# Molecular Modeling, Visualization, and Analysis in VMD

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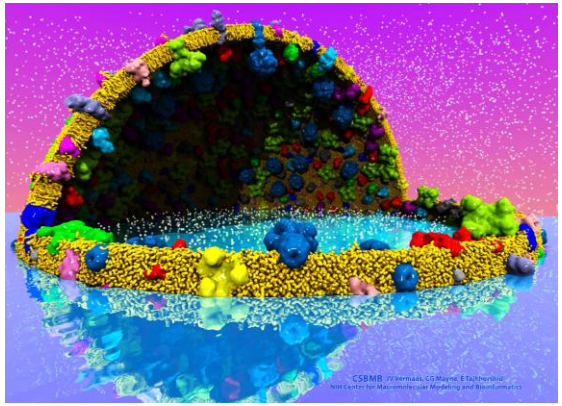
http://www.ks.uiuc.edu/Research/vmd/

**MMBioS – Computational Biophysics Virtual Workshop 2021**

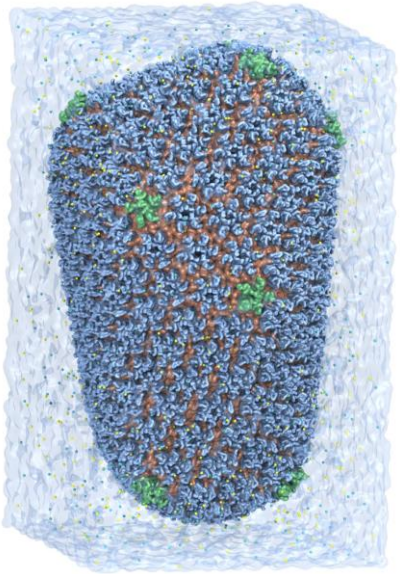
**June 30th, 2021**

# VMD – “Visual Molecular Dynamics”

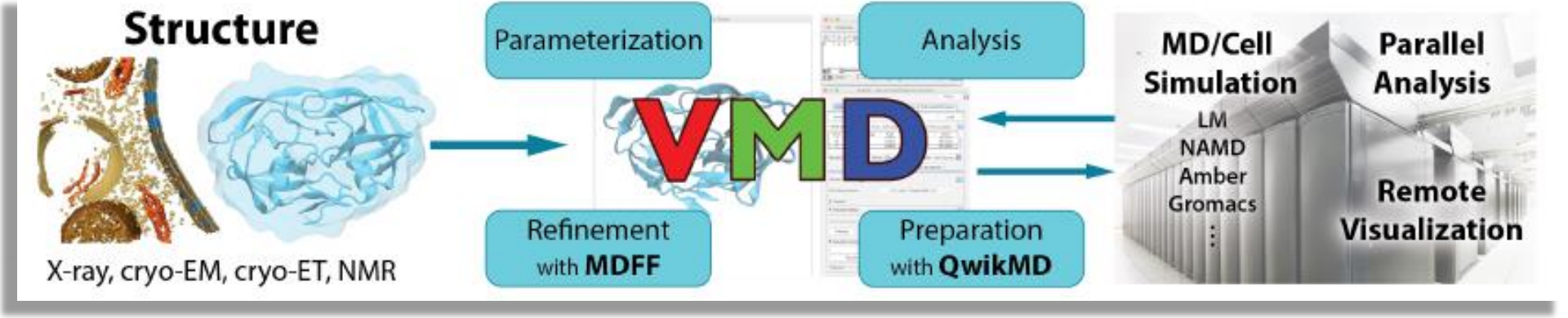
- 125,000 active users worldwide
- Visualization and analysis of:
  - Molecular dynamics simulations
  - Lattice cell simulations
  - Quantum chemistry calculations
  - Cryo-EM densities, volumetric data
- User extensible scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



Cell-Scale Modeling



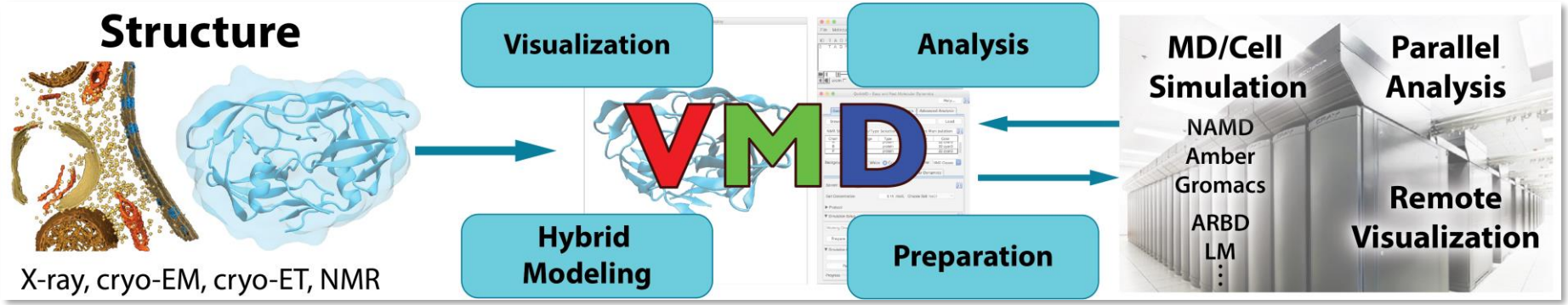
MD Simulation



# VMD Hands-On Tutorials

- 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

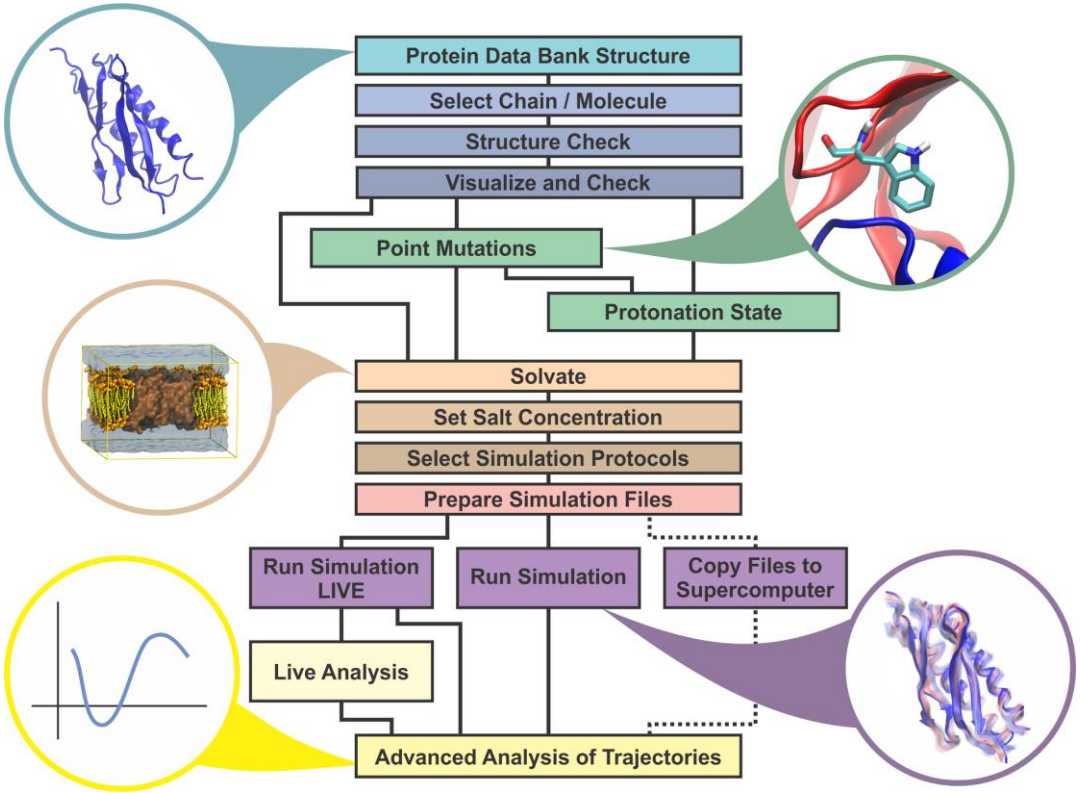
# QwikMD: Guided MD Simulation and Training

Smooths 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




Ribeiro, et al. QwikMD - Integrative Molecular Dynamics Toolkit for Novices and Experts. ***Sci. Rep***. 6, 26536, 2016

# 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
- RNAView
- Solvate
- SSRestraints
- Topotools

**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**

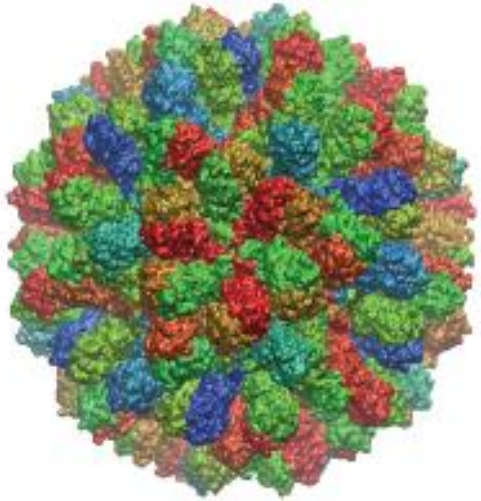
- Check sidechains
- MultiMSMS
- Interactive Essential Dynamics
- Mead Ionize
- Clustering Tool
- iTrajComp
- Swap RMSD
- Intervor
- SurfVol
- vmdICE

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

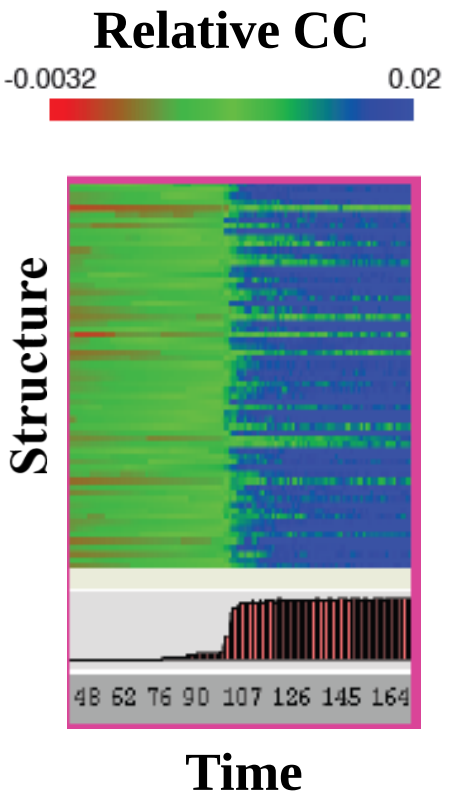
http://www.ks.uiuc.edu/Research/vmd/plugins/

# Parallel MDFF Cross Correlation Analysis on Cray XK7

| Rabbit Hemorrhagic Disease Virus (RHDV) | |
|---|---|
| Traj. frames | 10,000 |
| Structure component selections | 720 |
| Single-node XK7 (projected) | 336 hours (14 days) |
| 128-node XK7 | 3.2 hours<br>105x speedup |
| 2048-node XK7 | 19.5 minutes<br>1035x speedup |



RHDV colored by relative CC

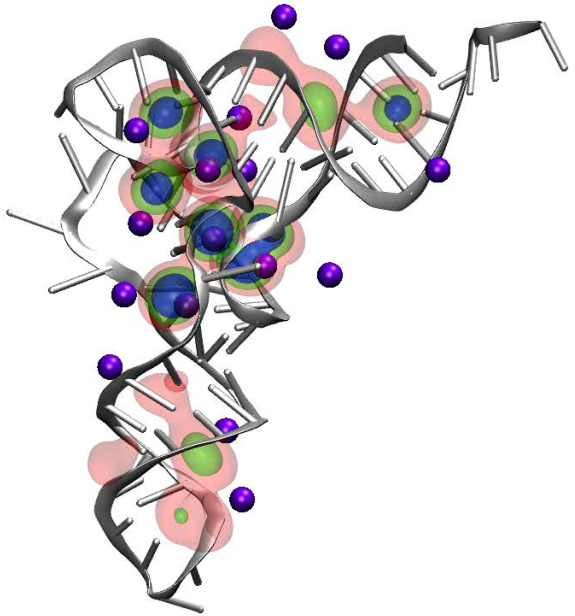



Calculation of 7M CCs would take **5 years** using serial CPU algorithm!

Stone et al., Faraday Discuss., 169:265-283, 2014.

# Time-Averaged Volumetric Properties

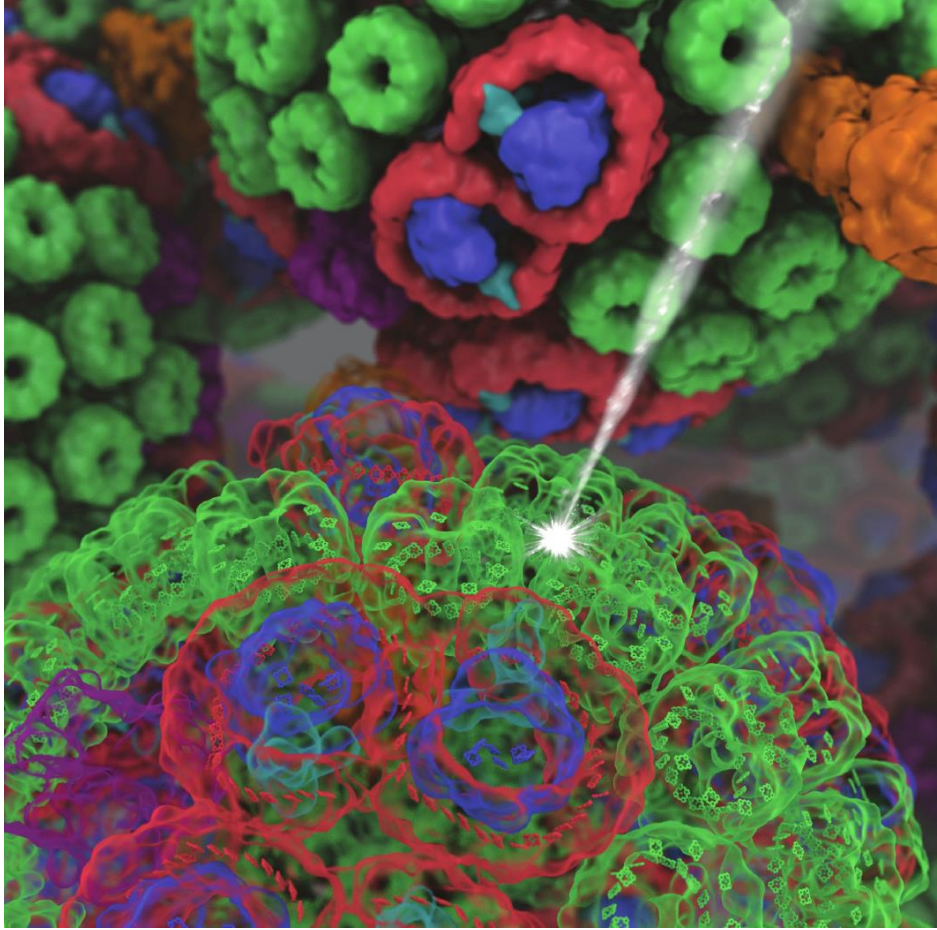
- Compute density, distance, occupancy, potential maps for a frame or averaged over a trajectory
- Example: display binding sites for diffusively bound ions as probability density isosurfaces



**tRNA magnesium ion occupancy: VMD volmap plugin**

# High Fidelity Ray Tracing

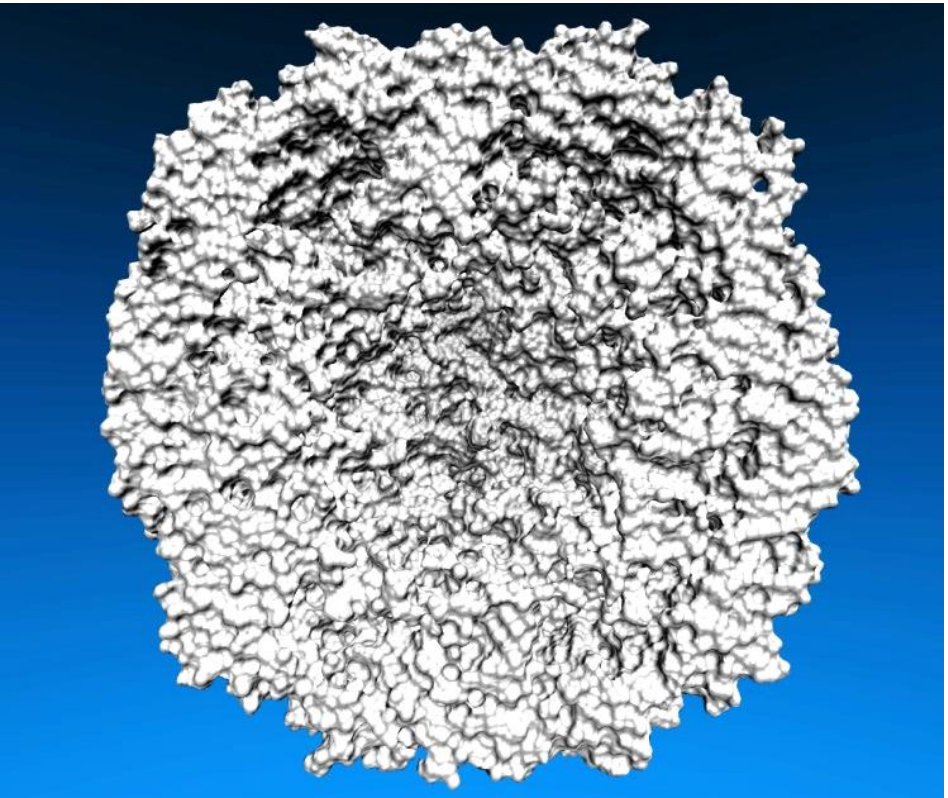
- Advanced rendering techniques save scientists time, produce images that are easier to interpret
- Ambient Occlusion, Depth of Field, high quality transparency, instancing, ….
- **Interactive RT** on laptops, desk, cloud, and **remote supercomputers**
- **Large-scale MPI parallel rendering:** in situ 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



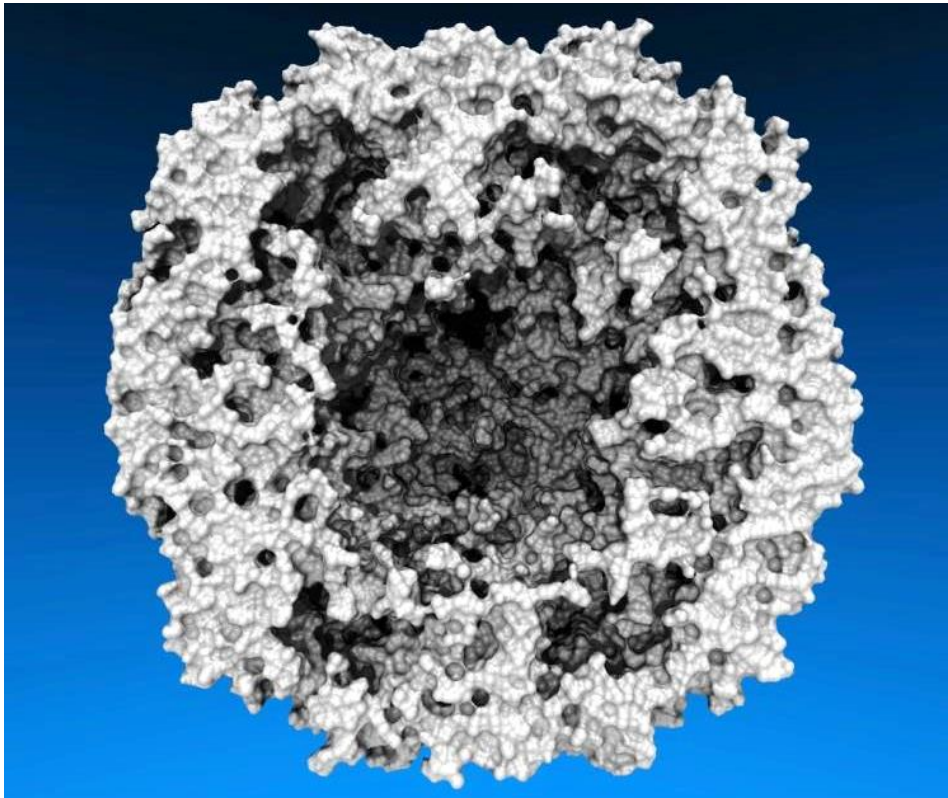
VMD/OptiX all-atom Chromatophore

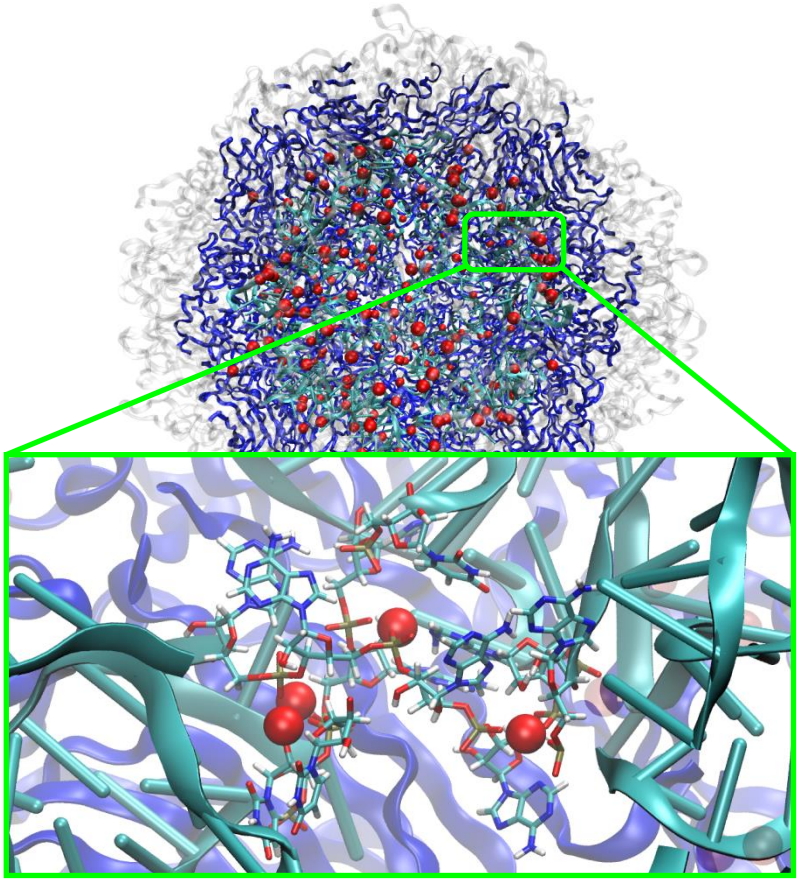
# Lighting Comparison, STMV Capsid

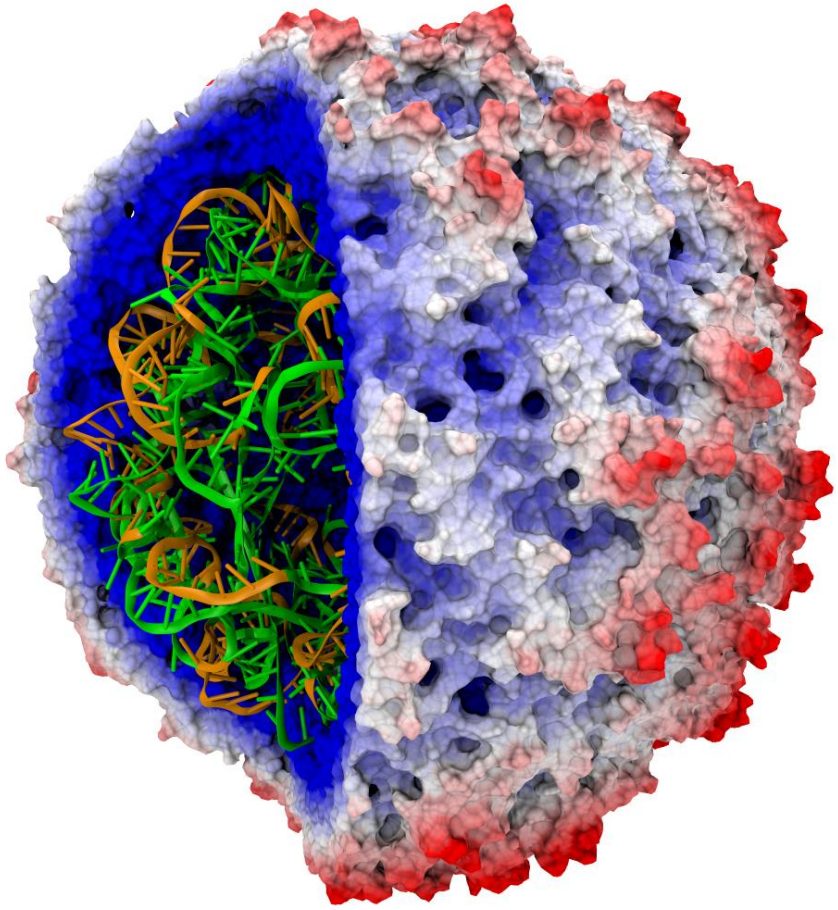
**Two lights, no shadows**



**Ambient occlusion + two lights, 144 AO rays/hit**

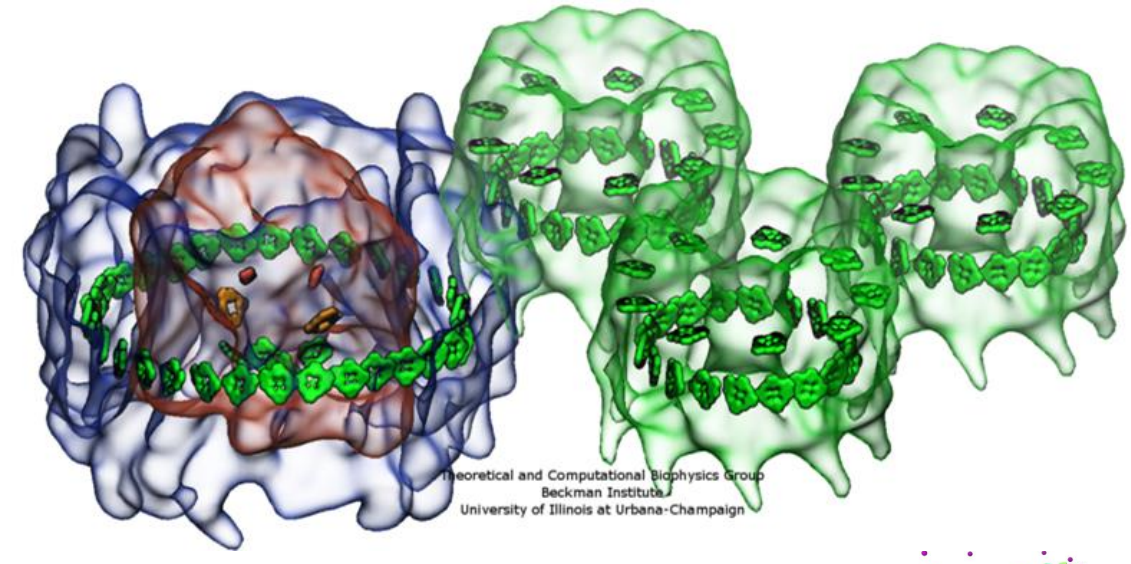


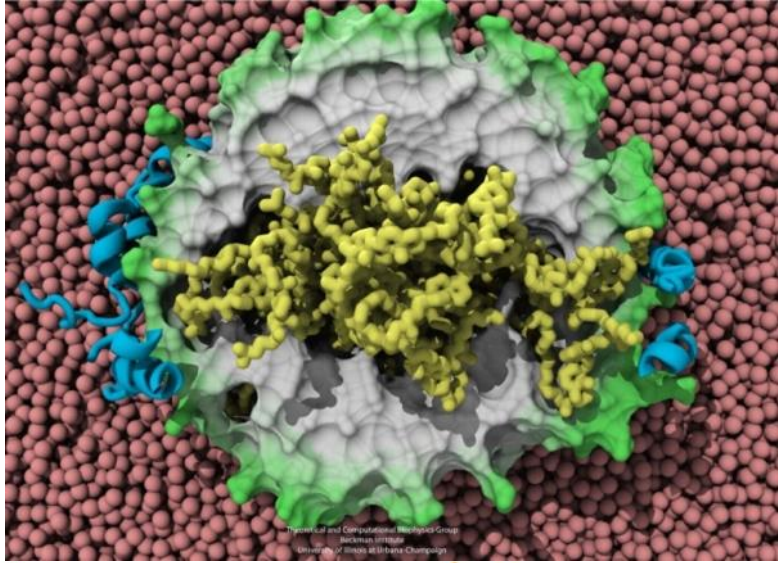


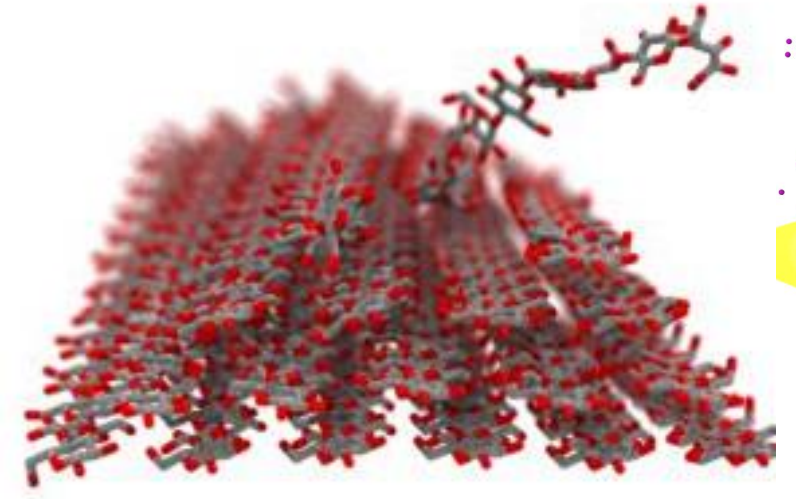


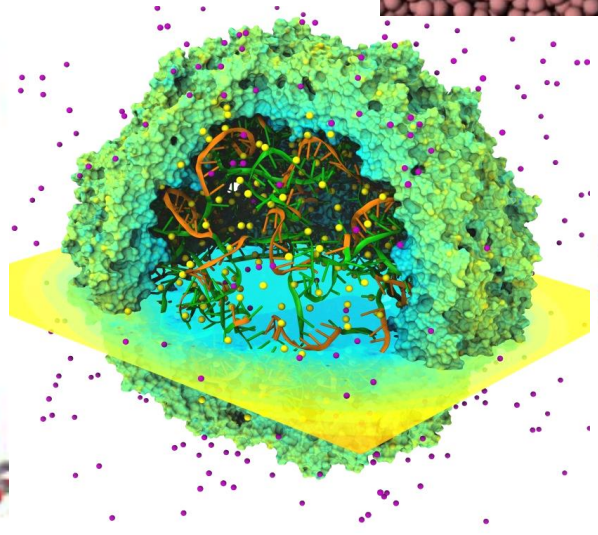
# Satellite Tobacco Mosaic Virus

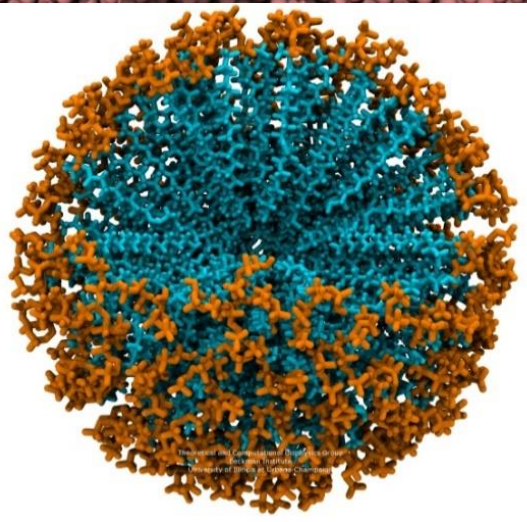
Biomedical Technology Research Center for Macromolecular Modeling and Bioinformatics
Beckman Institute, University of Illinois at Urbana-Champaign - www.ks.uiuc.edu


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



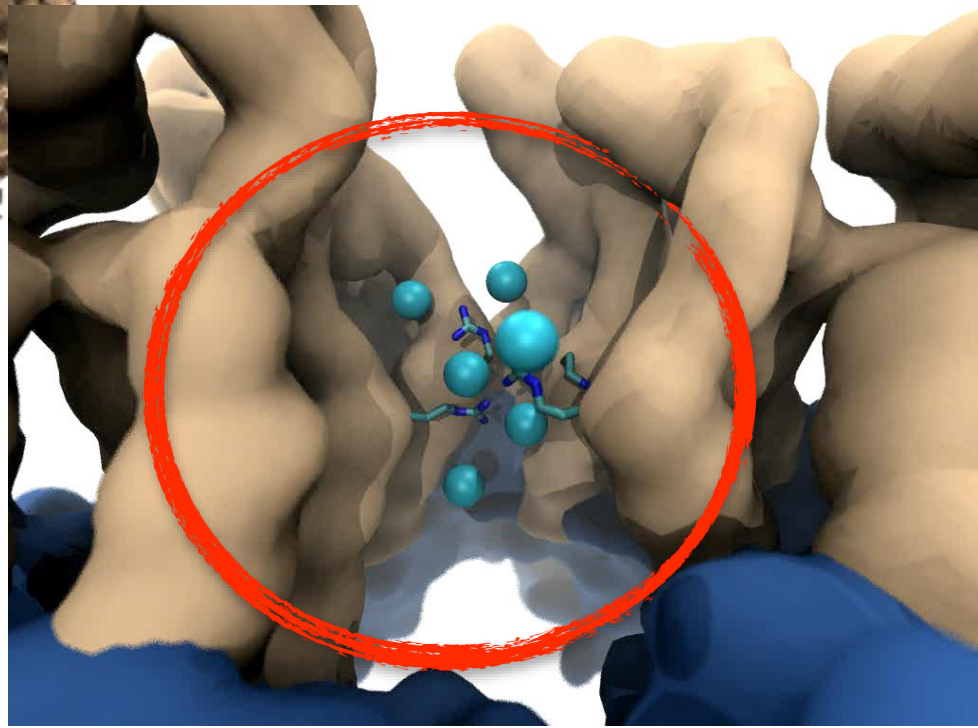






# Goal: Intuitive interactive viz. in crowded molecular complexes

Results from 64 M atom, 1 μs sim!



- Close-up view of chloride ions permeating through HIV-1 capsid hexameric centers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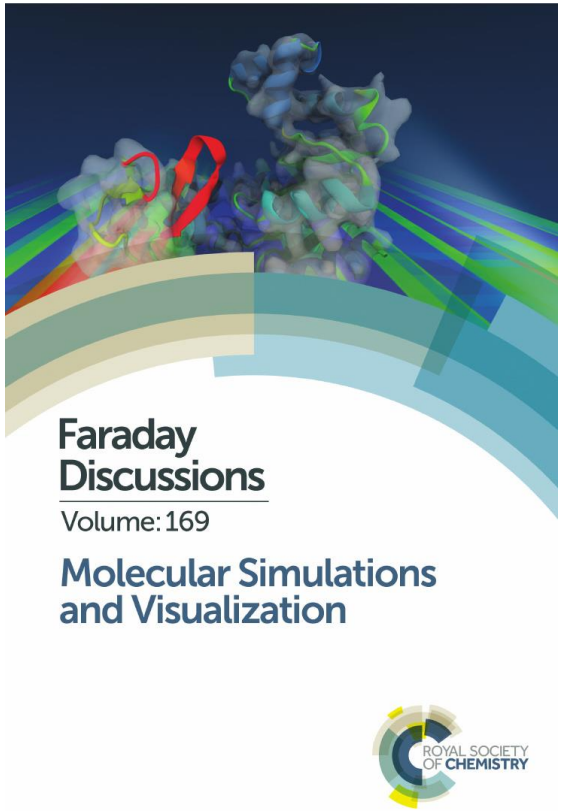
Faraday Discussions
Volume: 169
Molecular Simulations and Visualization
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THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
THE HIV-1 CAPSID
Atomic structure of the AIDS pathogen's protein coat
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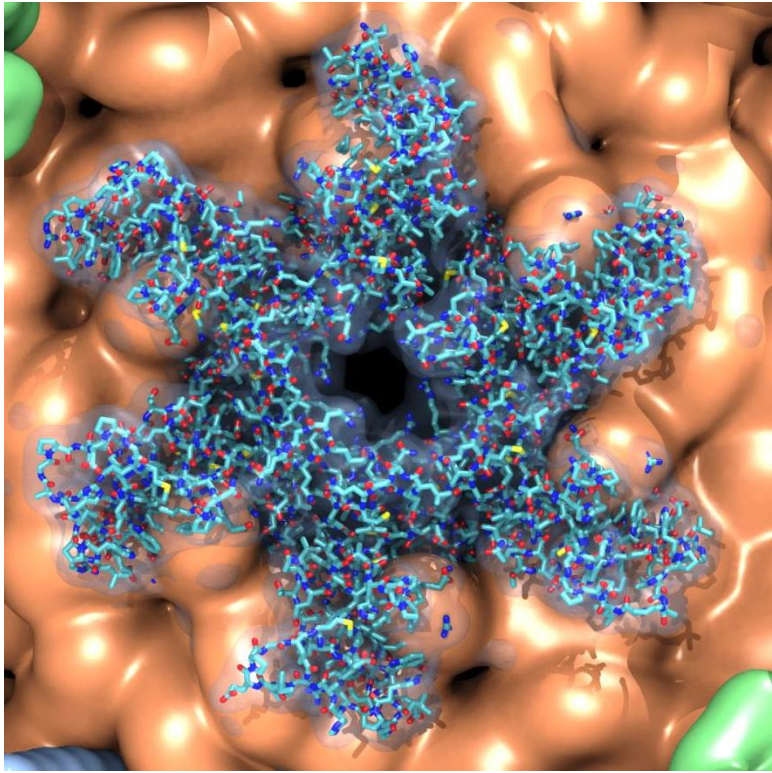
A SITTING TARGET
An indirect hit on 'undruggable' KRAS protein
PAGES 577 & 638
NATURE.COM/NATURE
30 May 2013

# VMD “Coming Soon”: VMD 1.9.4 and VMD-Next

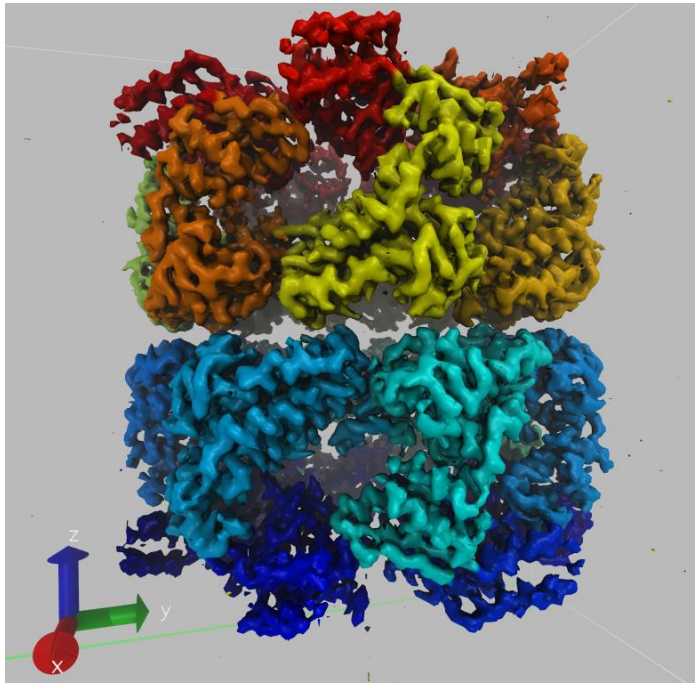
# VMD 1.9.4, and VMD-Next

- 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

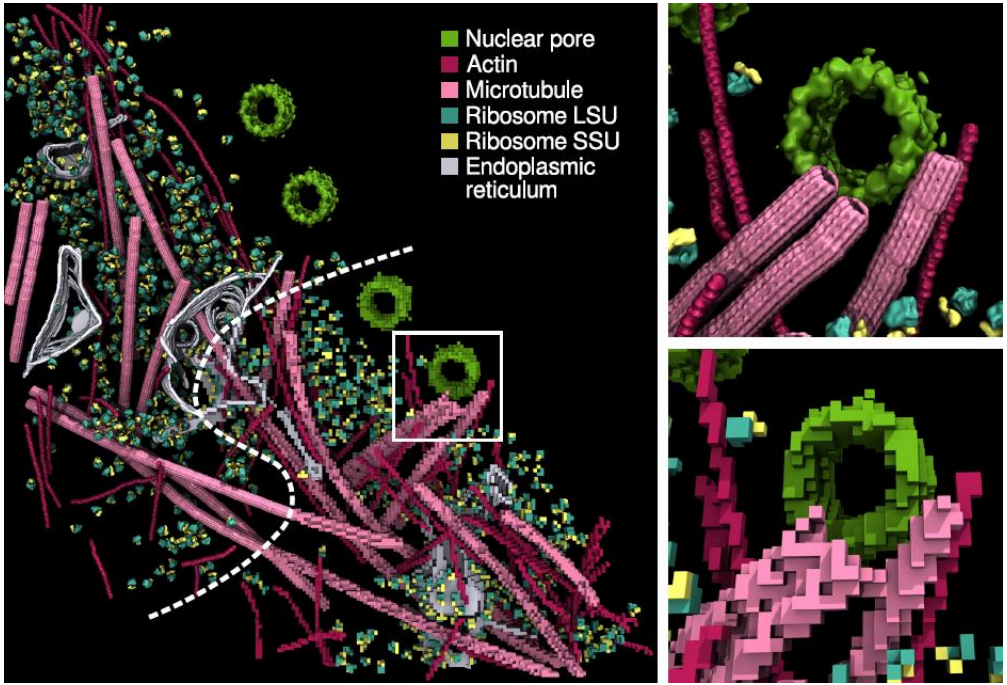


GPU Ray Tracing of
HIV-1 Capsid Detail

# Density Map Segmentation



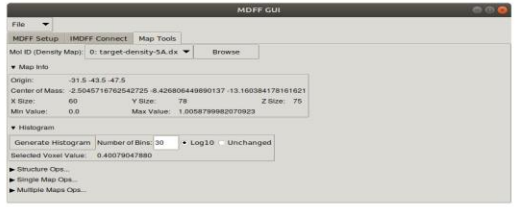

**VMD GPU-accelerated density map segmentation of GroEL**

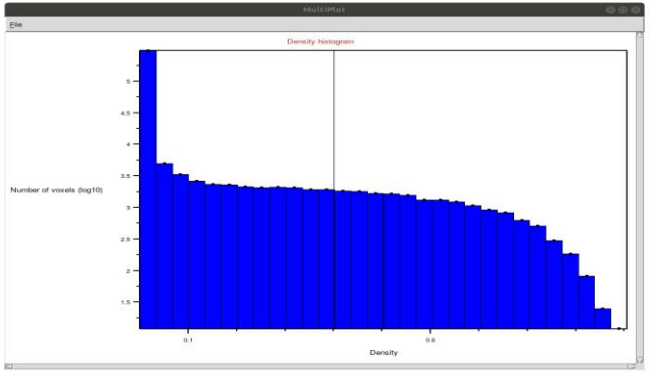


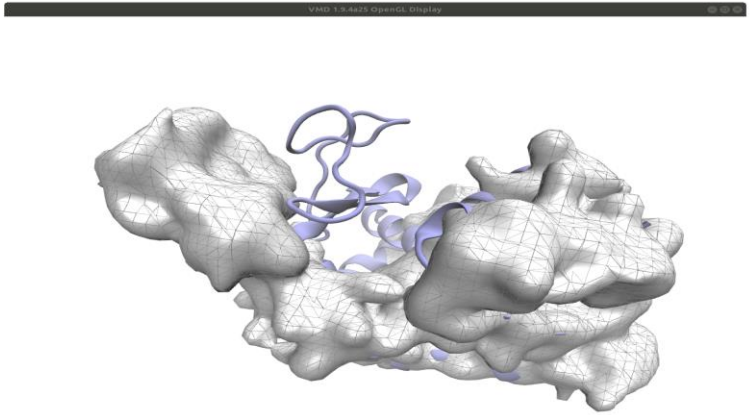

**Earnest, et al. J. Physical Chemistry B, 121(15): 3871-3881, 2017.**

# 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



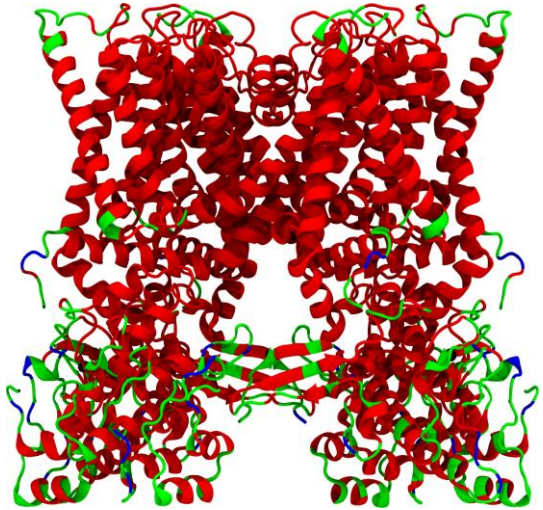



# New Density Map Tools - Masking

Easily select and mask density map regions with VMD selection language

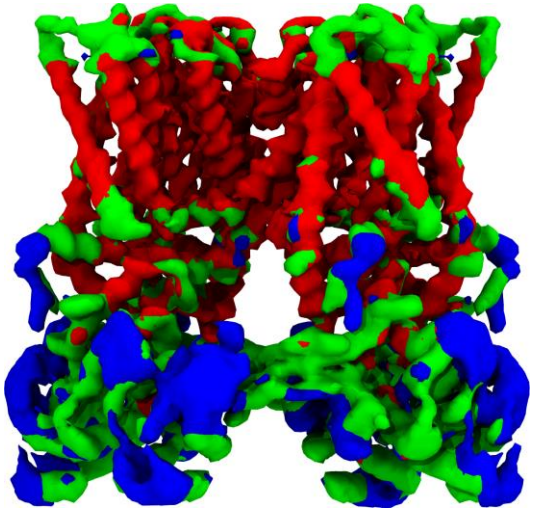
TRPV1 structure (3J5P) and cryo-EM density (emd-5778) colored by local resolution obtained by ResMap



High Res
(~3 Å)

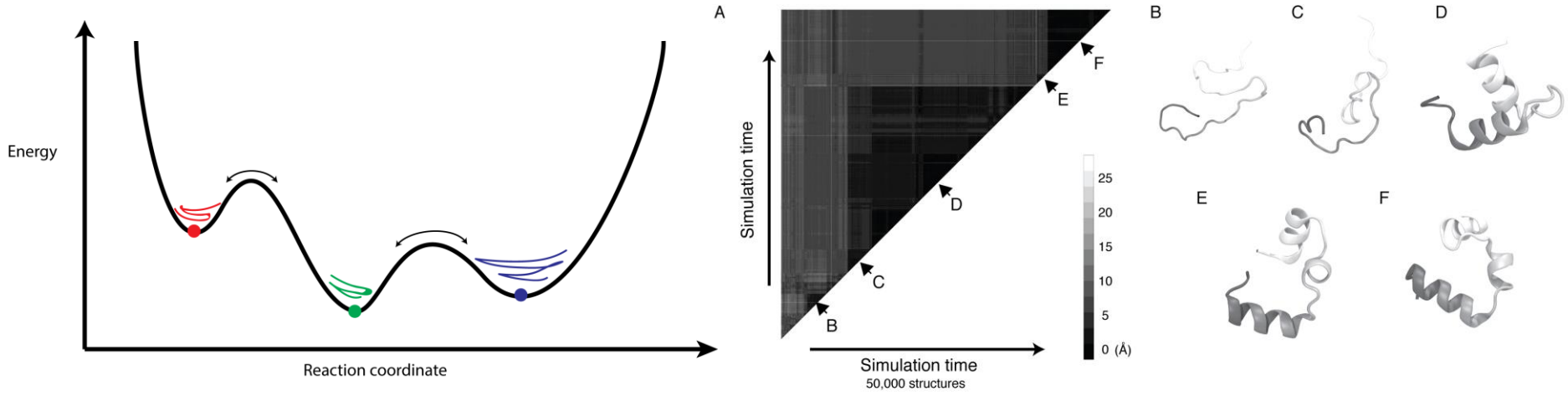
Med Res
(~4 Å)

Low Res
(~5 Å)



A. Kucukelbir, F.J. Sigworth, H.D. Tagare, Quantifying the Local Resolution of Cryo-EM Density Maps, Nature Methods, Volume 11, Issue 1, Pages 63-65, 2014.

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

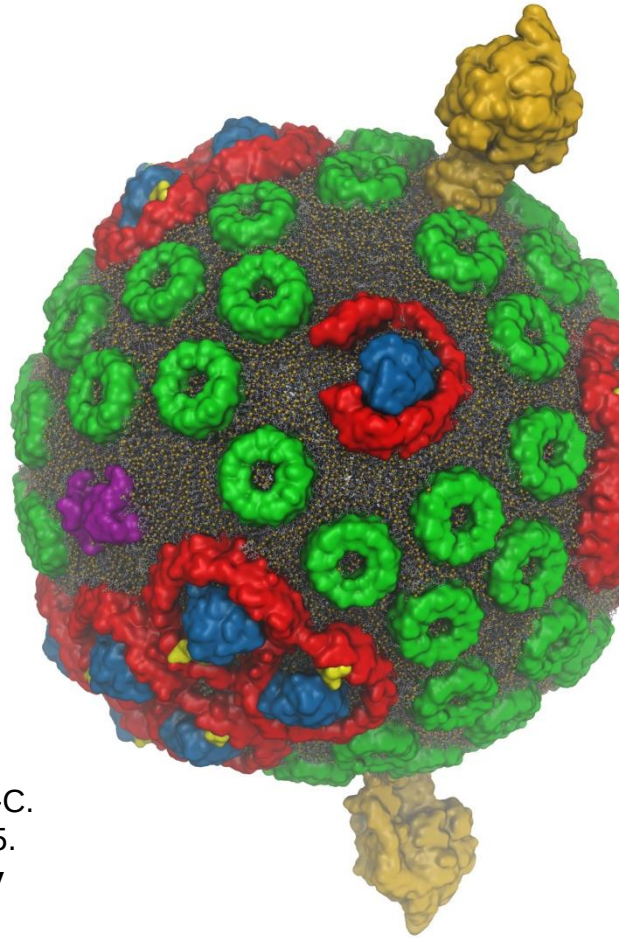



**GPU-Accelerated Molecular Dynamics Clustering Analysis with OpenACC.** J.E. Stone, J.R. Perilla, C. K. Cassidy, and K. Schulten. In, Robert Farber, ed., Parallel Programming with OpenACC, Morgan Kaufmann, Chapter 11, pp. 215-240, 2016.

# VMD w/ OptiX RTX Ray Tracing

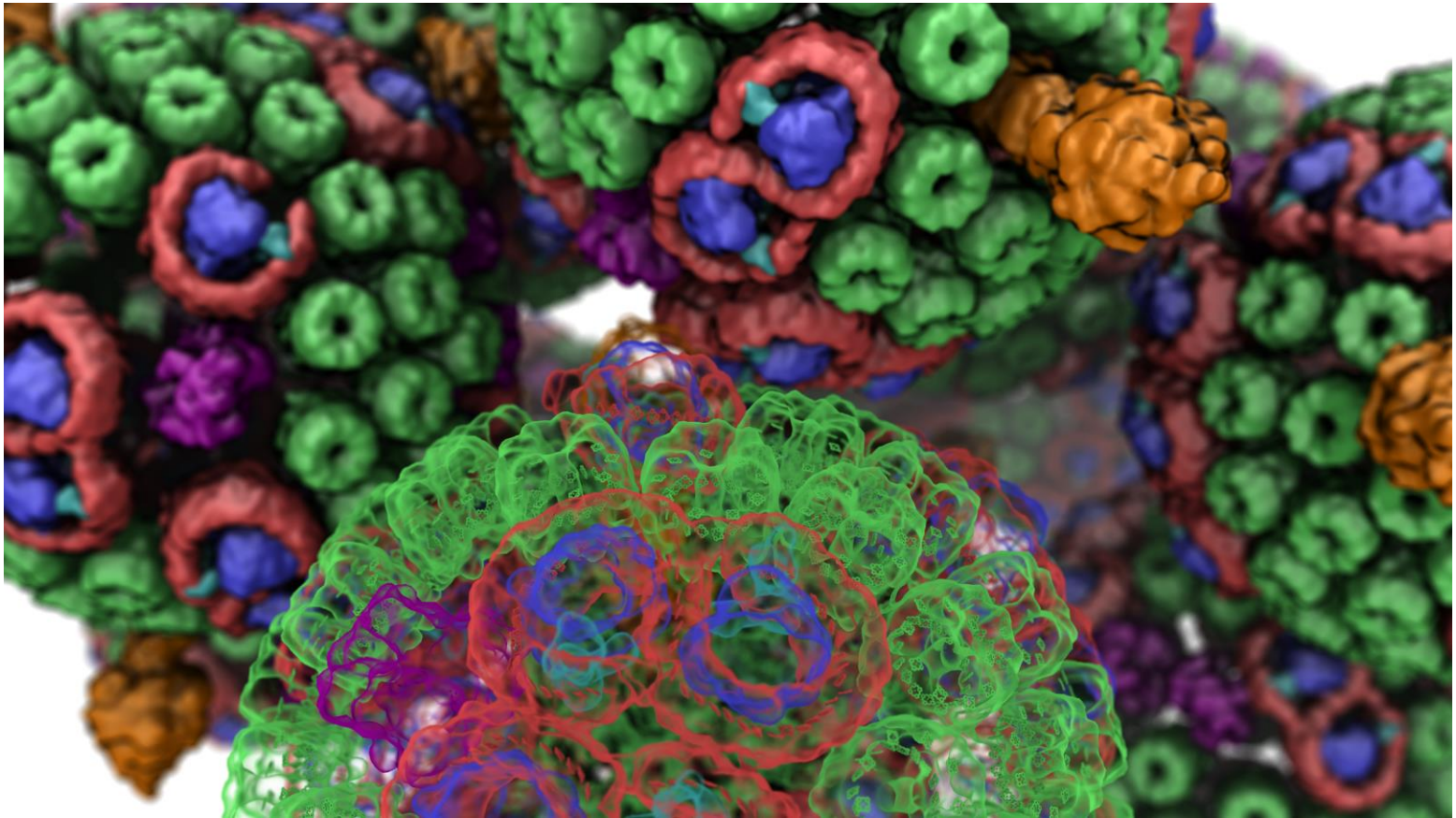
- Interactive RT on laptops, desktops, and cloud
- Large-scale parallel rendering: in situ or post hoc visualization
- **Remote ray tracing with NvPipe video streaming**
- Stereoscopic panoramic and full-dome projections
- **Omnidirectional VR for YouTube, VR HMDs**
- VMD+OptiX NGC container: https://ngc.nvidia.com/registry/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

**GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.** J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, pp. 6:1-6:8, 2013.
**Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.** M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.
**Chemical Visualization of Human Pathogens: the Retroviral Capsids.** J. R. Perilla, B.-C. Goh, J. E. Stone, and K. Schulten. SC'15 Visualization and Data Analytics Showcase, 2015.
**Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.** J. E. Stone et al., J. Parallel Computing, 55:17-27, 2016.
**Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering** J. E. Stone, W. R. Sherman, and K. HPDAV, IPDPSW, pp. 1048-1057, 2016.

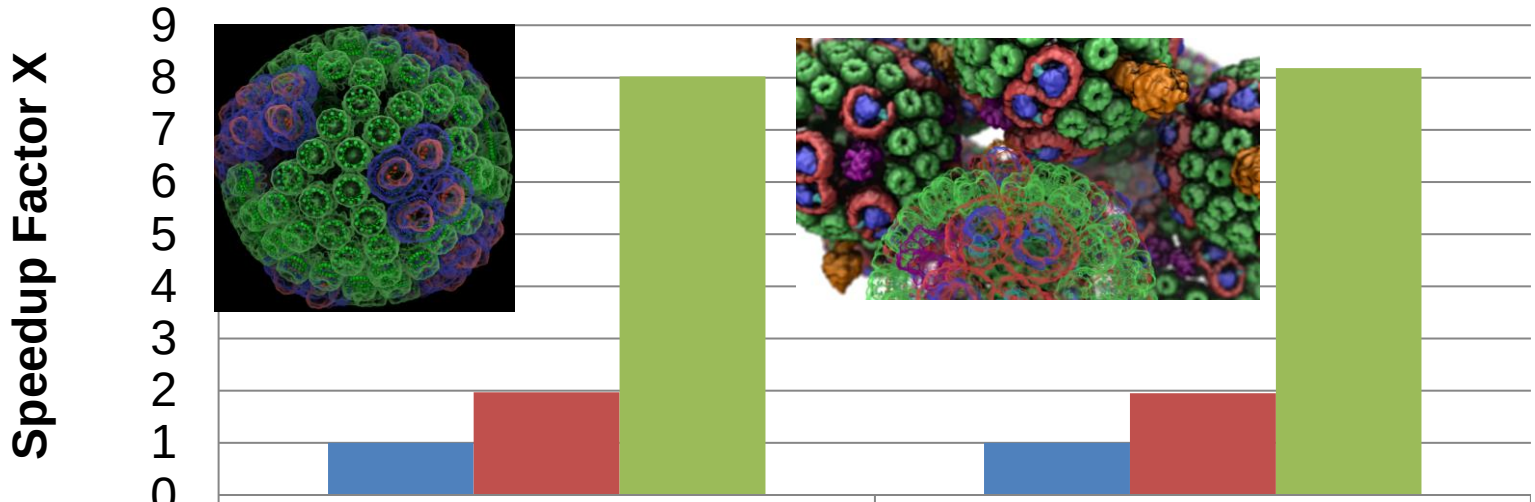


**VMD/OptiX GPU Ray Tracing of all-atom Chromatophore w/ lipids.**

# VMD/OptiX RTX Acceleration



# VMD OptiX RT performance on Quadro RTX 6000



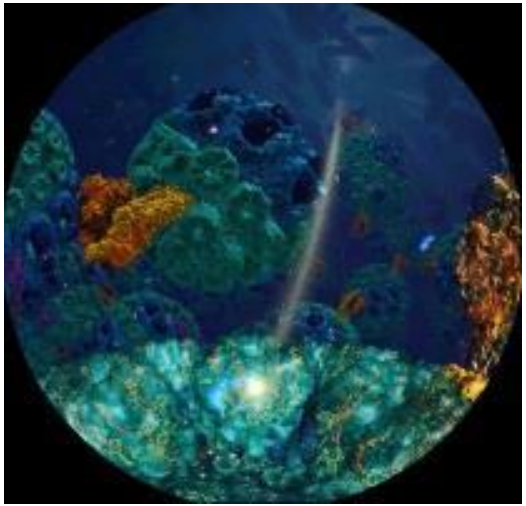

| | Chromatophore @ 4Kx4K | Chrom Cell, 512x DoF @ 1080p |
|---|---|---|
| Quadro GV100 | 1 | 1 |
| 2x Quadro GV100 | 1.97 | 1.95 |
| Quadro RTX 6000 | 8.02 | 8.18 |

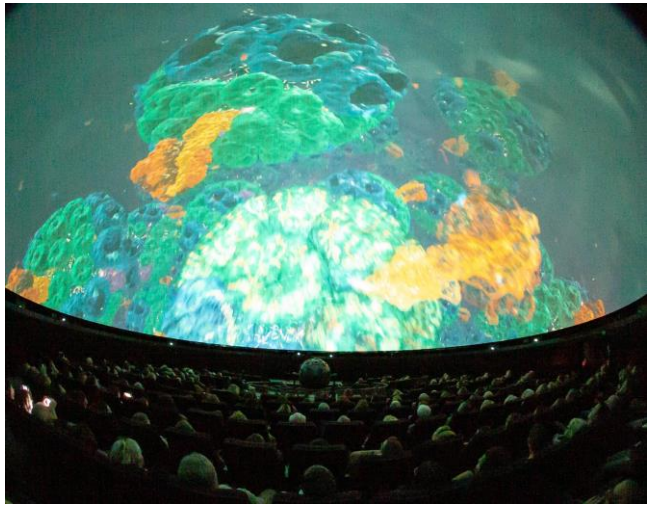
# VMD Cinematic Molecular Visualization and Rendering: “Birth of Planet Earth” Fulldome Show

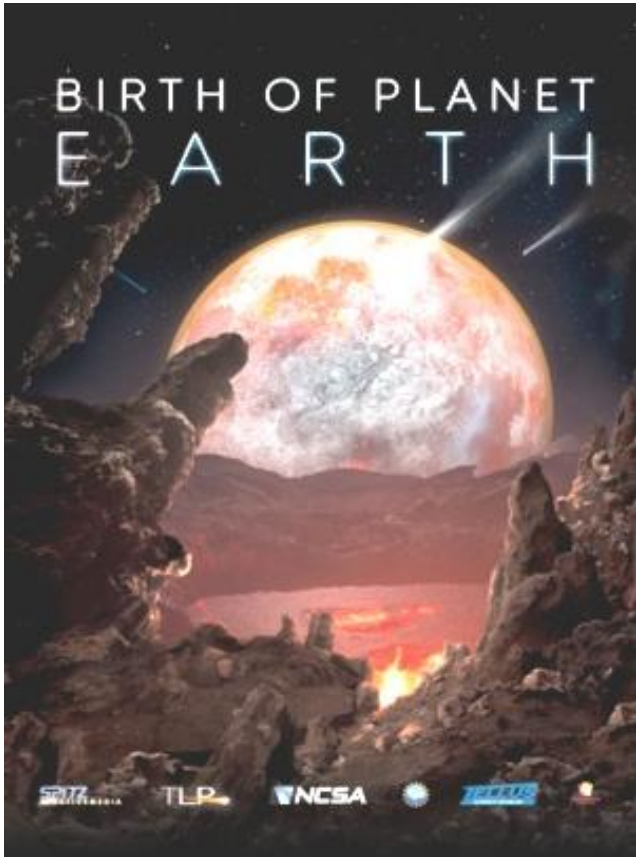
https://www.youtube.com/watch?v=NTgAok6n7I4

## 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!**



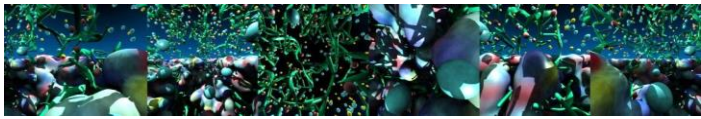


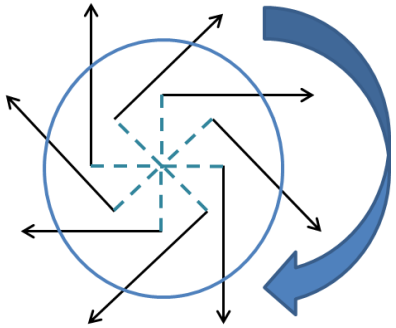


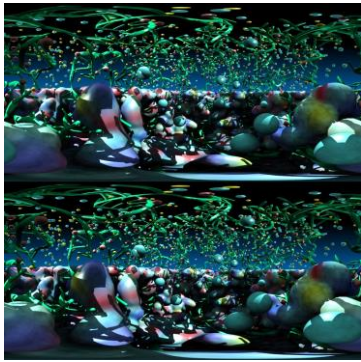

**Multiscale modeling and cinematic visualization of photosynthetic energy conversion processes from electronic to cell scales.**
M. Sener, S. Levy, J. E. Stone, et al., J. Parallel Computing, 2021.

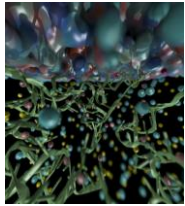
# Omnidirectional Stereoscopic Ray Tracing

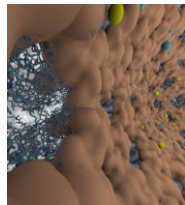
- **Ray trace 360° images and movies for Desk and VR HMDs: Oculus, Vive, Cardboard**
- Stereo spheremaps or cubemaps allow very high-frame-rate interactive OpenGL display
- **AO lighting, depth of field**, shadows, transparency, curved geometry, …
- **Summit 6x Tesla V100 GPU nodes:**
  - **Render many 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**











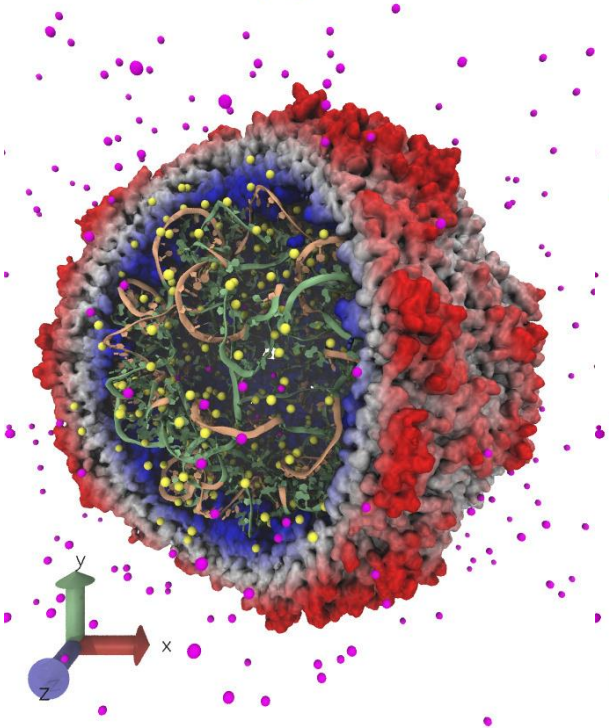
**Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing.** J. E. Stone, et al. J. Parallel Computing, 55:17-27, 2016.

**Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering.** J. E. Stone, W. R. Sherman, and K. Schulten. High Performance Data Analysis and Visualization Workshop, IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), pp. 1048-1057, 2016.

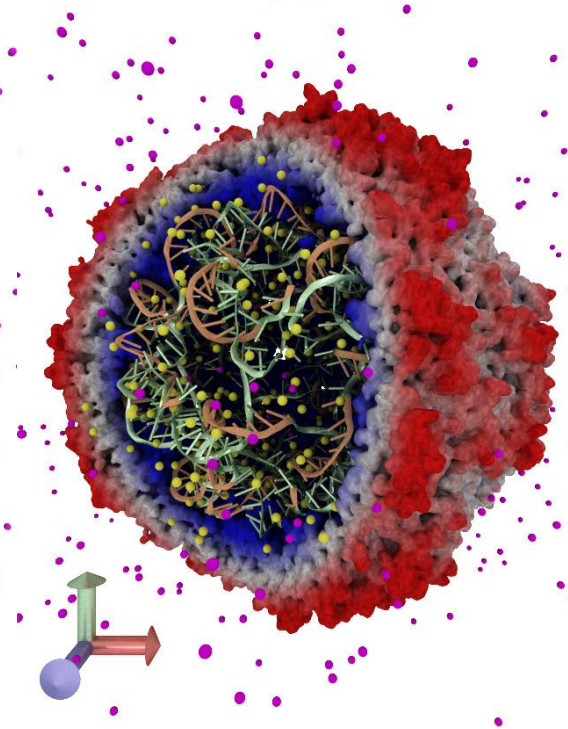
# VMD Examples from In-Progress ANARI Renderers

https://www.khronos.org/anari

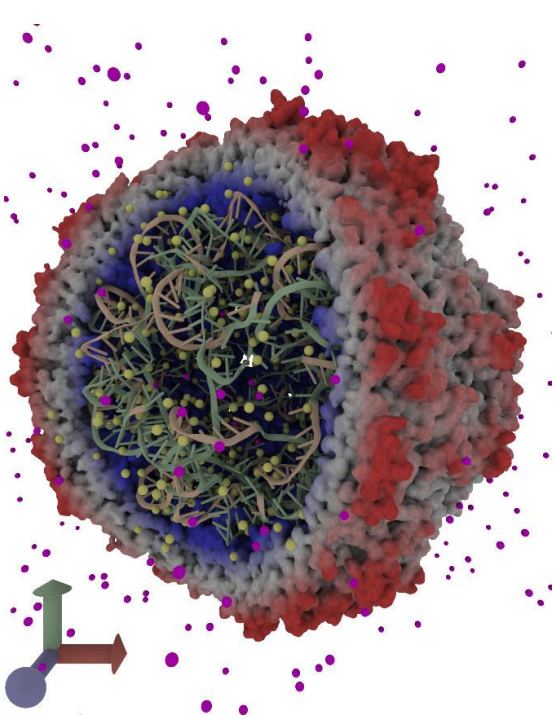
Tachyon Ray Tracer




OSPRay Path Tracer



OptiX Path Tracer



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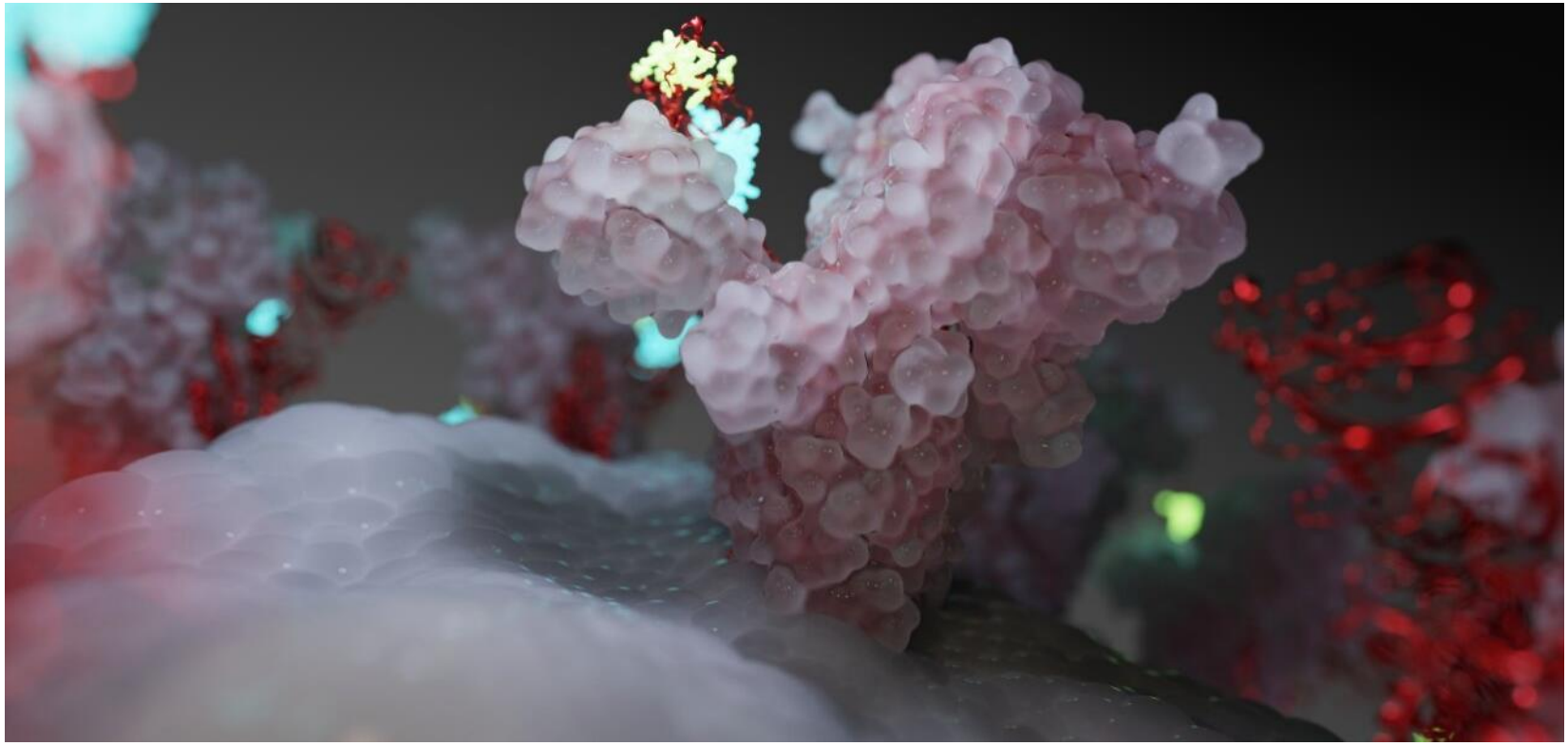
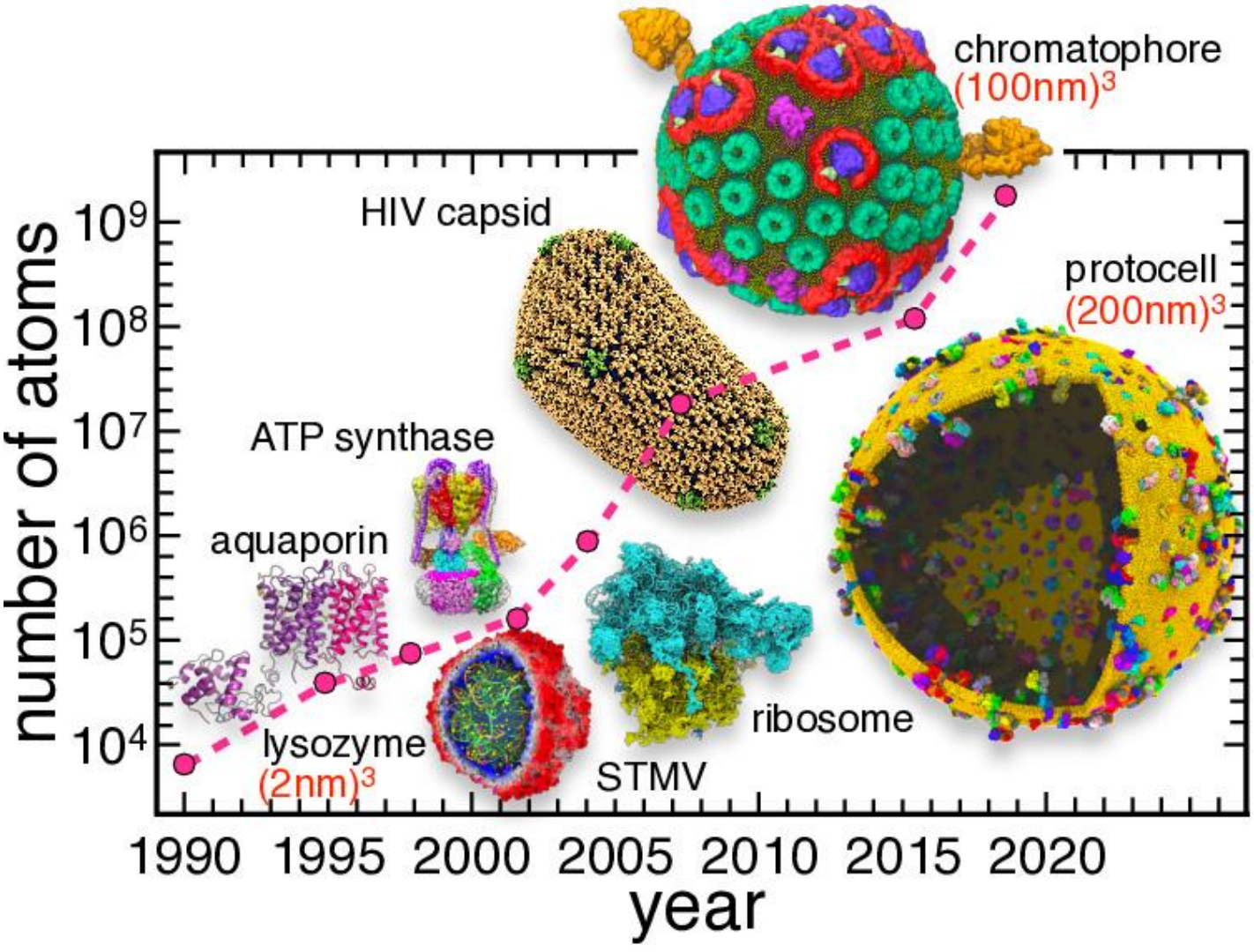
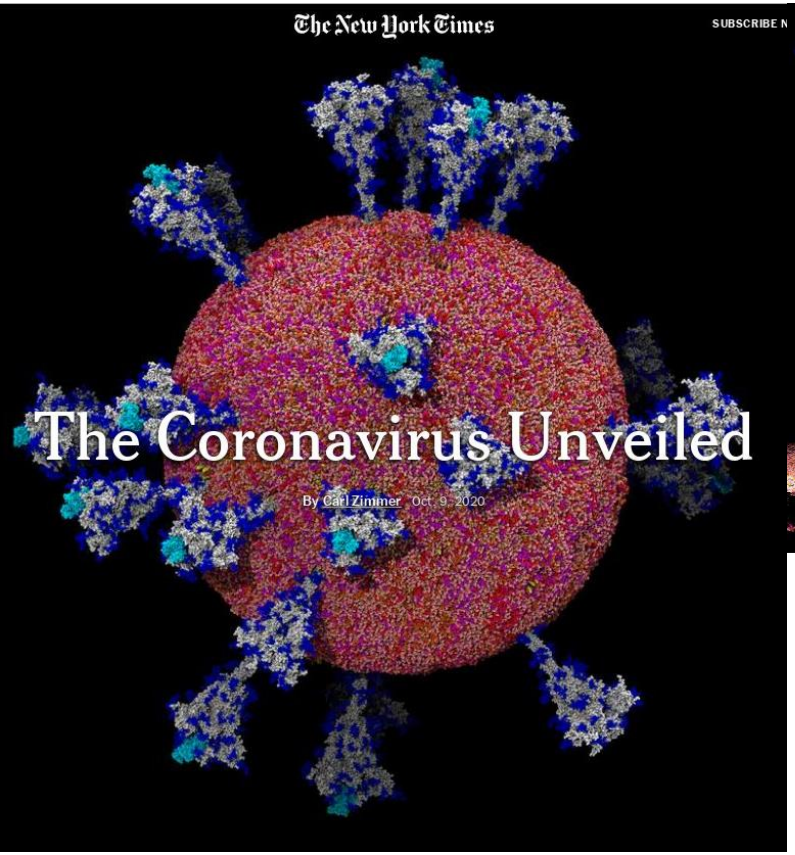
# VMD+Folding@Home w/ NVIDIA Omniverse+Maya

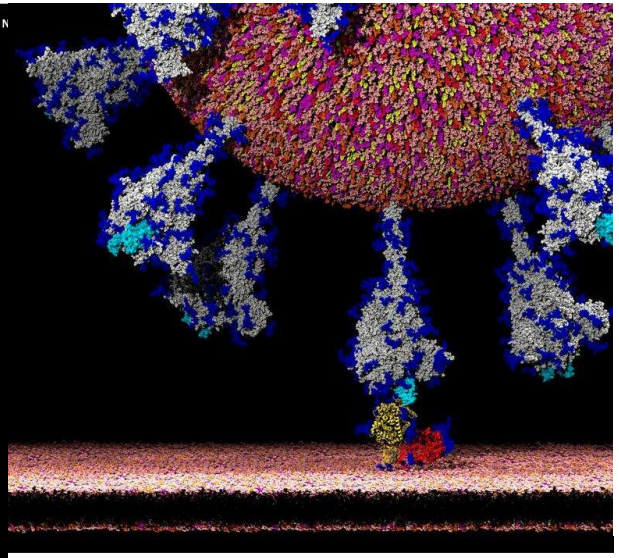
- https://blogs.nvidia.com/blog/2020/10/07/foldingathome-omniverse-coronavirus/
- Movie (YouTube): https://youtu.be/Y9N_lmvwnUI



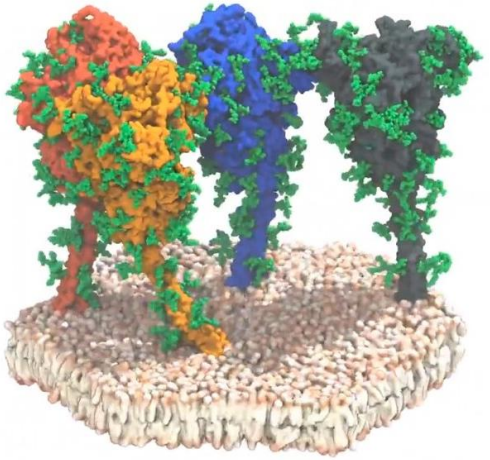

chromatophore
(100nm)3
HIV capsid
protocell
(200nm)3
ATP synthase
aquaporin
ribosome
lysozyme
(2nm)3
STMV
number of atoms
10^9
10^8
10^7
10^6
10^5
10^4
1990
1995
2000
2005
2010
2015
2020
year

https://www.nytimes.com/interactive/2020/health/coronavirus-unveiled.html

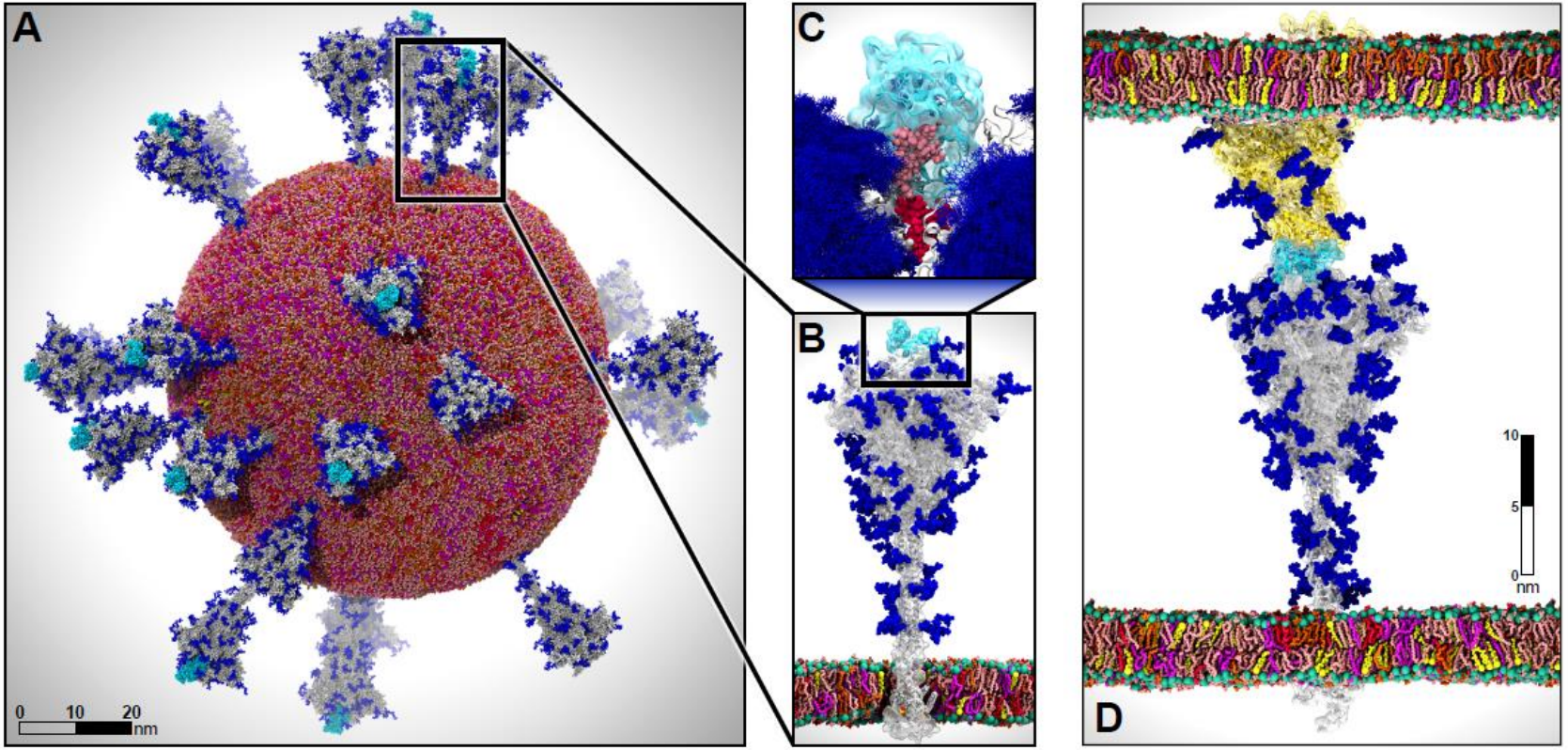


Latching on to an ACE2 receptor, in yellow, allows the coronavirus to enter human cells. Lorenzo Casalino, Amaro Lab, U.C. San Diego.



A simulation of four spike proteins, each bending on three hinges. Sören von Bülow, Mateusz Sikora and Gerhard Hummer, Max Planck Institute of Biophysics




**AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics.**
**L. Casalino, A. Dommer, Z. Gaieb, et al., IJHPCA, 2021.**
**https://dx.doi.org/10.1177/10943420211006452**

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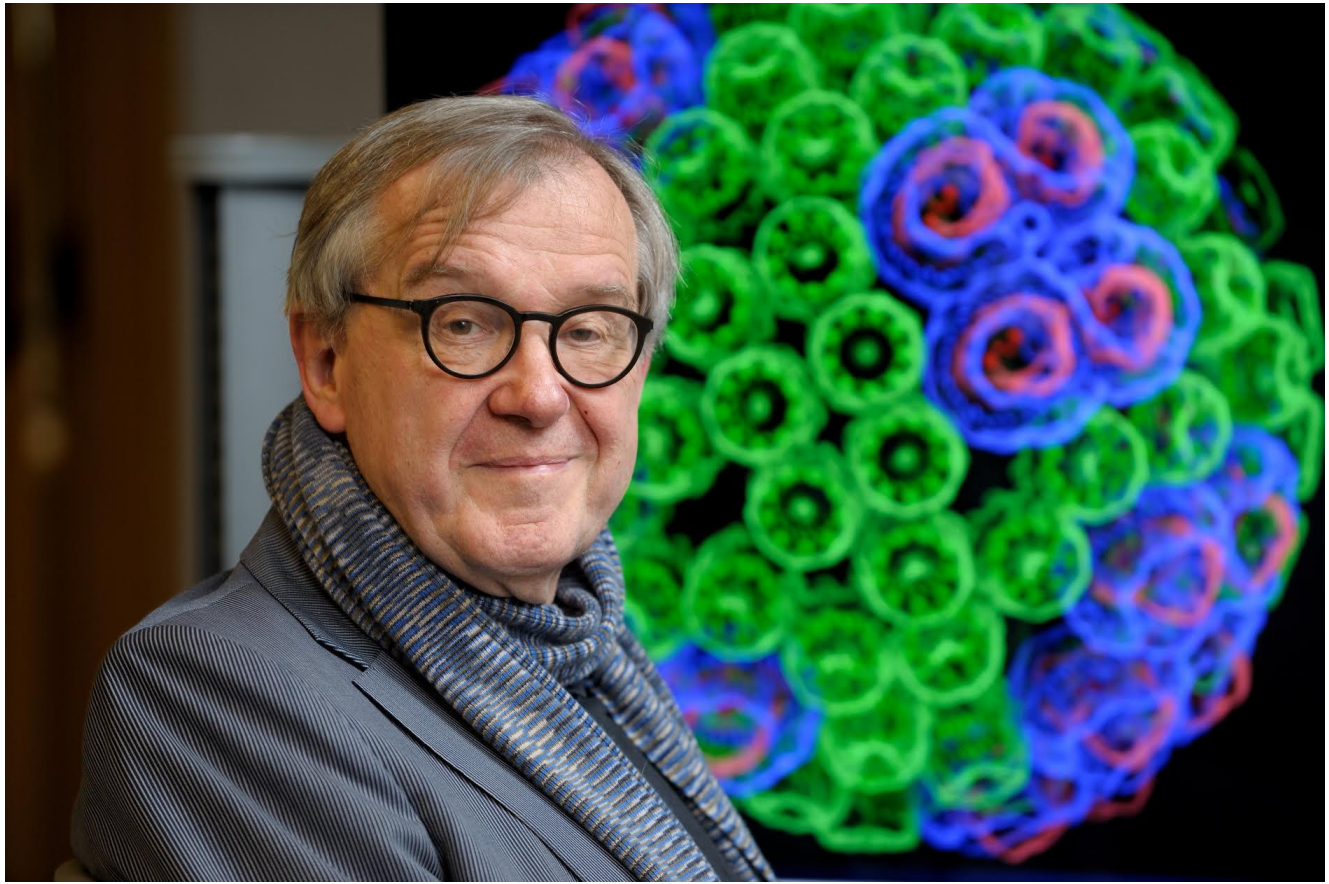
    ACI-1238993, ACI-1440026
  - NSF Support: CADENS award ACI-1445176



*“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*