S5246—Innovations in OptiX

Guest Presentation: Integrating OptiX in VMD

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S5246, GPU Technology Conference

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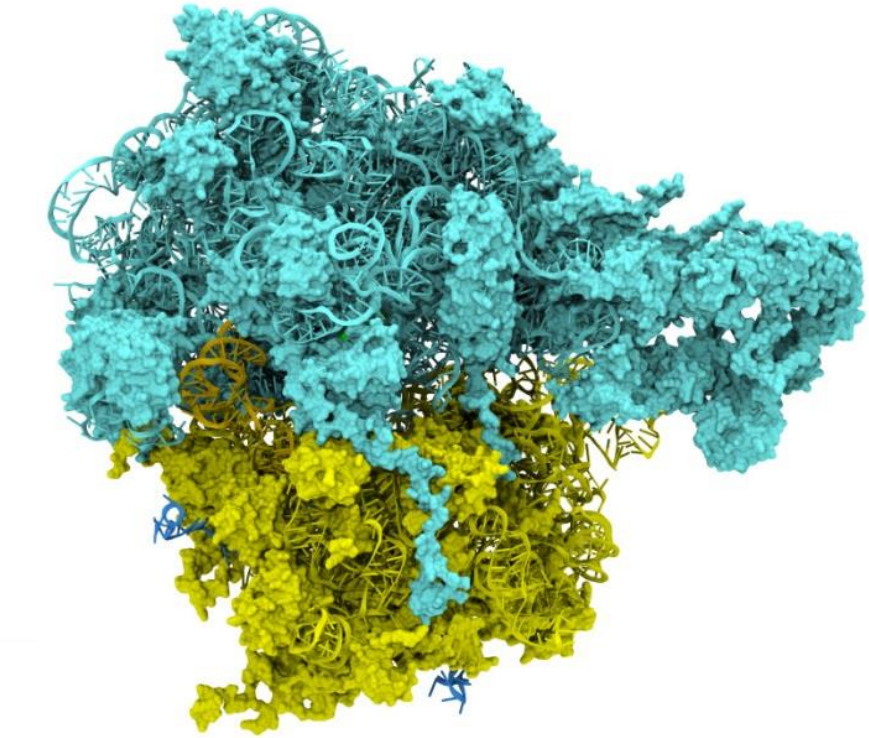
VMD – “Visual Molecular Dynamics”

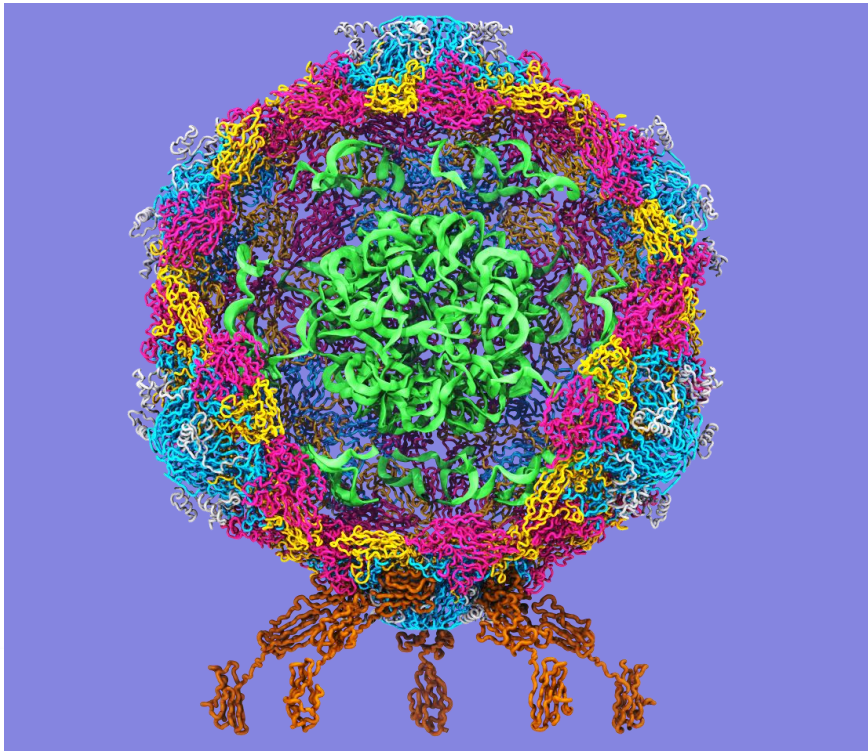
Goal: A Computational Microscope

Study the molecular machines in living cells

Ribosome: target for antibiotics



Poliovirus

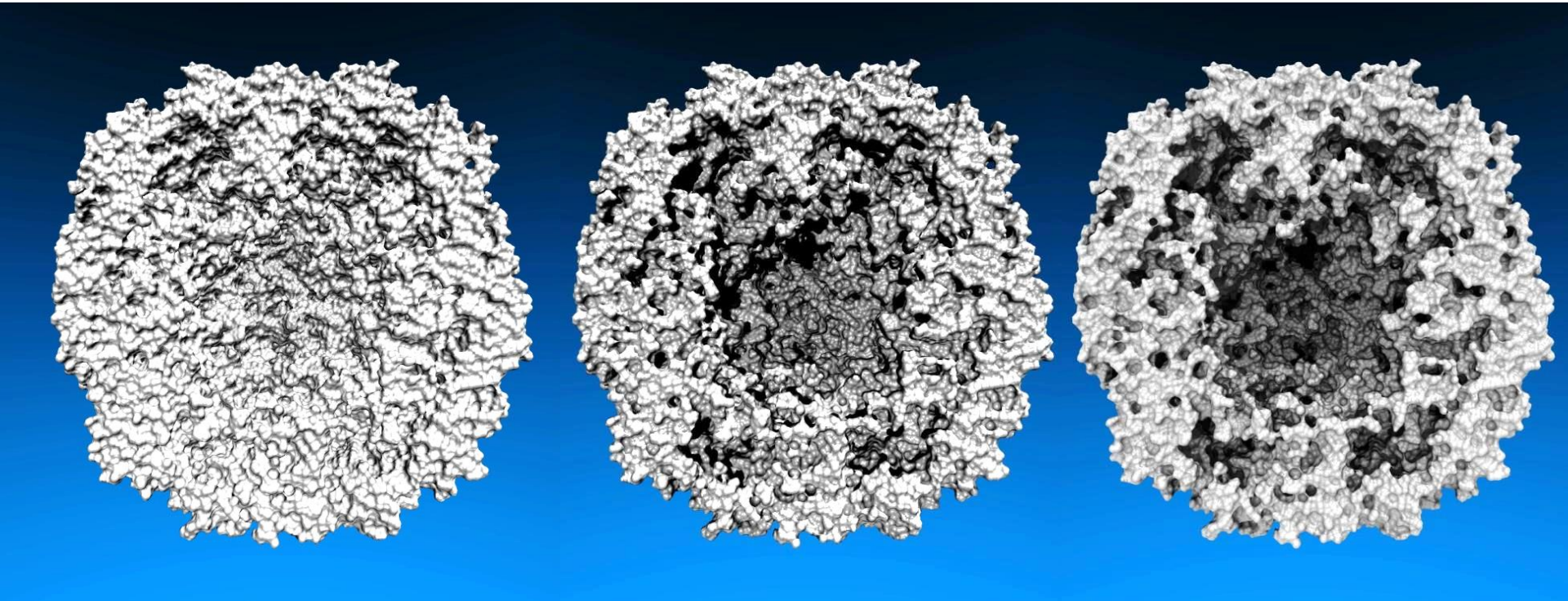


Lighting Comparison

Two lights, no shadows

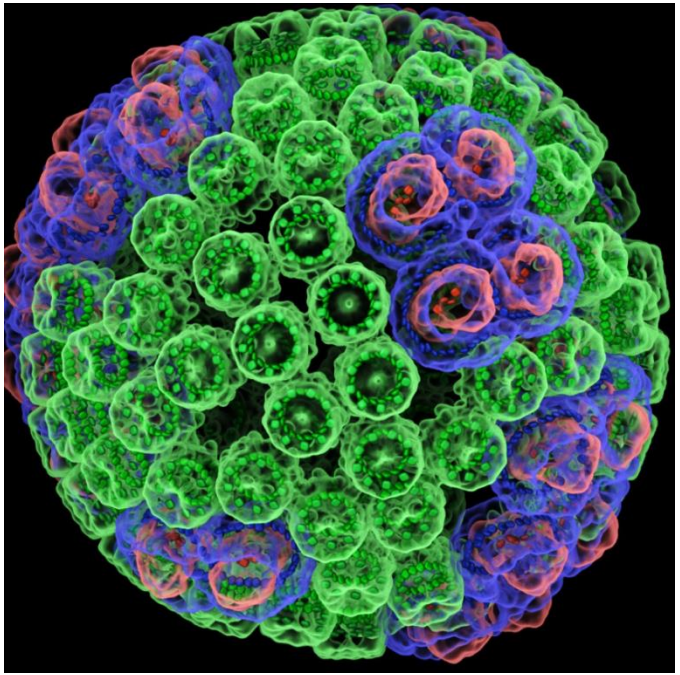
Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit



VMD Chromatophore Rendering on Blue Waters

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

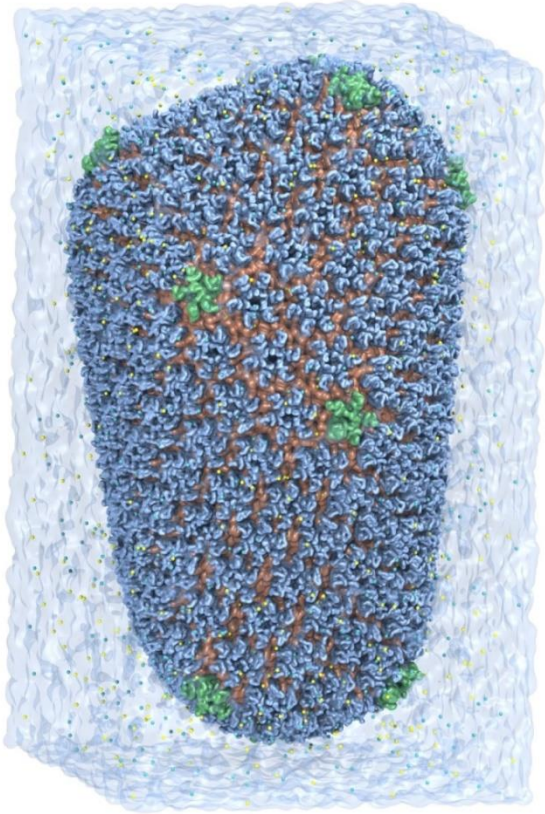


GPU-Accelerated Molecular Visualization on Petascale Supercomputing Platforms.
J. E. Stone, K. L. Vandivort, and K. Schulten. UltraVis'13, 2013.

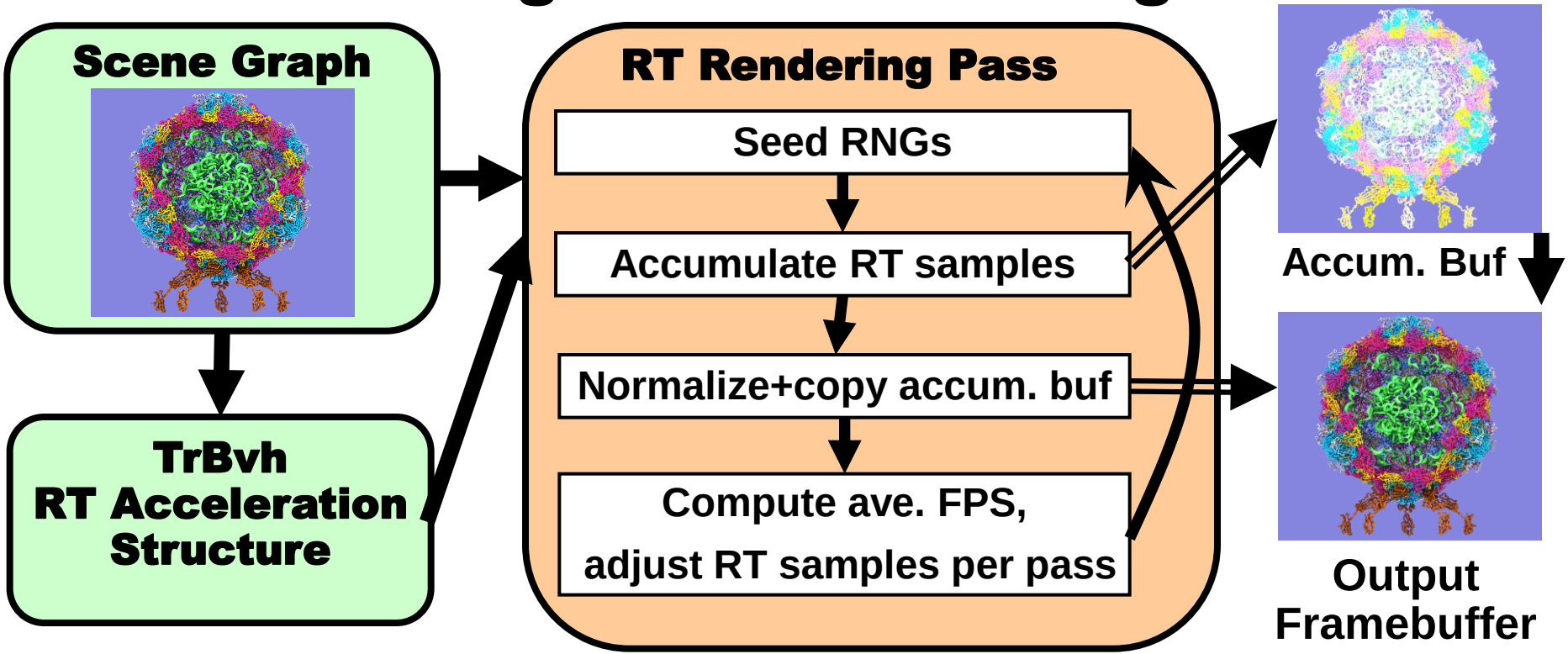
Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail.
M. Sener, et al. SC'14 Visualization and Data Analytics Showcase, 2014.
*****Winner of the SC'14 Visualization and Data Analytics Showcase**

VMD 1.9.2 Interactive GPU Ray Tracing

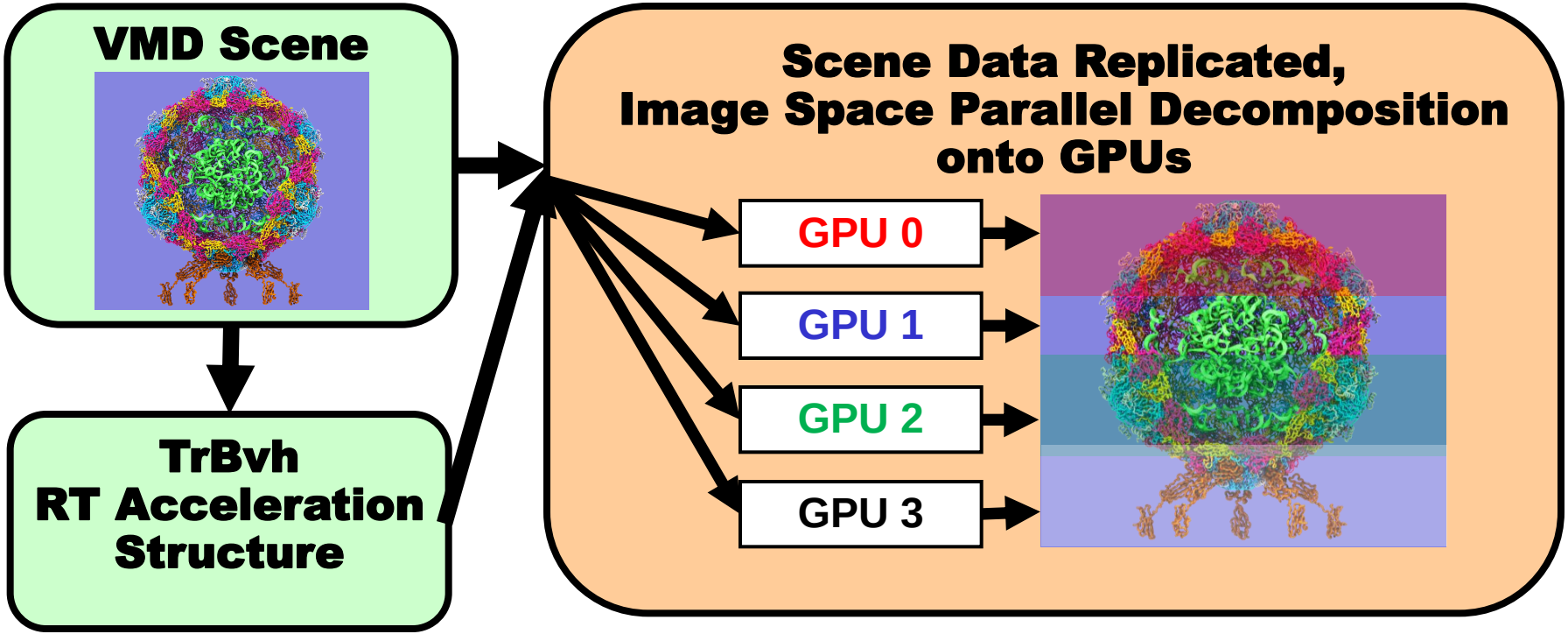
- Ray tracing heavily used for VMD publication-quality images/movies
- High quality lighting, shadows, transparency, depth-of-field focal blur, etc.
- VMD now provides –***interactive***– ray tracing on laptops, desktops, and ***remote*** visual supercomputers



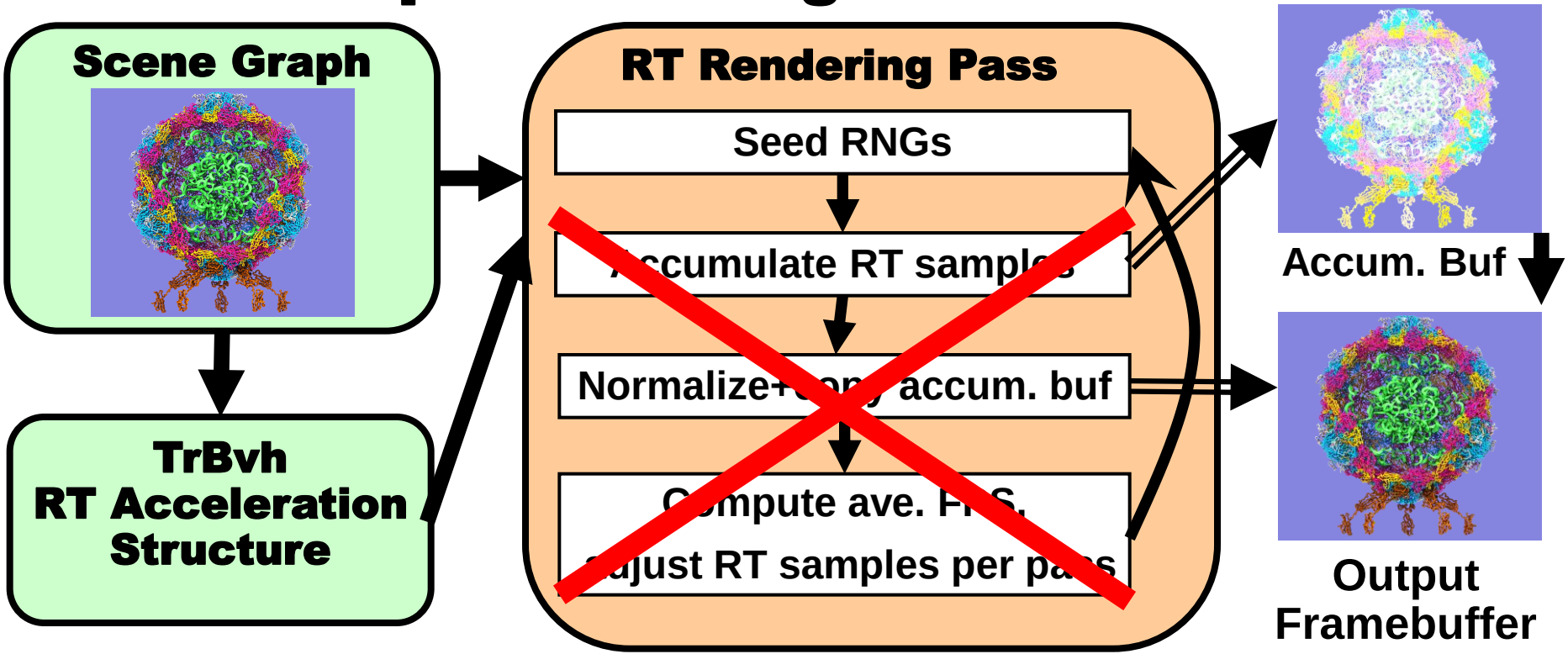
VMD TachyonL-OptiX Interactive RT w/ Progressive Rendering



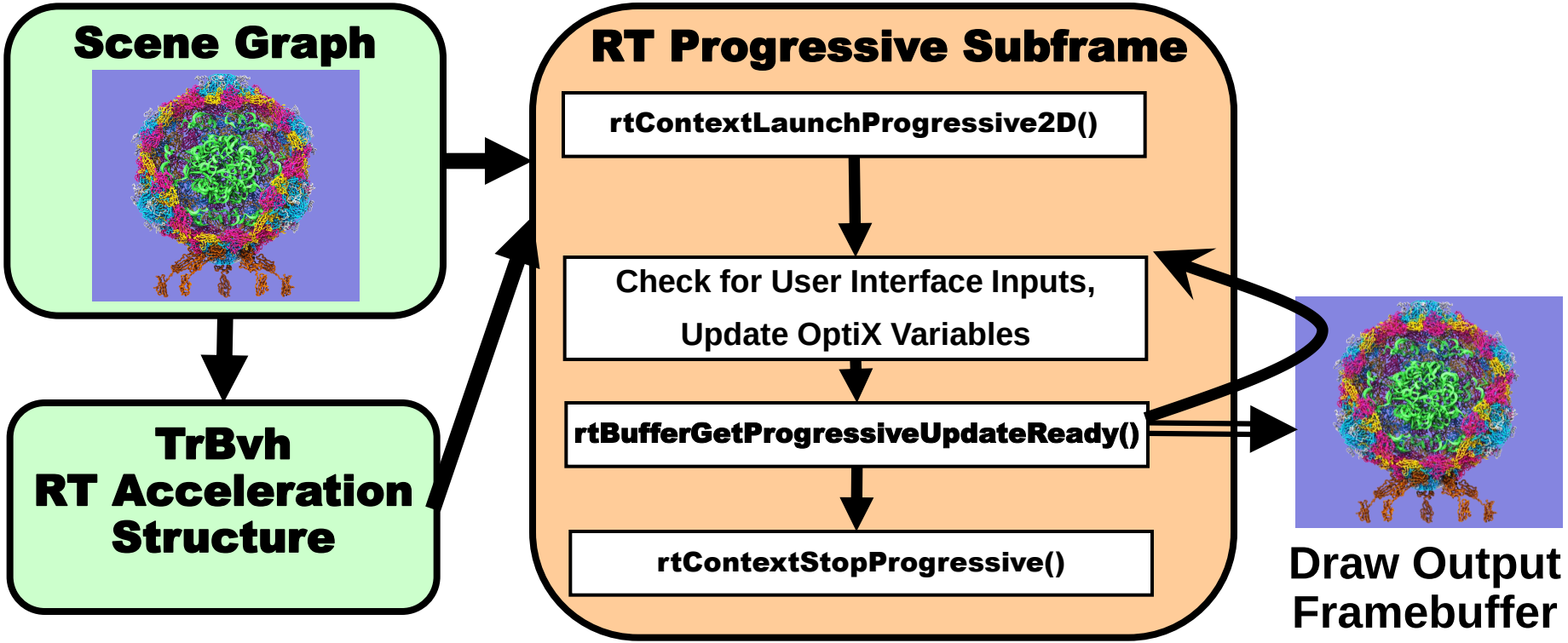
VMD TachyonL-OptiX: Multi-GPU on a Desktop or Single Node



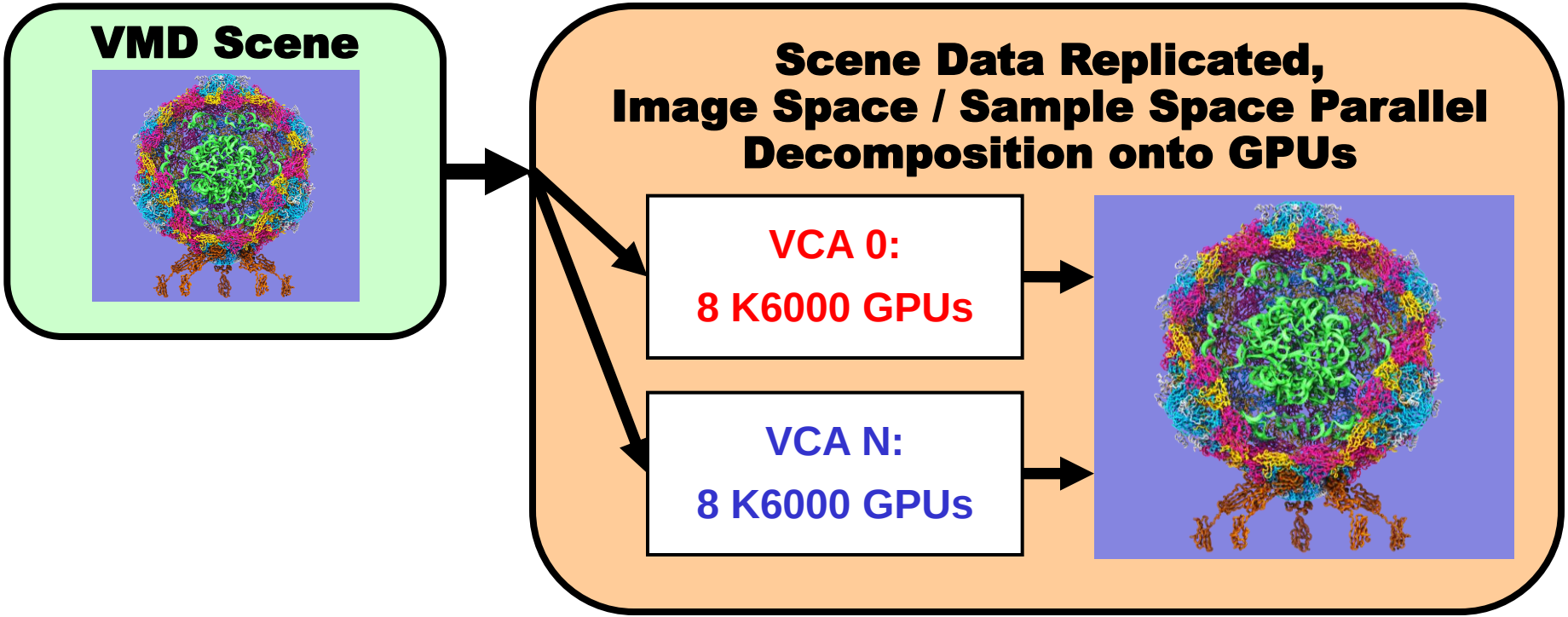
VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



VMD TachyonL-OptiX Interactive RT w/ OptiX 3.8 Progressive API



VMD TachyonL-OptiX: Multi-GPU on NVIDIA VCA Cluster



Future Work

- Improved performance / quality trade-offs in interactive RT stochastic sampling strategies
- Optimize GPU scene DMA and BVH regen speed for time-varying geometry, e.g. MD trajectories
- Continue tuning of GPU-specific RT intersection routines, memory layout
- GPU-accelerated movie encoder back-end
- Interactive RT combined with remote viz on HPC systems, much larger data sizes

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