Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail

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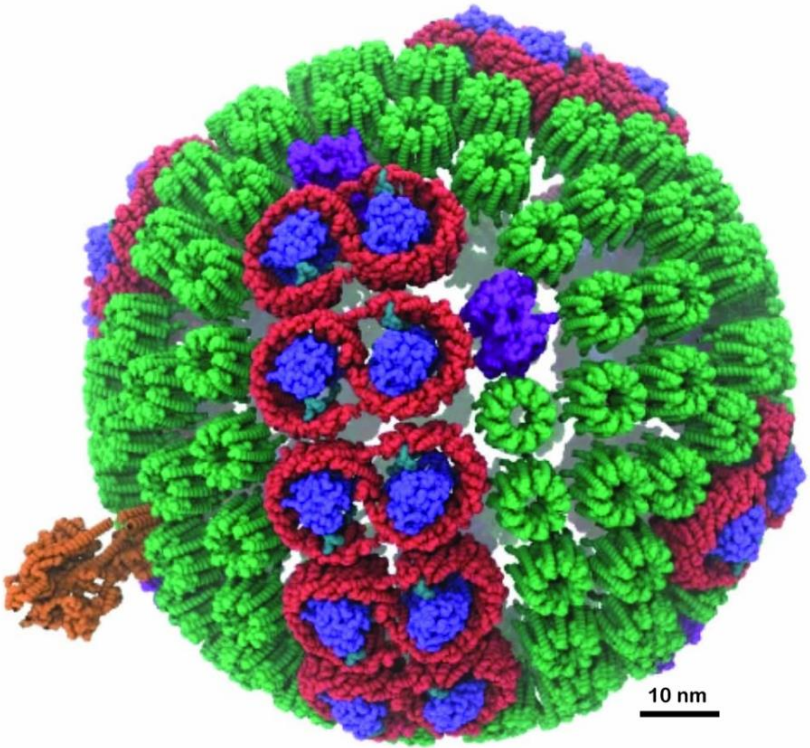
Nature's Use of Solar Energy

- Solar energy powers life on Earth
- **120,000 TW** average solar irradiance
- Natural light harvesting systems use quantum mechanical phenomena to convert light into chemical energy, to be *stored* and *consumed* by cells…
- Use insights from nature to engineer bio-hybrid or synthetic devices to help feed our **>15 TW** power demand

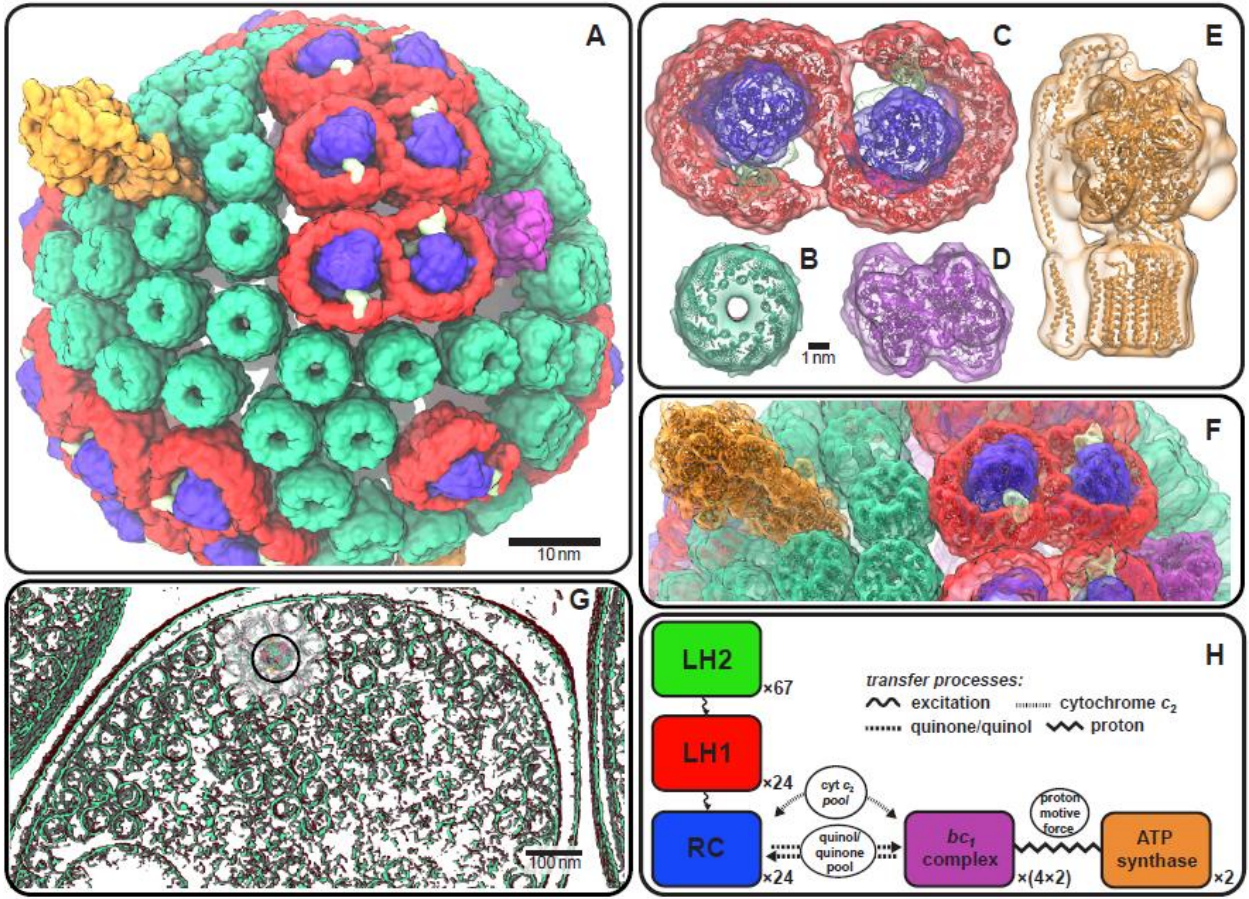
Blankenship et al., Science 332(6031):805-809, 2011.

Photosynthetic Chromatophore of Purple Bacteria

- Purple bacteria live in light-starved conditions at the bottom of ponds, with ~1% sunlight
- Chromatophore system
  - 100M atoms, 700 $Å^3$ volume
  - Contains over 100 proteins, ~3,000 bacteriochlorophylls for collection of photons
  - Energy conversion process synthesizes ATP, which fuels cells…



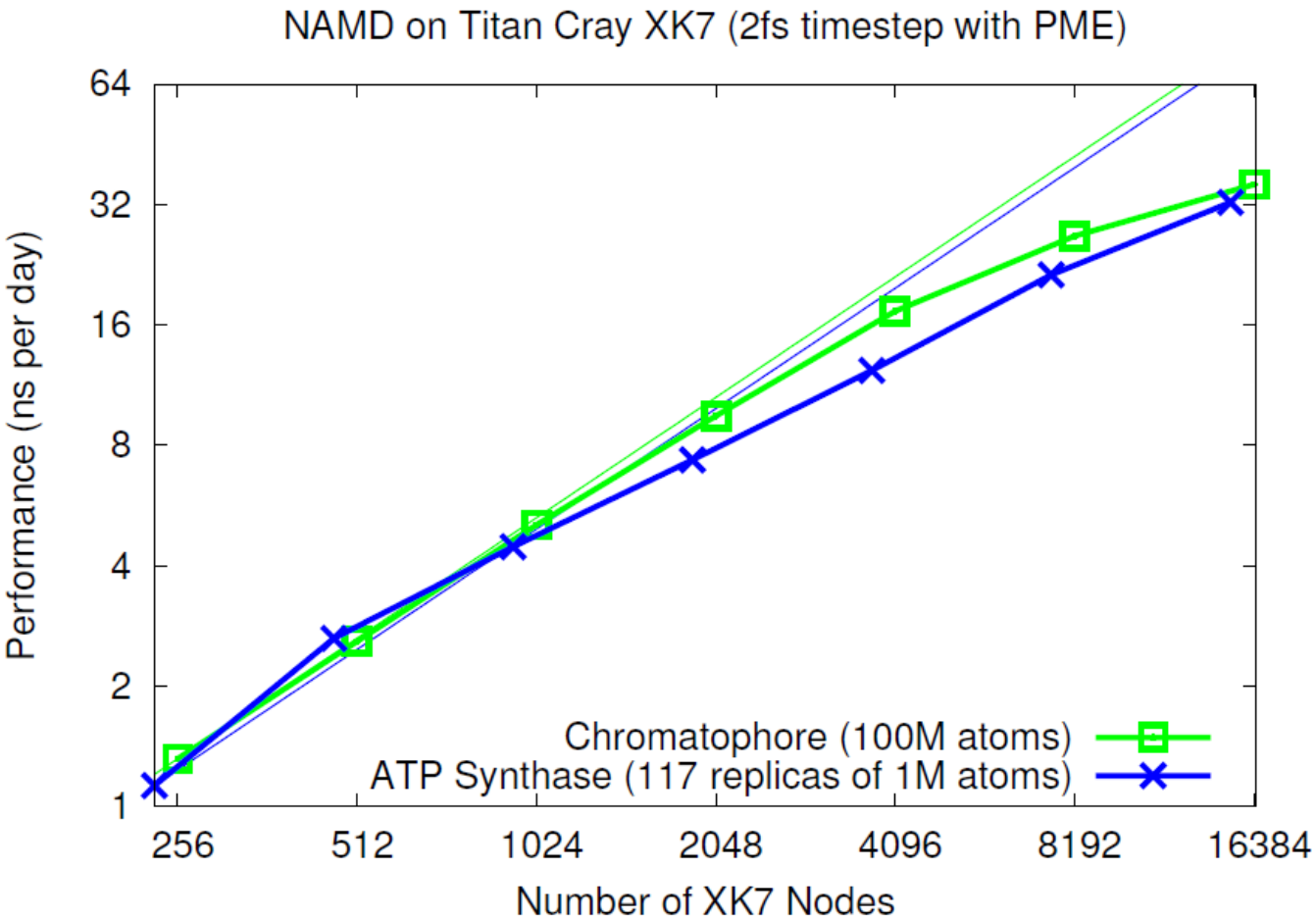
- Movie sums up ~40 papers and 37 years of work by Schulten lab and collaborators
- Driving NAMD and VMD software design:
  - Two decades of simulation, analysis, and visualization of individual chromatophore components w/ NAMD+VMD



Chromatophore Challenges

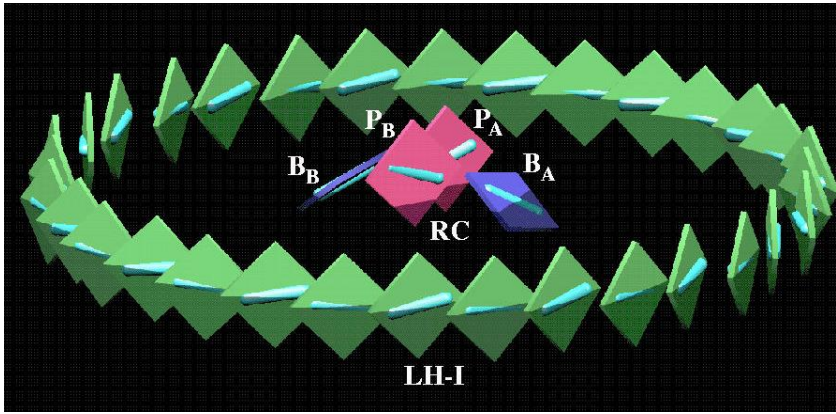
- Combines structure data from many imaging modalities: AFM, cryo-EM, Tomography, X-Ray Crystallography, …
- NAMD+VMD structure building tools, file formats, analysis algorithms reworked to handle >100M-atom scales
  - Simulation of complete chromatophore requires **petascale computing** on Blue Waters and Titan
  - New algorithms for efficient use of GPUs, Cray XK7 for all stages of simulation, analysis, and visualization
- Study of quantum dynamics required development of completely new software (HEOM) on large shared memory parallel computers

NAMD Chromatophore Runs on Titan w/ 16,384 GPUs



Role of Visualization

- MD simulation, analysis, visualization provide researchers a so-called ***"Computational Microscope"***
- Visualization is heavily used at every step of structure building, simulation prep and run, analysis, and publication

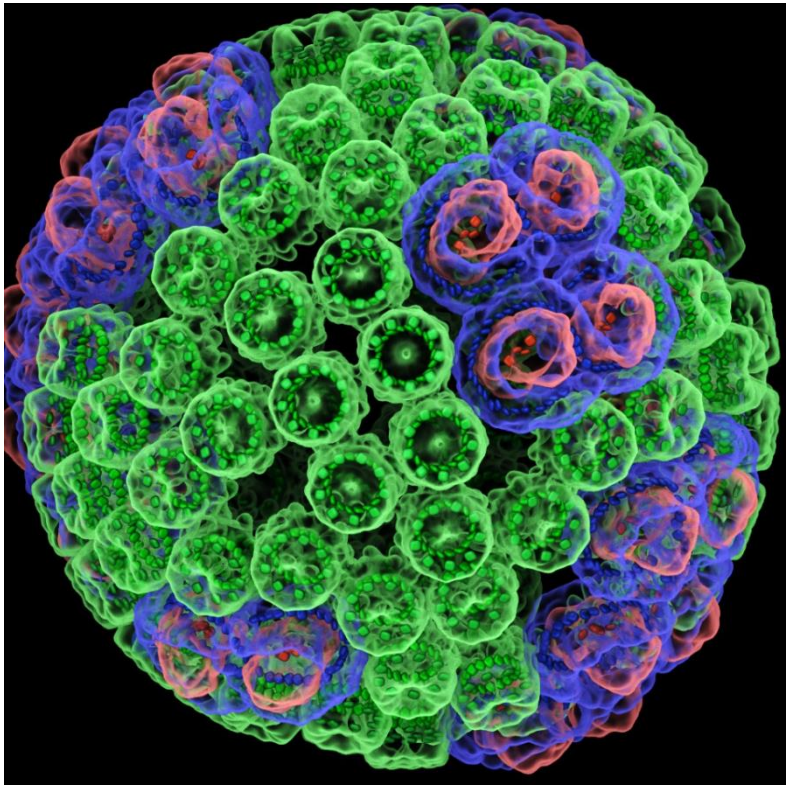


1998 VMD rendering of LH-I

SGI Onyx2 InfiniteReality w/ IRIS GL

VMD Parallel Rendering on Blue Waters

- New graphical representation schemes, transparent surface shaders
- GPU-accelerated molecular surface calculations, memory-efficient algorithms for huge complexes
- VMD + GPU-accelerated Tachyon ray tracing engine based on CUDA+OptiX w/ MPI+Pthreads
- ***Each revision:*** 7,500 frames render on 96 Cray XK7 nodes in 290 node-hours, 45GB of images prior to editing



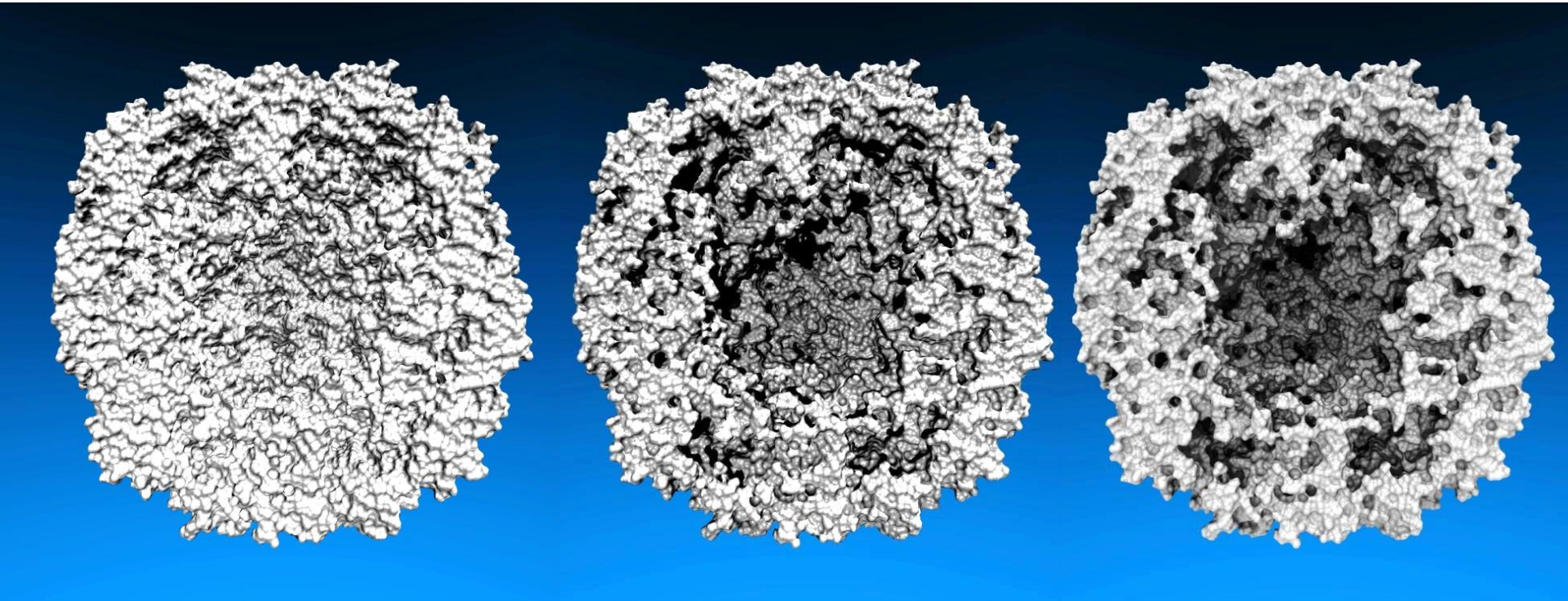
GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms. J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

Lighting Comparison

Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit



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