

Tips and Tricks to Render Images of Biomolecules in VMD

João V. Ribeiro

www.ks.uiuc.edu/~jrubeiro

jrubeiro@illinois.edu

May 25nd, 2018

Hands-on Workshop on Computational Biophysics 2018

Pittsburgh Supercomputing Center

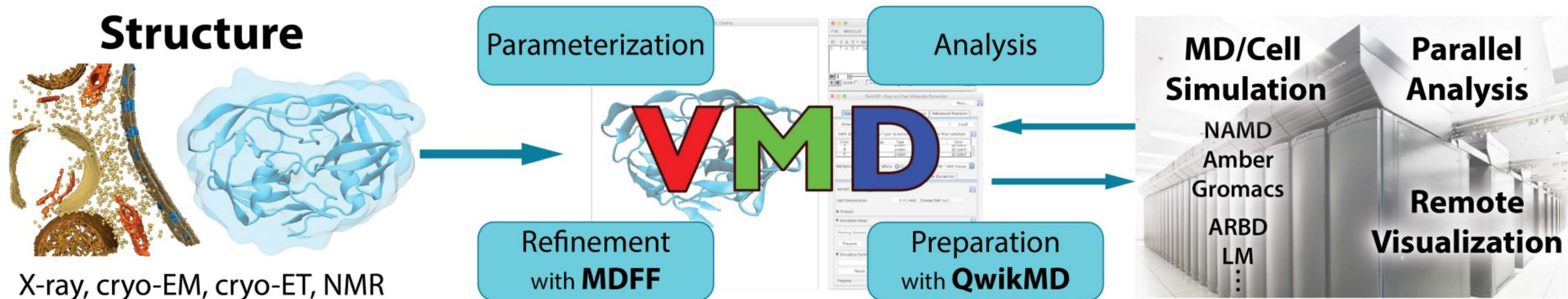
Pittsburgh, PA

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

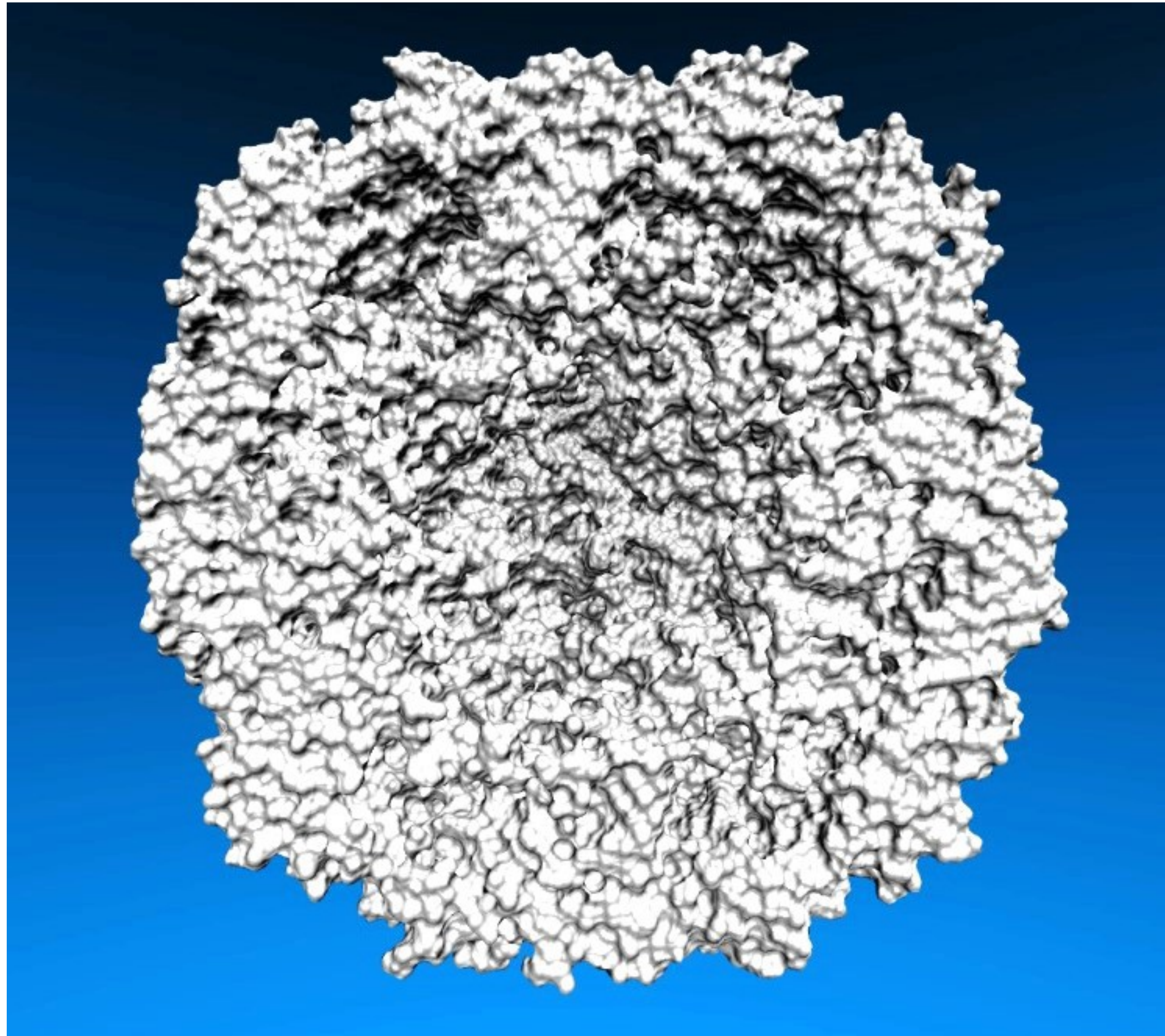
VMD Interoperates with Mainstream Research Tools

- 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

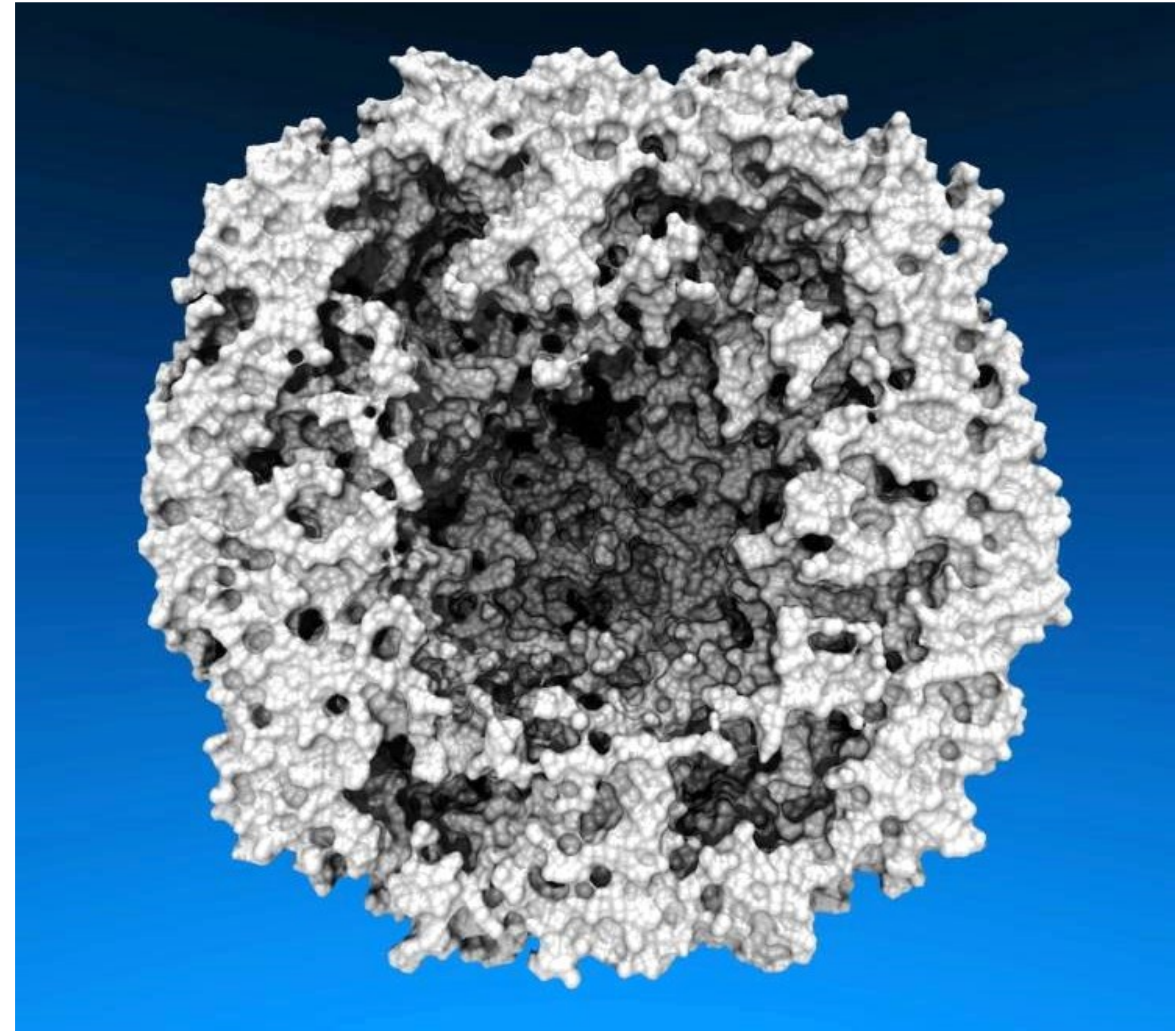


***Interactive* Ray Tracing, Lighting Comparison: STMV Capsid**

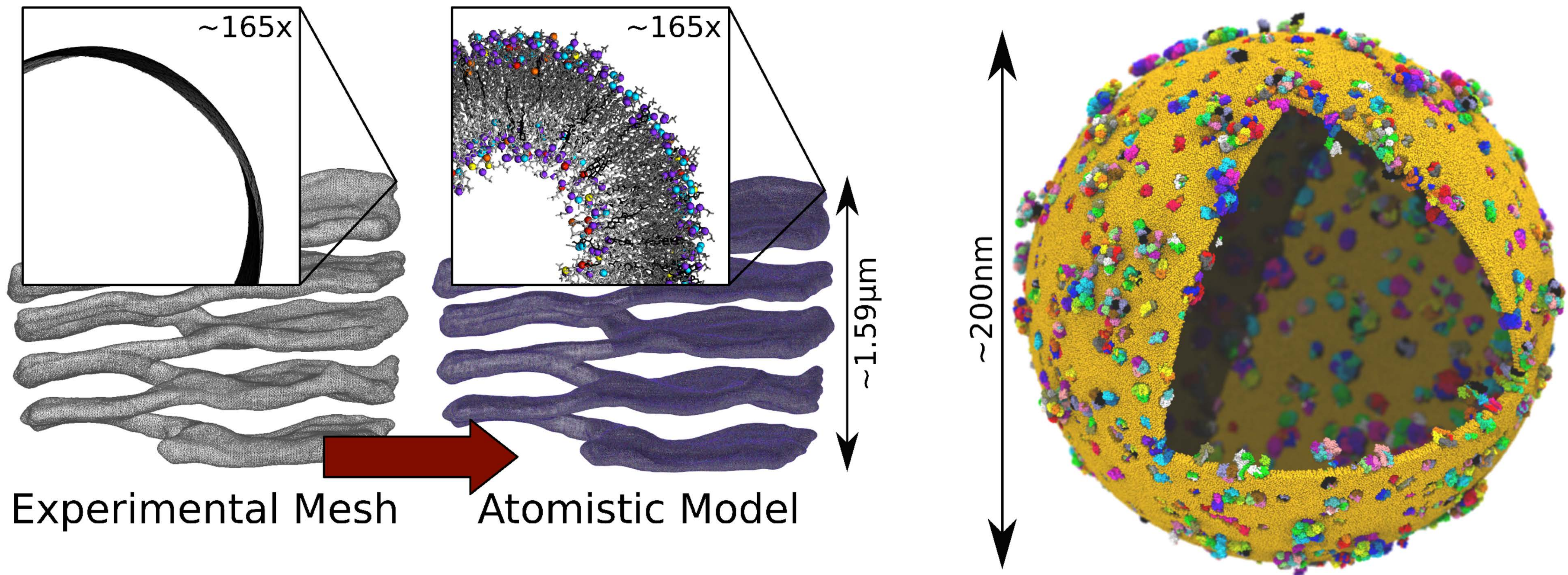
**Two lights, no shadows
(e.g. as used by OpenGL)**



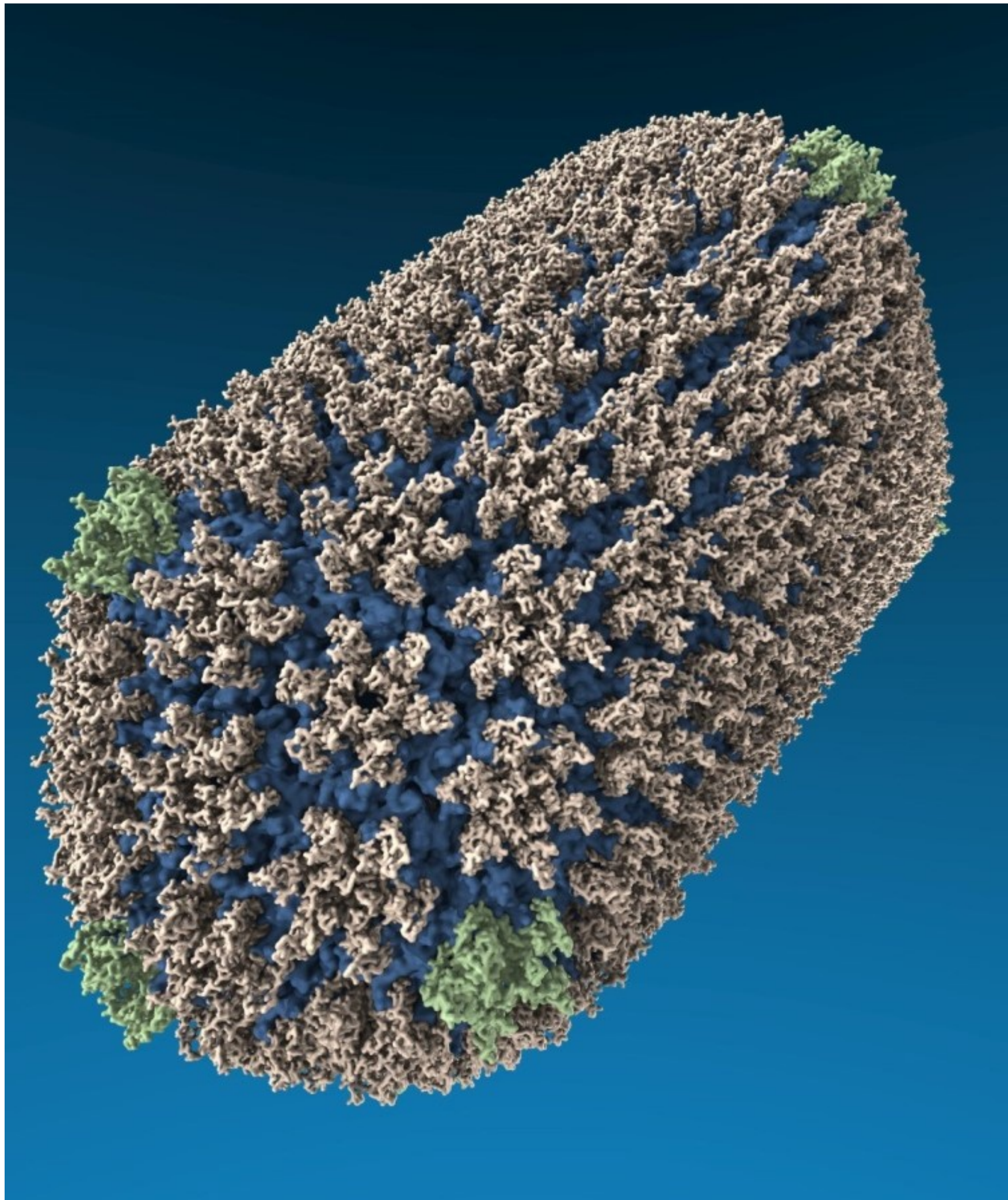
**Ambient occlusion lighting
and shadows w/ RT**



Multi-Billion Atoms System Visualization



Multi-Million Atoms System Visualization



nature
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE

THE HIV-1 CAPSID

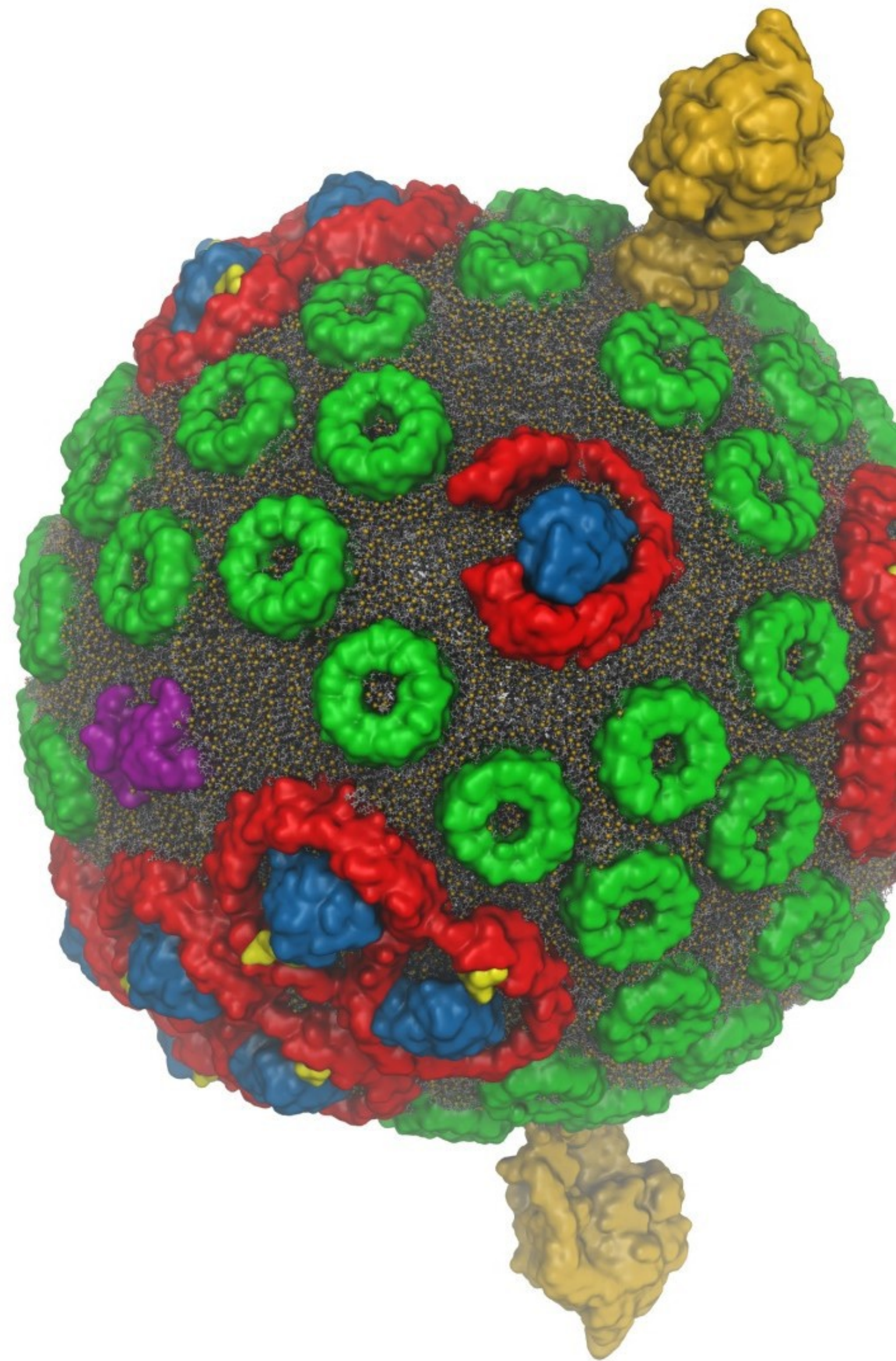
Atomic structure of the AIDS pathogen's protein coat
PAGE 643

COSMOLOGY
THE FIRST LIGHT
In pursuit of the most distant galaxies
PAGE 554

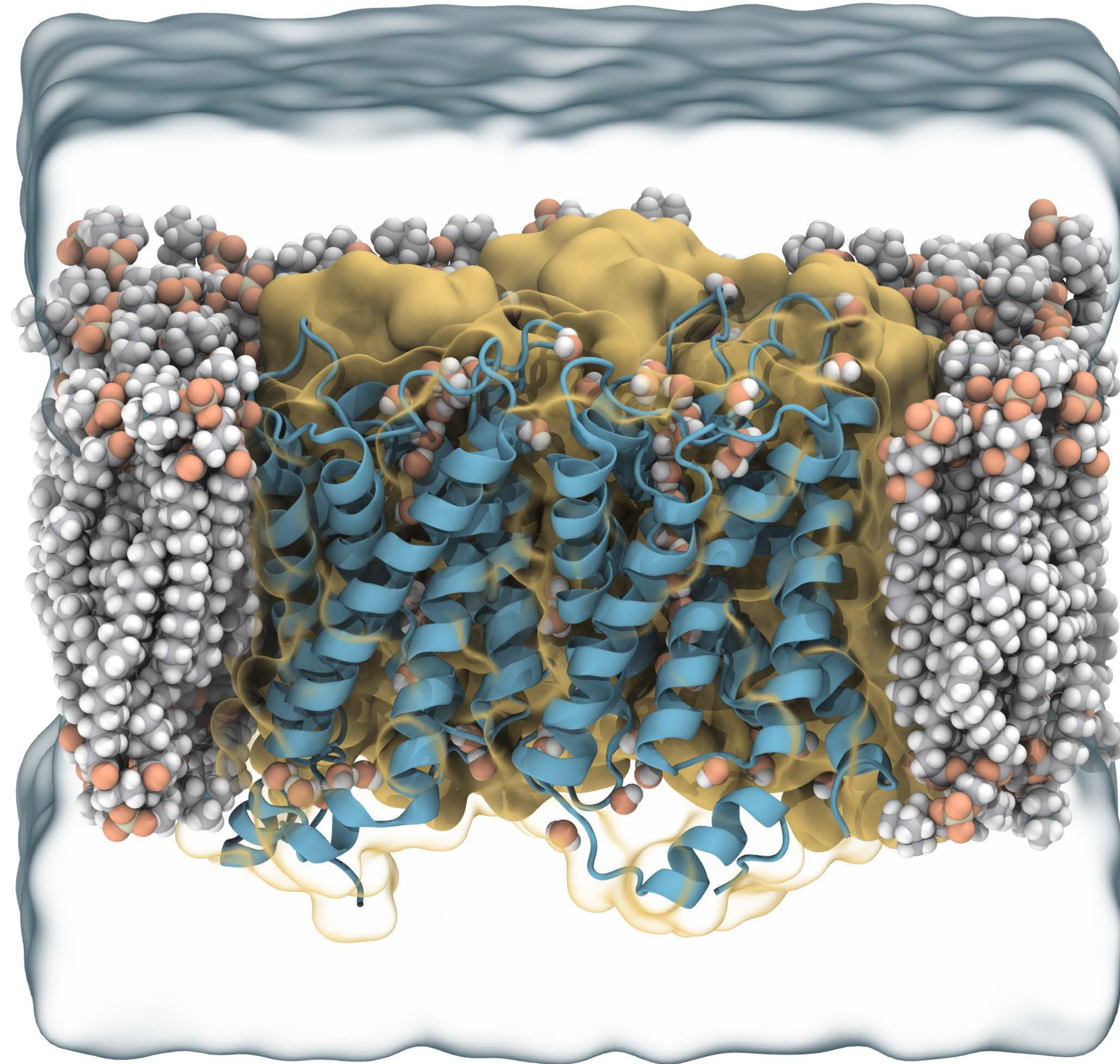
CITATION
CROSSING THE BORDERS
International collaborations make the most impact
PAGE 557

ANTICANCER DRUGS
A SITTING TARGET
An indirect hit on 'undruggable' KRAS protein
PAGES 577 & 638

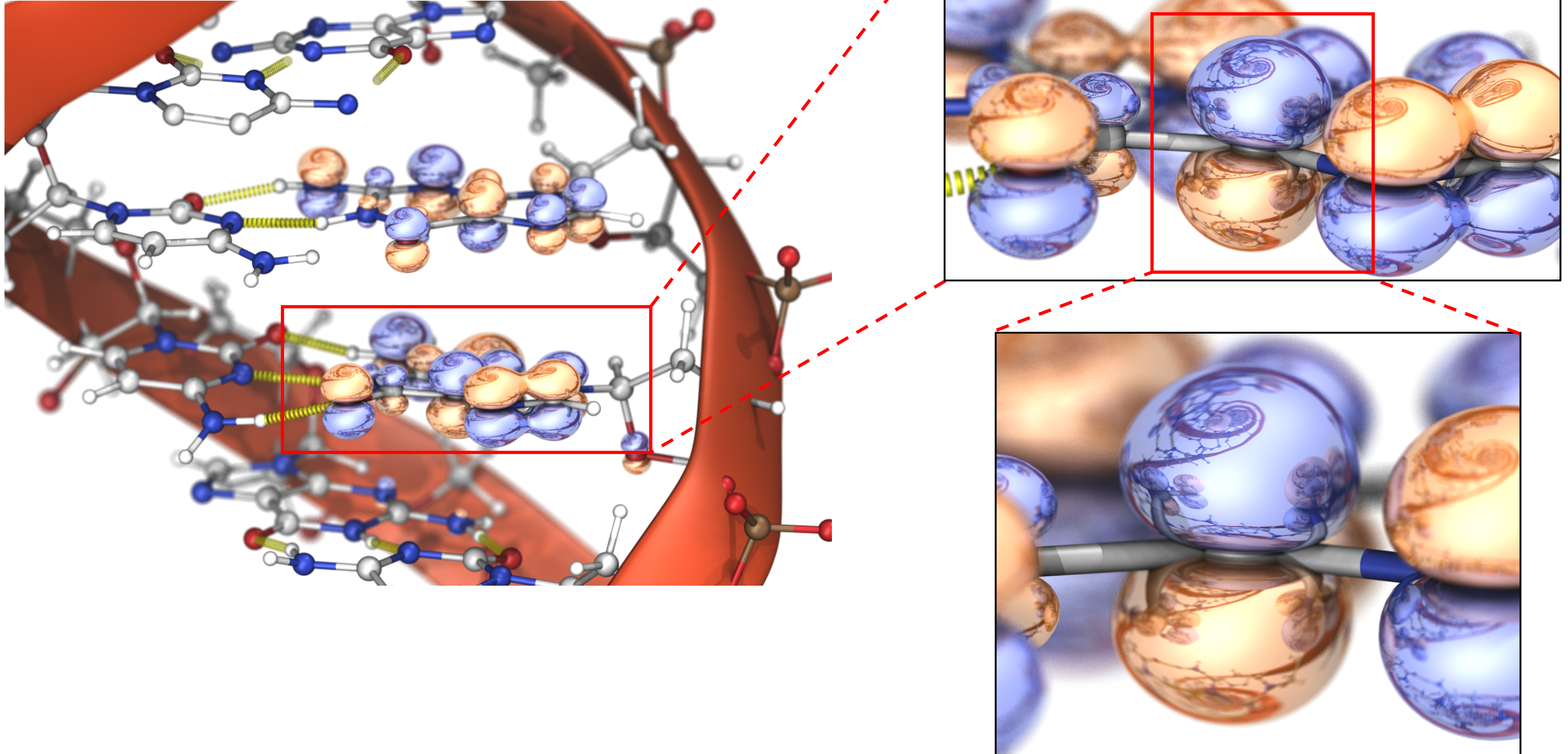
NATURE.COM/NATURE
30 May 2013
\$10.00US \$12.99CAN 2.20
0 71486 03070 6



Membrane Proteins



As Small As QM Orbitals

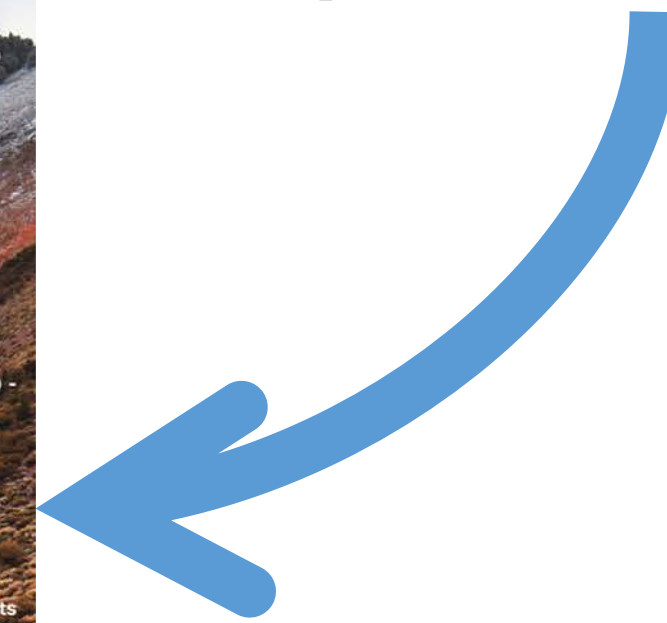


Remote Visualization and Analysis

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



Clusters,
Supercomputers



A screenshot of a VMD (Visual Molecular Dynamics) session running on a workstation. The main window displays a 3D molecular model of a protein-ligand complex with various atoms and bonds. The interface includes several panels: 'QwikMD - Easy and Fast Molecular Dynamics' with tabs for 'Easy Run', 'Advanced Run', 'Basic Analysis', and 'Advanced Analysis'; 'Graphical Representations' with options for 'Style', 'Color', and 'Selected Molecule'; 'File Render Controls' with a 'Render Command' field; 'VMD Main' with a table of molecule and atom information; and 'VMD Plots' with a graph of 'Orbital Energy' vs 'Time'. The desktop background shows a mountain landscape. The taskbar at the bottom includes 'VNC Server (Virtual...', 'Terminal', 'VMD', 'VMD Main', 'Graphical Represent...', 'QwikMD - Easy and F...', 'File Render Controls', 'VMD TachyonL-OptiX ...', 'chir', and 'mnt3'. The system tray shows the date 'Tue May 1, 15:45' and the user 'Joao Ribeiro'.

Workstations,
Servers, Cloud



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)

