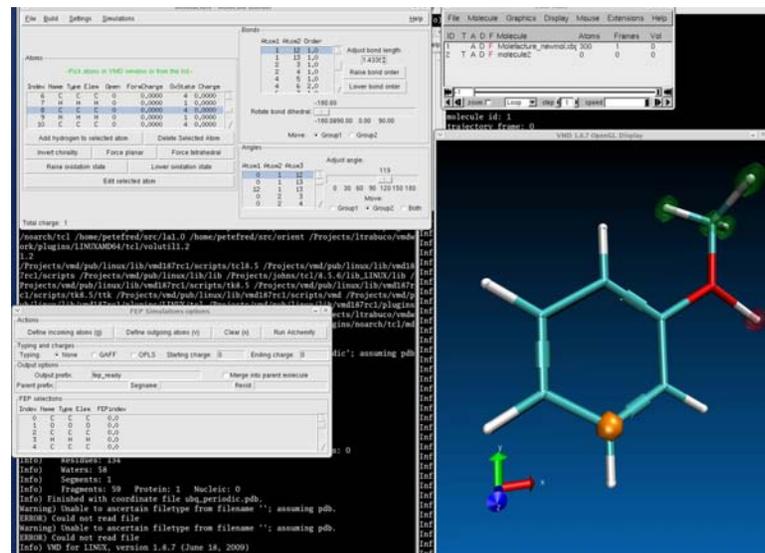 - "vx", "vy", "vz" – per-atom, per-timestep velocities

New/Updated Analysis Features

- Meausre commands:
  - "measure surface" – find atoms on the surface of a selection
  - "measure inertia" – compute COM, axes of inertia, moments of inertia, etc
  - "measure symmetry" – finds molecular symmetry for an atom selection
- Many others, see VMD User's Guide for details on new and updated measure commands, atom selection keywords, etc.

New and Updated Plugins:
http://www.ks.uiuc.edu/Research/vmd/plugins/

- Structure building

- Analysis

- Visualization

- Further discussion of new plugins in Wednesday and Friday sessions

Future VMD Development…