Tips and Tricks to Render Images of Biomolecules in VMD

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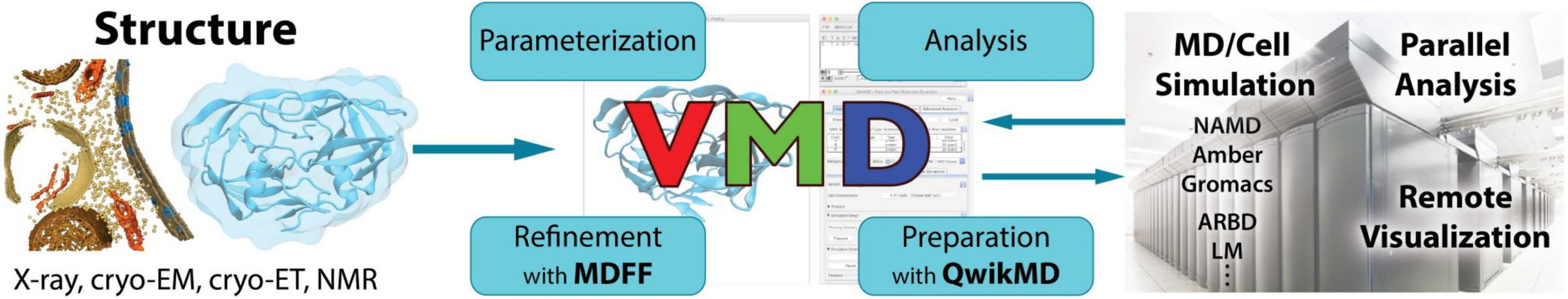
VMD Tutorial Home Page

- http://www.ks.uiuc.edu/Training/Tutorials/
  - Main VMD tutorial
  - QwikMD simulation preparation and analysis plugin
  - VMD images and movies tutorial
  - Structure check
  - Parameterizing small molecules using ffTK

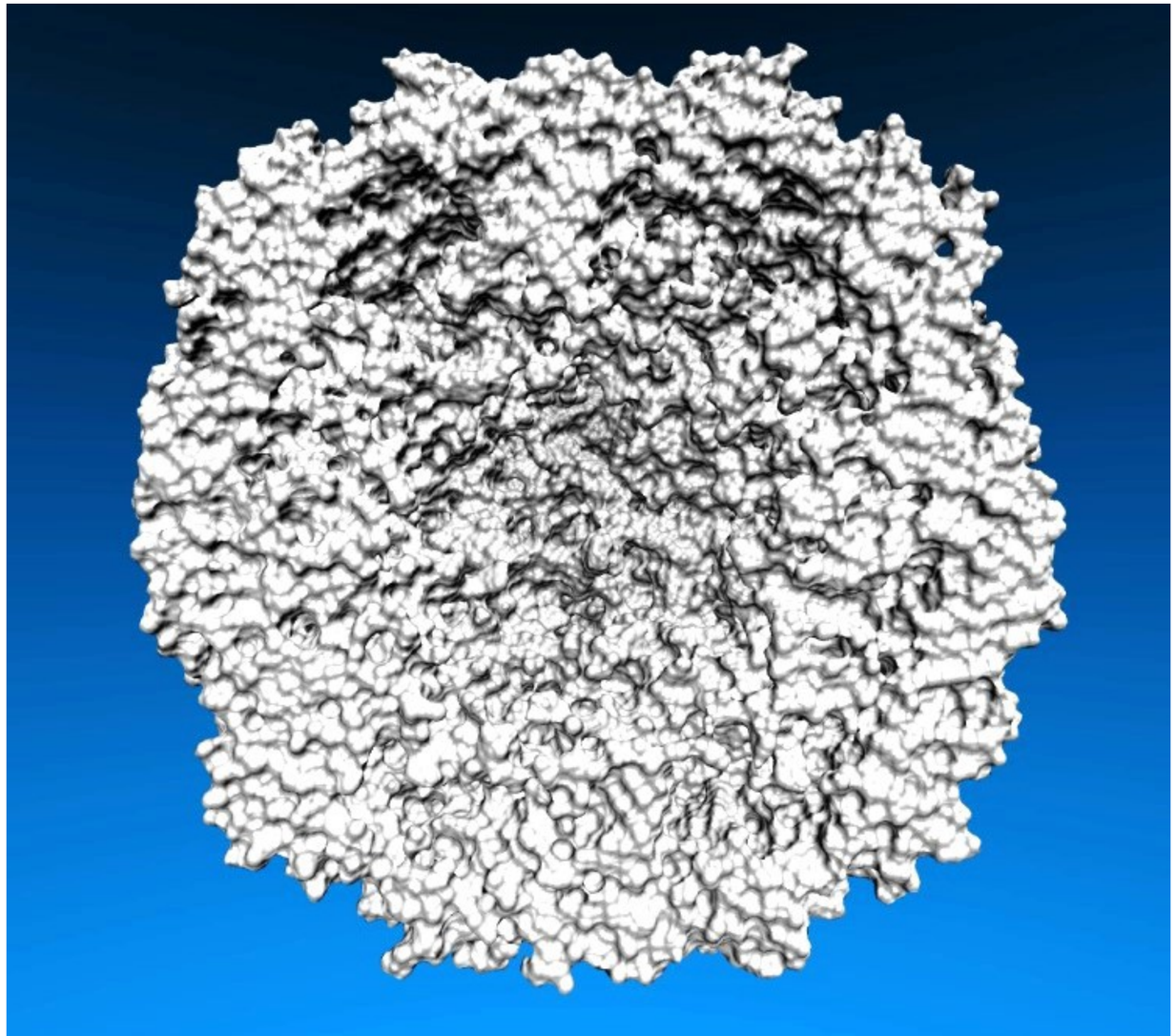
VMD Interoperates with Mainstream Research Tools

- 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

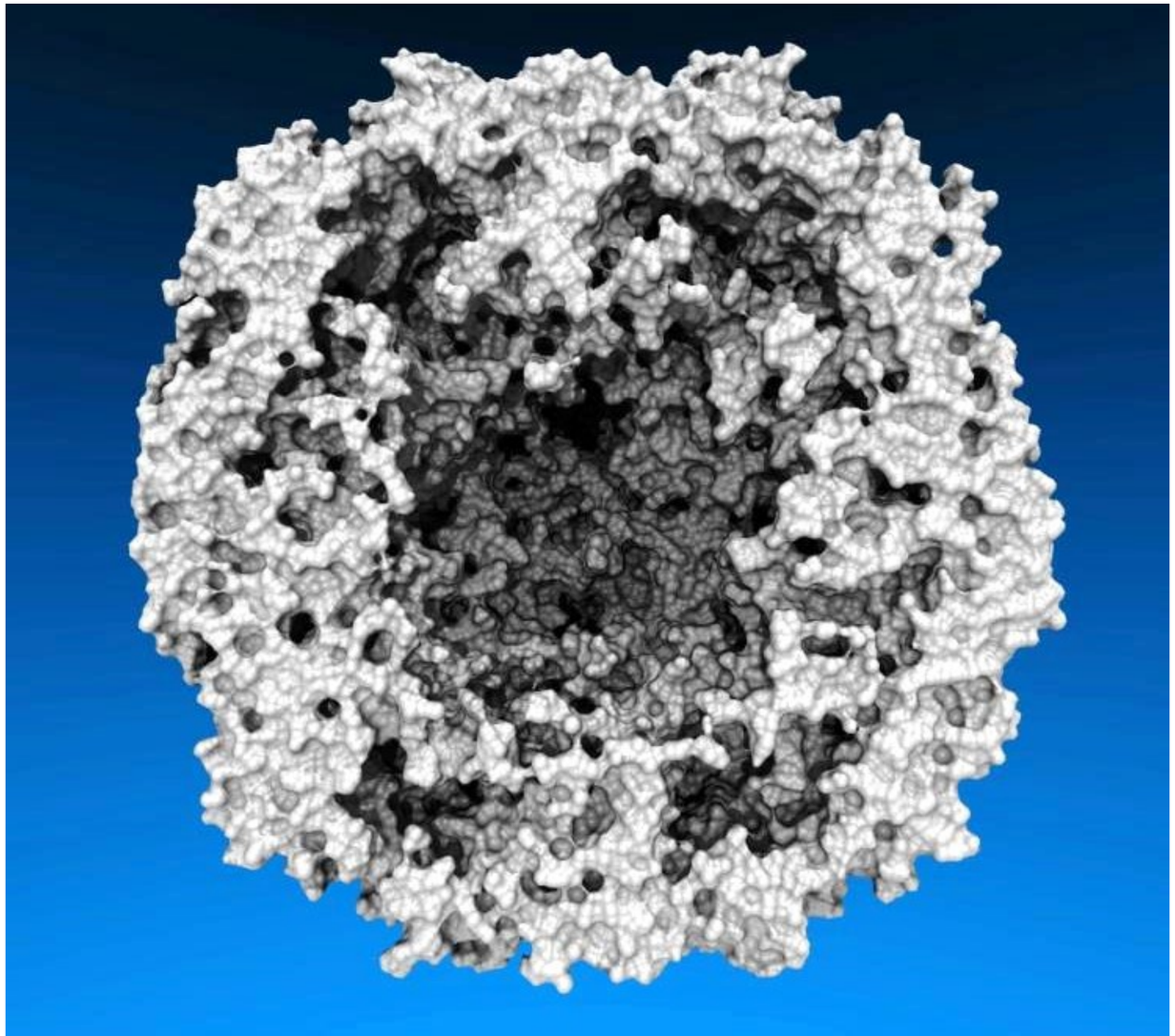


Interactive Ray Tracing, Lighting Comparison: STMV Capsid

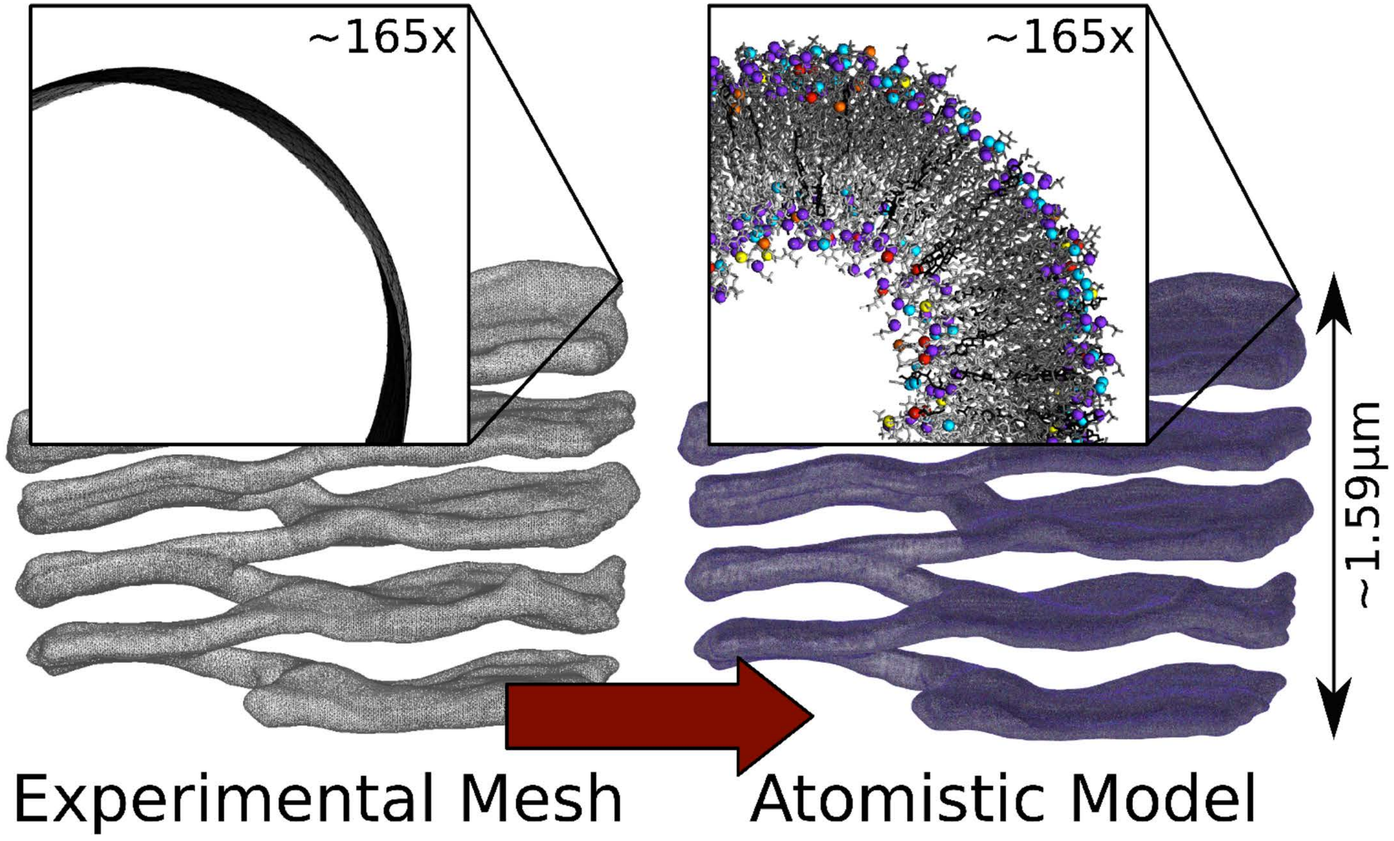
Two lights, no shadows (e.g. as used by OpenGL)

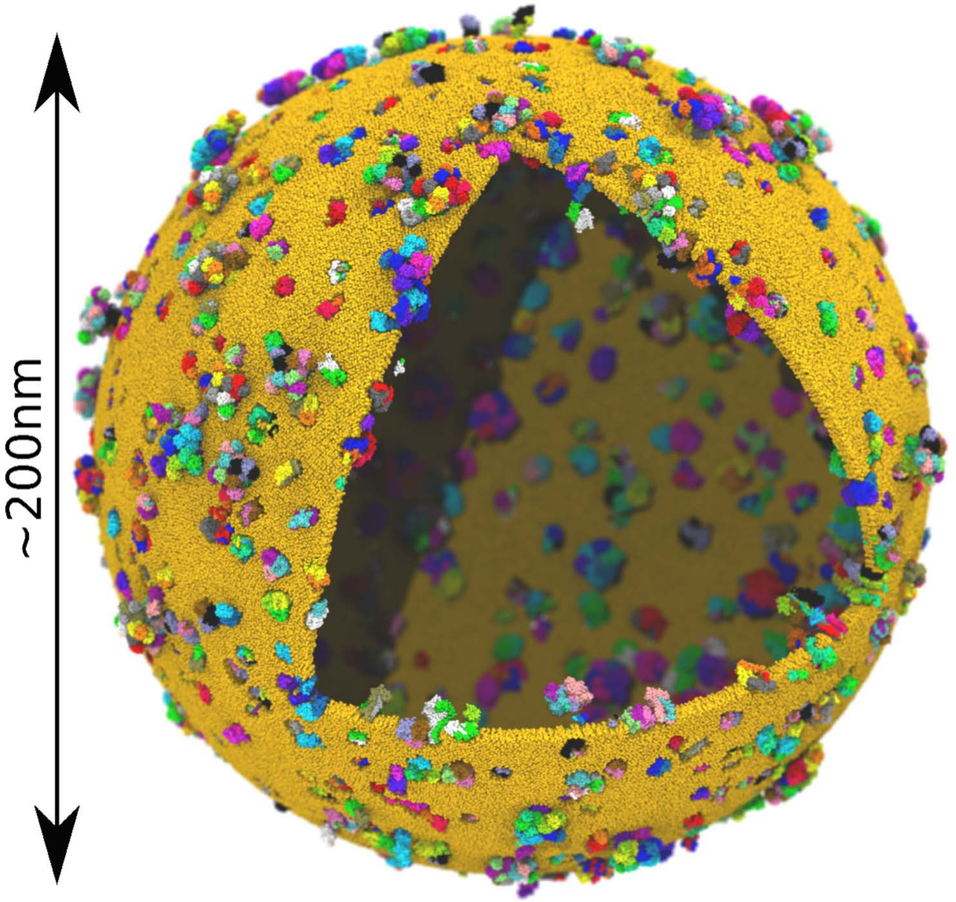


Ambient occlusion lighting and shadows w/ RT

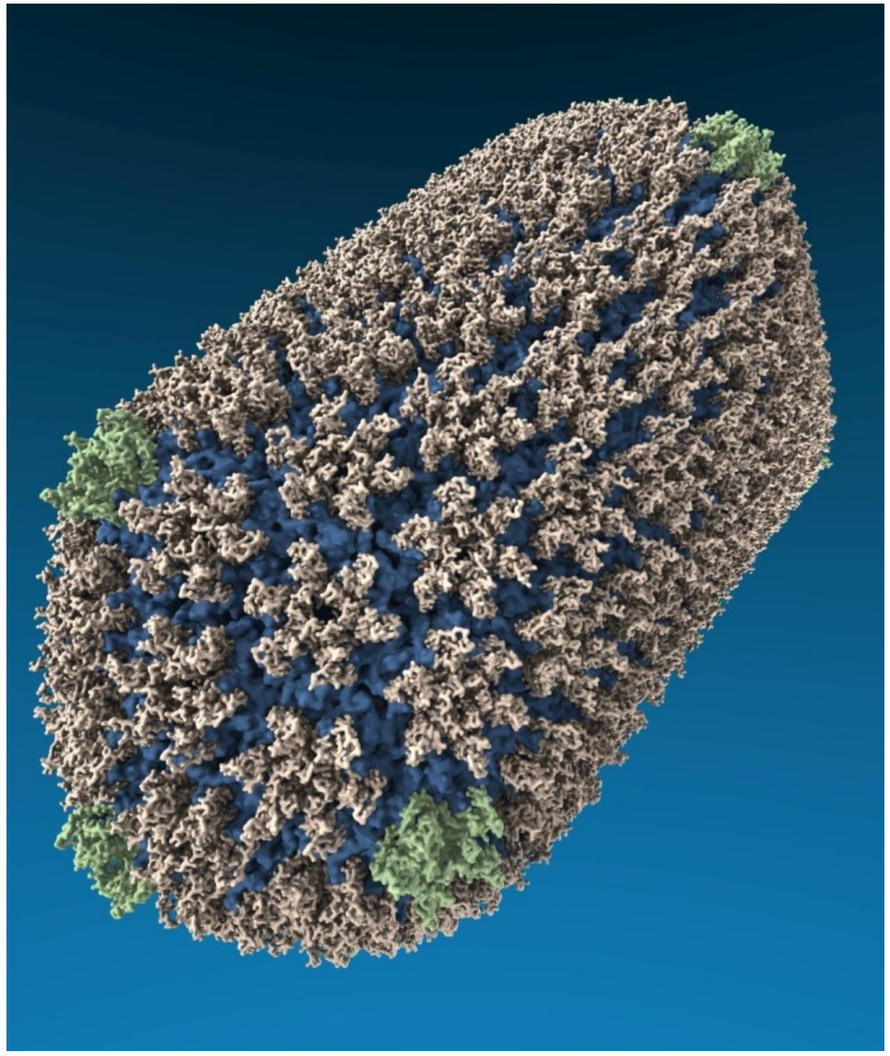


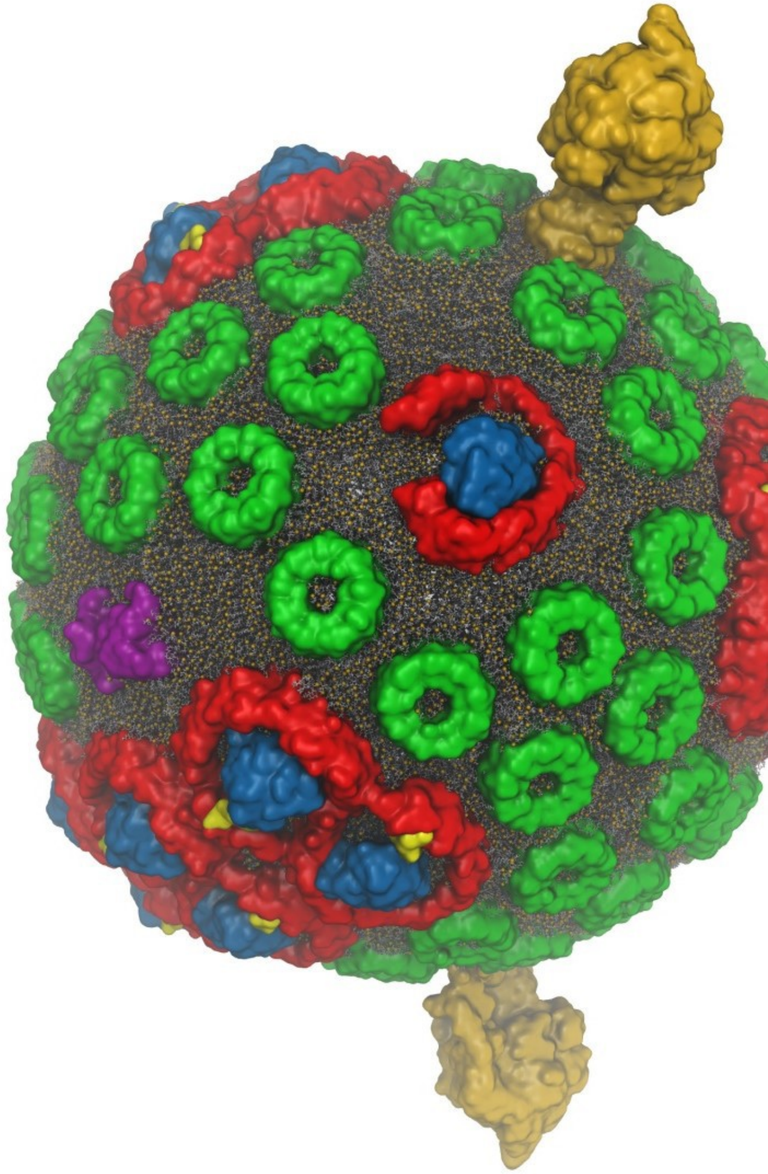
Multi-Billion Atoms System Visualization



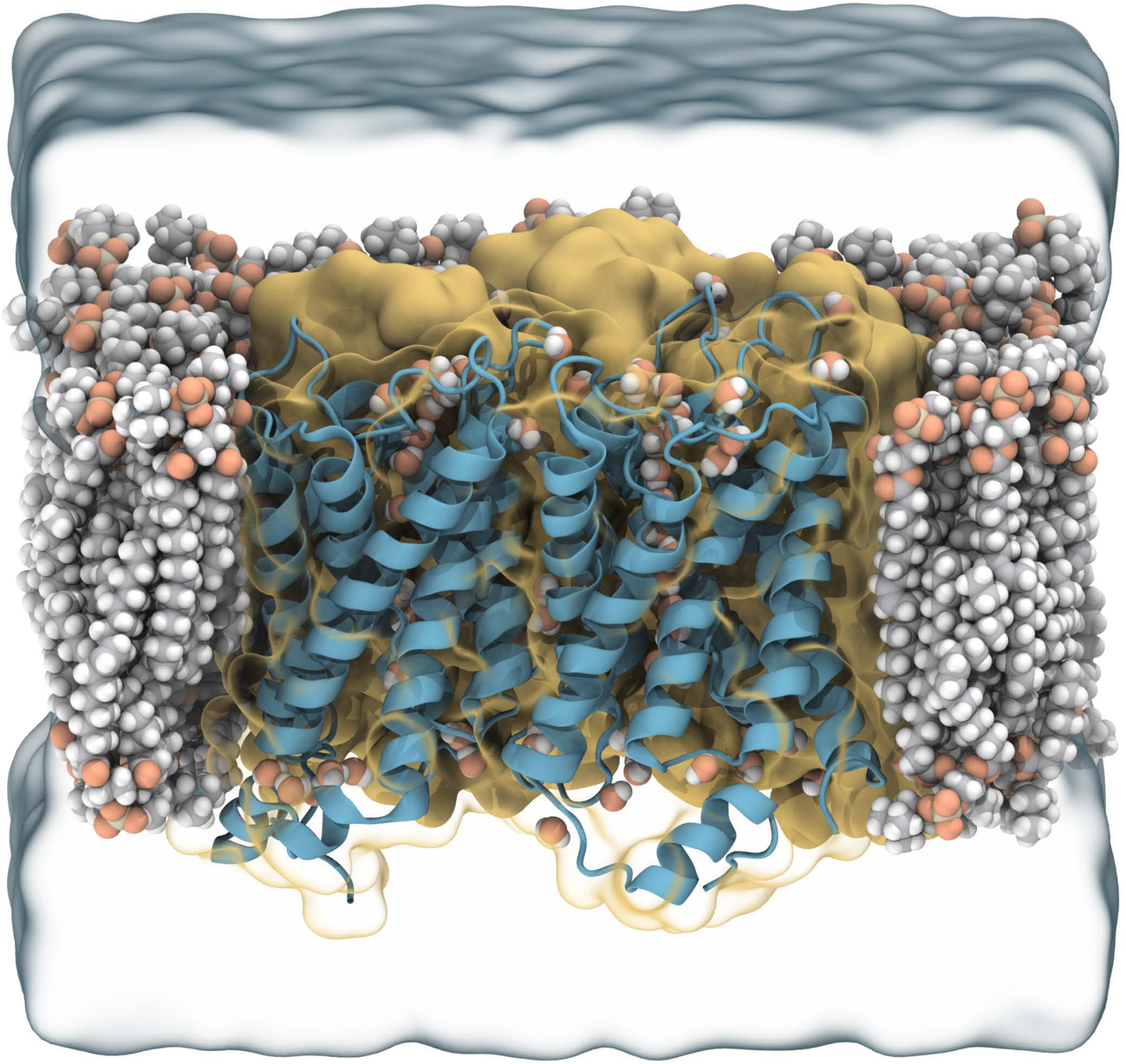


Multi-Million Atoms System Visualization

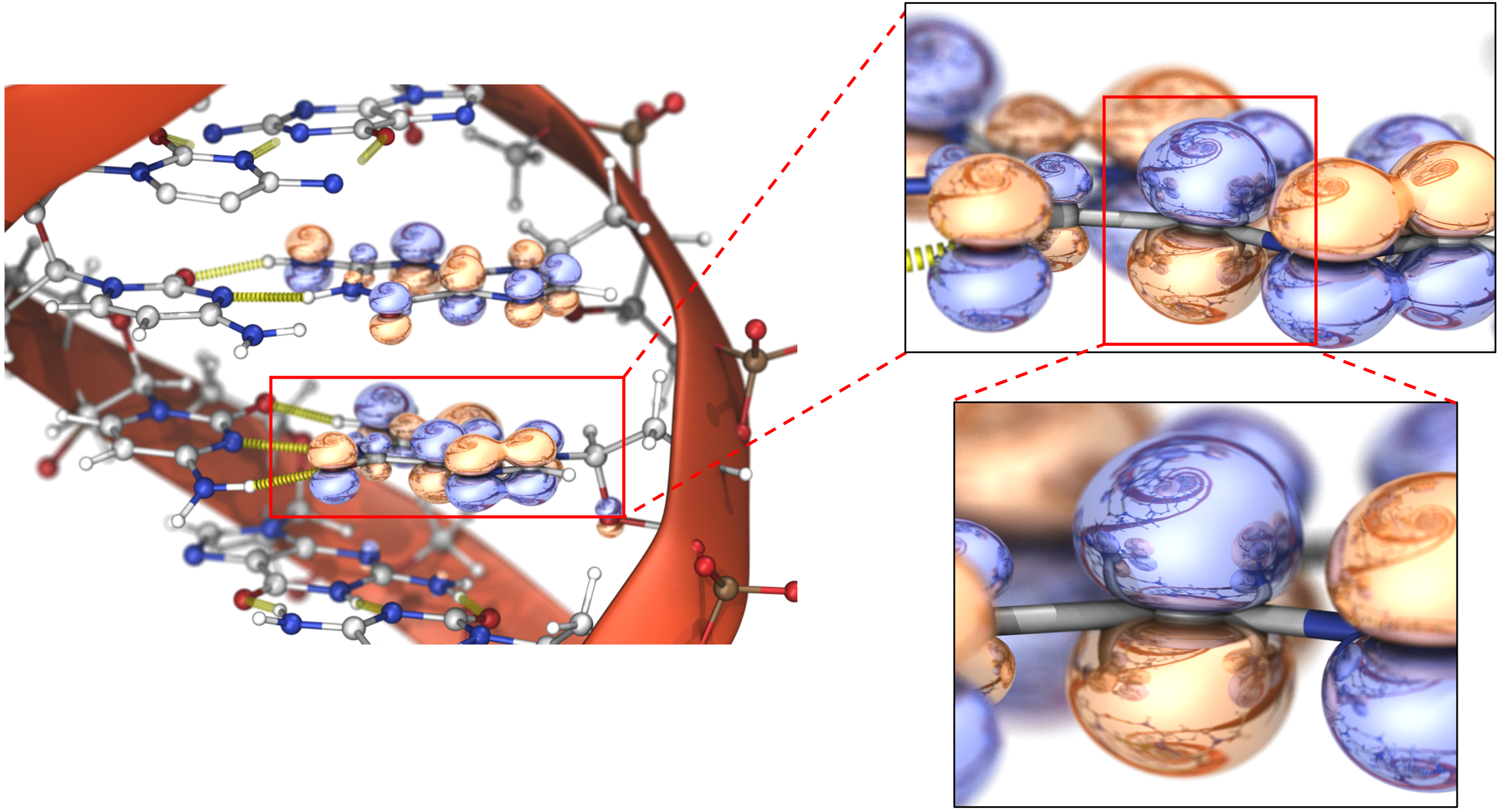




Membrane Proteins



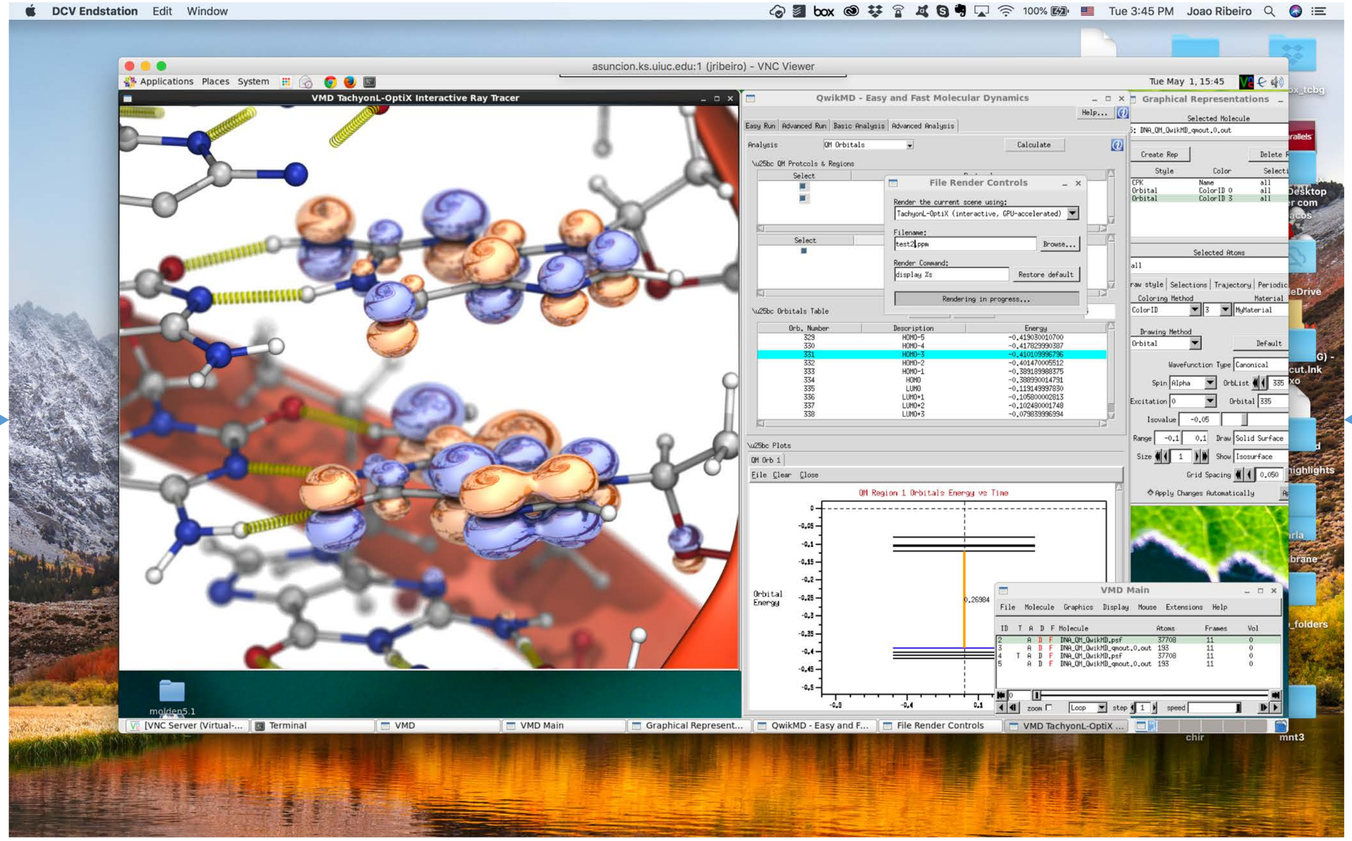
As Small As QM Orbitals



Remote Visualization and Analysis

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

Workstations,
Servers, Cloud



Clusters,
Supercomputers

amazon
web services

Tachyon-OptiX interact Rendering Commands

General Controls:

space: save numbered snapshot image
=: reset to initial view
h: print this help info
p: print current rendering parameters
ESC,q: quit viewer

Mouse Controls:

f: mouse depth-of-field mode
r: mouse rotation mode
s: mouse scaling mode
t: mouse translation mode

Display Controls:

F1: override shadows on/off (off=AO off too)
F2: override AO on/off
F3: override DoF on/off
F4: override Depth cueing on/off
F12: toggle full-screen display on/off
1-9,0: override samples per update auto-FPS off
Up: increase DoF focal distance
Down: decrease DoF focal distance
Left: decrease DoF f/stop
Right: increase DoF f/stop
S: toggle stereoscopic display on/off (if avail)
a: toggle AA/AO auto-FPS tuning on/off (on)
g: toggle gradient sky xforms on/off (on)
l: toggle light xforms on/off (on)