CINEMATIC SCIENTIFIC DATA VISUALIZATION FOR CADENS

Allocation: Illinois/275 Knh
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EXECUTIVE SUMMARY

The Advanced Visualization Lab (AVL) continues work on the NSF-funded CADENS project (the Centrality of Advanced Digitally Enabled Science, ACI-1445176). AVL co-produced and rendered visualization scenes for the upcoming full-dome planetarium show, *Birth of Planet Earth*. We have used Blue Waters for processing data as well as rendering scenes in 4K monoscopic and full-dome formats.

RESEARCH CHALLENGE

Drawing on data from scientists involved in high-performance computing-based research, the AVL creates visualizations in a cinematic style intended for public outreach, through flat-screen science documentaries, films, and full-dome planetarium shows.

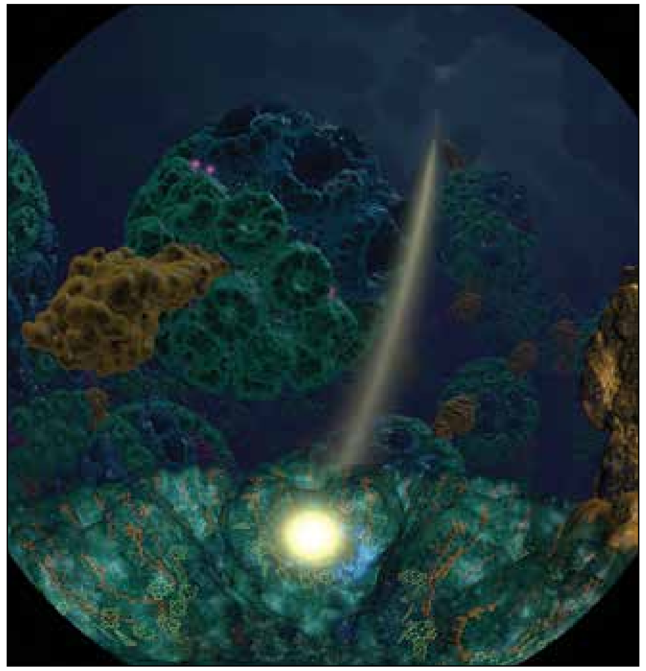

Figure 1: Photosynthetic energy harvesting in the purple bacterium *Rba. sphaeroides* [1]. Adapted from a visualization [2] of the structure [3] of chromatophores—photosynthetic vesicles—illustrating energy conversion steps from the capture of sunlight to the synthesis of ATP. This segment is dedicated to Klaus Schulten, as its content had been a lifetime passion for studies [1–3] in his Theoretical and Computational Biophysics Group until his passing in 2016. (To appear in *Birth of Planet Earth*.)

METHODS & CODES

Our Blue Waters visualization work depends on several externally provided packages: Houdini, a commercial visual effects software package from SideFX; yt, the data analysis and visualization package (yt-project.org) for ingesting and re-gridding some types of data; VMD, the Visual Molecular Dynamics package from John Stone of the Theoretical Biophysics group at the University of Illinois at Urbana-Champaign (www.ks.uiuc.edu); and Python with numpy and scipy for many sorts of data preprocessing from the formats provided by the scientists into formats usable by Houdini. We have developed our own software tools, including Ytini for yt–Houdini integration, and Blurend to organize the Houdini rendering workflow for the Blue Waters environment.

Visualizing energy harvesting in a photosynthetic purple bacterium [1] involved combining structural models from atomic, protein, organelle, and cell scales using multiple software tools [2]. The construction of structural models [3] was performed with VMD [2] and Mathematica, which was also used for the determination of relevant energy conversion steps [1]. Multiple copies of a static chromatophore model [3] were assembled in Houdini to emulate the interior of a low light-adapted purple bacterial cell. Dynamic elements—photons, electronic excitations, protons, quinols/quinones, ATP—were choreographed using Houdini to illustrate energy conversion processes for a lay viewer. Since the timescales for these conversion processes span almost 12 orders of magnitude (femtoseconds to milliseconds) [1], the animations deliberately represent a simplified visual narrative rather than the results of a specific simulation at one timescale. Some visual elements were rendered using Houdini, others with VMD.

We also relied on Blue Waters' capacity to create a high-quality visualization of Robin Canup's Moon-forming collision [4], as explained below.

RESULTS & IMPACT

Blue Waters enabled us to create and refine two data-driven cinematic animations, both appearing in the forthcoming full-dome planetarium show, *Birth of Planet Earth*, to be released in 2019:

- Formation of the Moon [4]—the first 24 hours after the collision that formed Earth's moon,
- Visualizing Energy Harvesting in a Photosynthetic Purple Bacterium [1–3].

Excerpts will be presented at the International Planetarium Society 2018 conference in Toulouse, France. In advance of the show's completion, a work-in-progress trailer is also available at https://vimeo.com/277190989, including contributions from AVL and other groups.

To suggest potential public impact for this work, we compare it with another full-dome planetarium show in the CADENS series, *Solar Superstorms*, for which AVL also relied on Blue Waters for data visualization. Since its 2015 release, it has been booked by over 70 planetaria and science museums in 15 countries, and translated into at least ten languages.

Further impact from past Blue Waters work involved two visualizations created during 2016–2017 and described in the *2017 Blue Waters Annual Report*: "First Light in the Renaissance Simulation" [5] and "Milky Way Analogue Isolated Disk Galaxy Visualization." These were later submitted to the Supercomputing 2017 conference's Scientific Visualization Showcase where they were awarded first and second place, respectively.

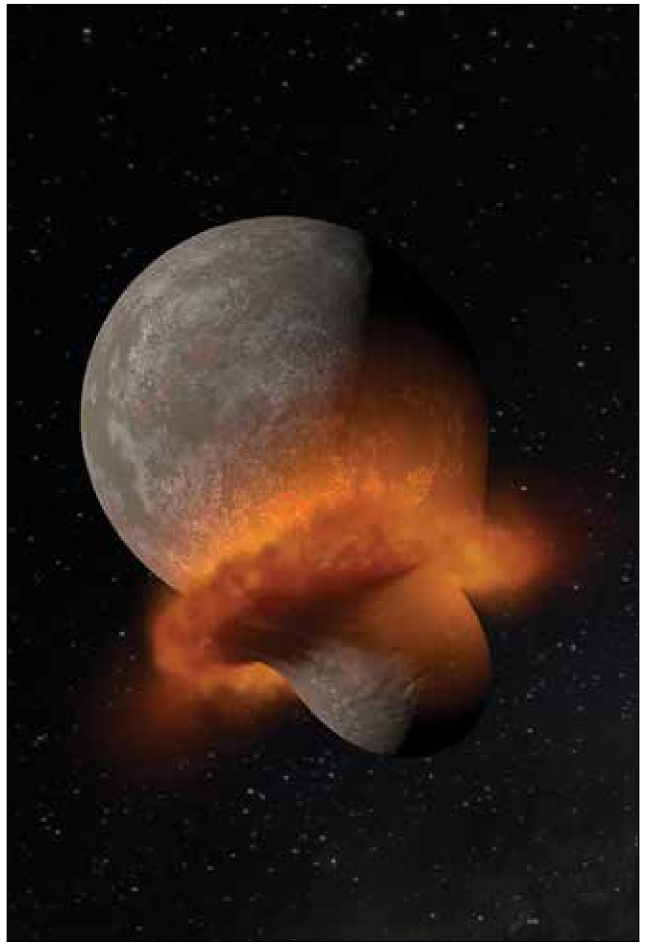

Figure 2: Visualizing the first 24 hours after the collision that formed Earth's moon, from a simulation [4] by Robin Canup of SWRI, as a Mars-sized body strikes the early Earth. (To appear in *Birth of Planet Earth*.)

In addition to full-length documentaries, two short videos using material created during this year's and last year's allocations appear in the Publications and Data Sets section.

WHY BLUE WATERS

Access to Blue Waters has allowed us to iterate quickly and meet deadlines. Over the course of a single weekend, we were able to render a Houdini scene involving a chromatophore model [3] and its surrounding environment that was made up of six separate render layers and a total of 20,870 image frames. The capability to render a large amount of images in a short period of time allowed us to make several iterations of the scene before finalizing a video to send to the IPS 2018 conference. This would not have been possible on our local cluster.

Furthermore, Blue Waters has made it possible to not sacrifice visual quality for render speed. One ~200-frame segment of our visualization of a planetary collision [4] was taking as many as 20 hours per frame to render. Blue Waters made it possible to render these images despite the long render time. Without Blue Waters, we would have had to either change many render settings and significantly decrease the render quality, change the camera position and lose the dramatic effect of having an arm of disk material pass closely overhead, or spend many days trying to come up with a different data representation of the simulation to make the render more manageable on our local cluster.

PUBLICATIONS & DATA SETS

Birth of Planet Earth, full-dome planetarium show directed by Thomas Lucas, to be distributed by Spitz, Inc. in 2019. A work-in-progress trailer appeared in June 2018: https://vimeo.com/277190989.

Cox, D., et al., First Light in the Renaissance Simulation Visualization: Formation of the Very First Galaxies in the Universe. *Supercomputing, Scientific Visualization Showcase Submission* (Denver, Colo., November 12–17, 2017).

Cox, D., et al., Milky Way Analogue Isolated Disk Galaxy Visualization. *Supercomputing, Scientific Visualization Showcase Submission* (Denver, Colo., November 12–17, 2017).

Collision that Formed the Moon, mini-documentary: https://www.youtube.com/watch?v=o2lRpiediP8.

Grand Journey to Understand the Evolution of the Universe, mini-documentary: https://www.youtube.com/watch?v=YyvZs3IBlLk.