

An accessible visual narrative for the primary energy source of life from the fulldome show *Birth of Planet Earth*

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Abstract—Conversion of sunlight into chemical energy, namely photosynthesis, is the primary energy source of life on Earth. An explanatory visualization depicting this process is presented in the form of an excerpt from the fulldome show *Birth of Planet Earth*. This accessible visual narrative shows a lay audience, especially children, how the energy of sunlight is captured, converted, and stored through a chain of proteins to power living cells. The visualization is the result of a multi-year collaboration among biophysicists, visualization scientists, and artists, which, in turn, is based on a decade-long experimental-computational collaboration on structural and functional modeling that produced an atomic detail description of a bacterial bioenergetic organelle, the chromatophore. The energy conversion steps depicted feature an integration of function from electronic to cell levels, spanning nearly 12 orders of magnitude in time scales modeled with multi-scale computational approaches. This atomic detail description uniquely enables a modern retelling of one of humanity’s earliest stories—the interplay between light and life.

I. INTRODUCTION

Public outreach of science, such as fulldome planetarium shows, fulfills a crucial educational need by bringing leading edge scientific discoveries to a populace that supported the research yet often remain unable to access it due to its inherent complexity [1]. Such a fulldome show, *Birth of Planet Earth*, introduces the story of life emerging on our planet and, particularly, how it is powered by harvesting the energy of sunlight, i.e., photosynthesis [2]. Here, an excerpt is presented as a stand-alone explanatory visualization (Fig. 1A). The accessible narrative of this visualization constitutes a modern extension of one of the oldest discoveries of humanity, namely, the relation between sunlight and the proliferation of life. (“The sun is not only the author of visibility in all visible things, but of generation and nourishment and growth.”—Plato, *The Republic*.) Thus, the visualization is a retelling of this ancient story of “nourishment and growth,” but with atomistic accuracy obtained by a decade of experimental and computational research [2]–[7], rendered accessible to children as a result of a multi-year collaboration between biophysicists, visualization scientists, and artists.

High performance computing (HPC) exhibits a dual role in the study of the complex biomolecular processes of photosyn-

thesis. On the one hand, HPC is a critical exploratory tool for building atomic detail structures and for multi-scale modeling of energy conversion steps from electronic interactions to cell level integration [2], [7]. On the other hand, HPC provides an explanatory tool for depicting the cascade of energy conversion steps in a continuous ‘powers of ten’ style visual narrative [8], [9]. Efficient harvesting and conversion of solar energy, thus depicted, may hold the key for a clean energy future for humanity [10] with biological systems outperforming comparable human technologies at systems-level [2].

The visualization presented here involved the development of novel workflows by a collaborating team of biophysicists (Fig. 1B) and visualization scientists (Fig. 1C), bridging multiple length and time scales as well as the corresponding data modalities and software tools. These workflows present an example for creating new visual narratives that bring complex processes in nature to broad audiences.

II. SUMMARY OF BIOENERGETIC PROCESSES DEPICTED

Bioenergetic processes in photosynthesis involve integration of function across hundreds of proteins [3], [4], [6] and span length and time scales ranging from electronic excitation transfer (picoseconds) [5] to organelle-scale diffusion of charge carriers [7] and ATP synthesis [11], [12] (milliseconds) to adaptive response of protein composition to changing environmental conditions at the cell level (hours) [2], [13]. A combination of experimental and theoretical approaches (Fig. 1B) involving multiple data modalities (Fig. 2A,B) are employed to determine structure and function at atomic, supra-molecular, organelle, and cell levels of organization [2], [7].

The visualization here is based on the photosynthetic purple bacterium, *Rba. sphaeroides*, resembling evolutionarily primitive light harvesting organisms [14]. The photosynthetic apparatus in this bacterium is organized in the form of spherical membrane vesicles of 60 nm diameter, called chromatophores (Fig. 1A), comprising of several hundred proteins containing an array of nearly 3,000 chlorophylls for light capture [3]. The chromatophore structural models permit the computation of electronic interactions between chlorophyll molecules (Fig. 2C) using effective Hamiltonian formulations [5] and, subsequently, the rate kinetics of electronic excitation transfer, i.e., delivery of the captured solar energy to reaction center

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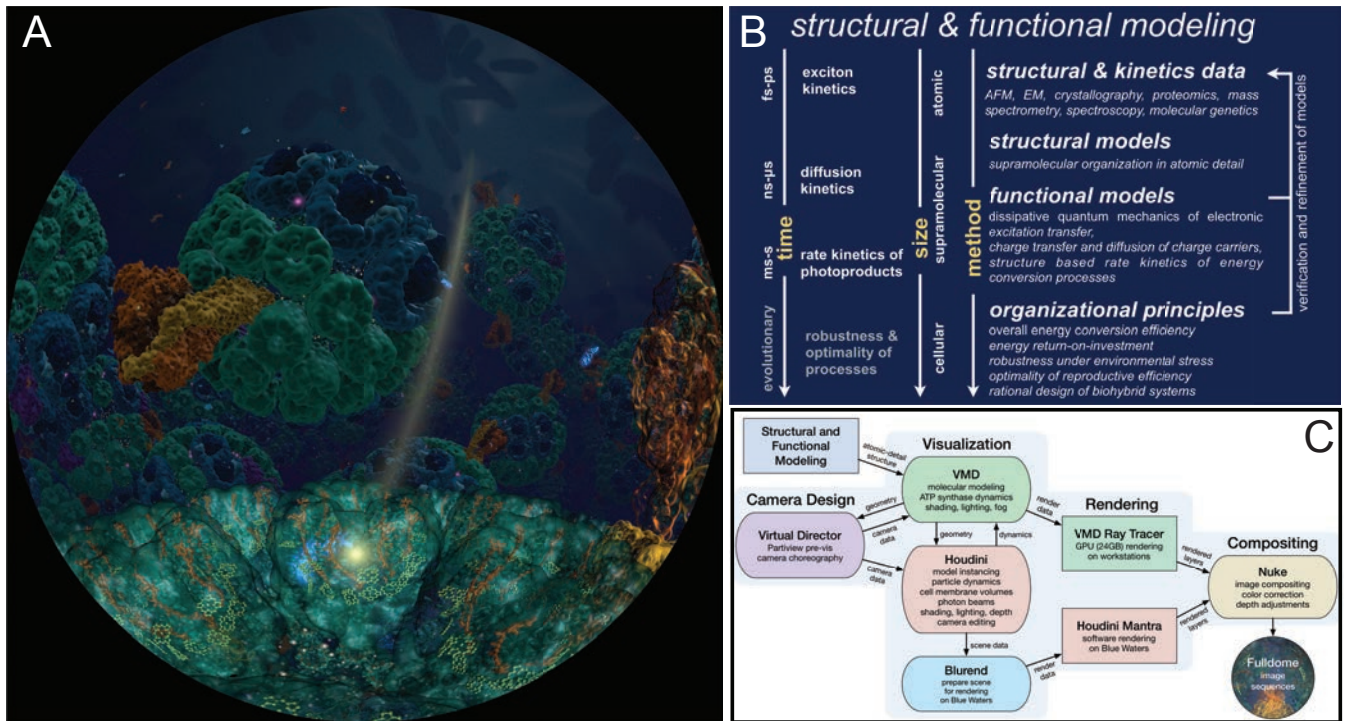


Fig. 1. High performance computing as an exploratory and explanatory tool for fundamental energy conversion processes powering life on Earth, from multi-scale rate kinetics models to accessible narratives for lay audiences. (A) Frame from the full-dome show *Birth of Planet Earth*, depicting the capture and transformation of solar energy by an array of proteins inside a biological cell. (B) Structural and functional modeling of photosynthetic energy conversion [2]–[4], [6], [7], combining experimental and computational approaches that correspond to time and size scales spanning electronic to cell levels. (C) From computational models to visual narratives [8], [9] using a chain of novel software solutions. Labelled arrows identify the flow and type of data exchanged between applications from scientific computation to full-dome visualization.

proteins that initiate charge transfer and diffusion steps [6]. (For a summary, see Refs. [2], [7].)

The interaction of the protein arrays across an entire chromatophore, integrated through multi-scale rate kinetics formulations [6], [7], determine the production rate of the final photoproduct, ATP, of energy conversion in a photosynthetic apparatus. ATP is the universal energy currency of all life on Earth [12]. The ATP production rate as a function of incident light intensity (Fig. 2D) provides a quantitative measure of efficiency for the chromatophore as an energy conversion device. A related performance metric, energy return-on-investment, permits a comparison with human made devices of similar purpose, where the chromatophore outperforms photovoltaic or fossil fuel based systems [2]. Combining the collective light-response of all chromatophores in an entire bacterium permits the computation of reproductive efficiency at cell level, related to the cell doubling time as a function of growth condition [2] (Fig. 2E).

This electronic-to-cell scale organization of energy conversion steps provides a natural event sequence for a storyboard (Fig. 2F), forming the basis for accessible narratives.

III. CONSTRUCTING ACCESSIBLE NARRATIVES

Communicating a complex biophysical process to a lay audience requires elements beyond those needed in an exploratory visualization aimed at a scientific audience [17]. A balance between accuracy and comprehensibility was sought

by the team in conceptualizing, researching, designing, choreographing, writing narration scripts, and testing audiences, iteratively for this explanatory visualization. The primary goals were to tell the story of how life is powered by sunlight in a way that was informative, but not burdensome; educational, but not didactic; scientifically and visually complex, but intuitively simple. All technical work described in Sec. IV below is rooted in these goals.

A. Accessibility of the narrative

Dome shows can reach millions of viewers between the target ages of 8 and 80, have a lifespan of over a decade, are translated into a dozen foreign languages, and are distributed worldwide. Creating a long-lasting visualization accessible to diverse audiences requires an understanding of human perception, education, psychology, and visual communication practices. An inspiring and engaging visualization additionally requires storytelling, cinematography, and production.

The first step in planning an accessible narrative is the storyboard (Fig. 2F). The storyboard is the basis for scene design and camera treatment to ensure accessibility for the target audience as they are exposed to multiple size and time scales in a complex process. A script for narration was co-developed alongside the storyboard with writer Thomas Lucas along with the biophysics and visualization teams, including the late Klaus Schulten. The final script was recorded by a professional actor, Richard Dormer, to ensure that the narration is performed with empathetic, emotional delivery that

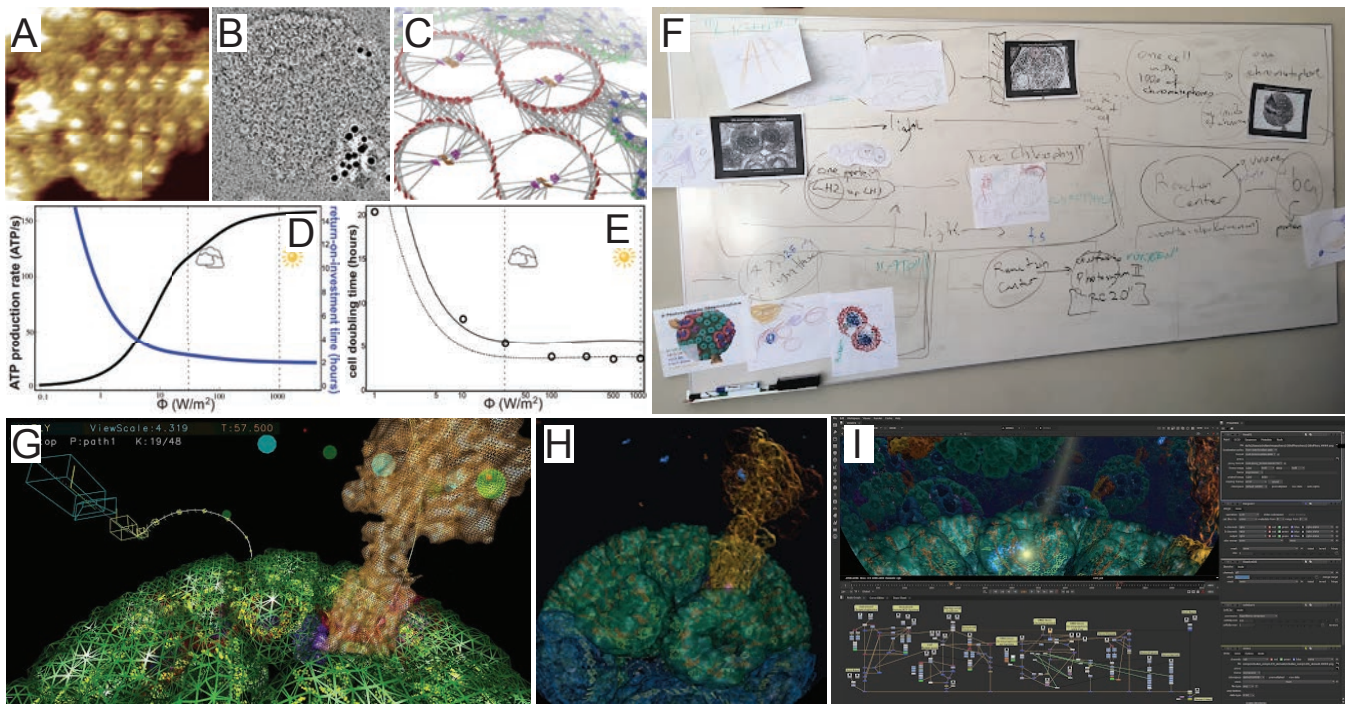


Fig. 2. Workflow from raw data to full-dome visualization represents over a decade of collaborative work. Structural information such as from atomic force microscopy (A) and negative stain electron microscopy (B) is used for the construction atomic detail structural models that form the basis of quantum mechanical computations for electronic couplings between chlorophylls (C) [3], [6]. Multi-scale modeling of energy conversion processes [7] culminates in the determination of system-level device performance metrics for the chromatophore (D), such as ATP production rate and return-on-investment time for energy as a function of incident light. Integrated at cell scale, reproductive efficiency is determined, expressed as doubling time (E) [2]. (F) This electronic-to-cell scale description of energy conversion steps translates to a storyboard, which is the basis of an accessible narrative for lay audiences. The storyboard is converted to an interactive pre-visualization in Virtual Director, shown with a camera path in (G), and a corresponding ray traced full-dome rendering in VMD [9], [15], [16] (H). Final images are composited using Foundry Nuke software (I), with nodes and connections representing the various Houdini and VMD image sequences being read in, processed, and merged to construct the final image sequence for the visualization, as shown for the frame in (Fig. 1A).

connects with the audience. Advance screenings for audience testing were held for the in-progress documentary where psychology researchers evaluated whether the visual narrative was enjoyable, met learning goals, and raised awareness of computational science. The show was revised accordingly.

B. Inclusion within a larger story

The present visualization must fit within a larger story as it is the culminating scene in how Earth came to be the cradle of life—starting with the remnants of a supernova, accretion of a molecular cloud that lends materials to the formation of the Solar System, the creation of our Earth-Moon system, and, at last, how early life was powered by photosynthesis.

The immediately preceding scene shows a pool of bubbling water surrounded by rocky, prehistoric-looking terrain created from reference photography in Iceland. Visual cues are made to flow smoothly between these two scenes as the camera smoothly zooms from the macroscopic to the atomic scale. To cross this scale gap between that of a pool and a solitary chromatophore, a larger contextual environment is constructed, consisting of (i) a bacterial cell model containing hundreds of chromatophores and (ii) a colony of hundreds of such bacteria, providing a background for the individual ‘hero’ chromatophore upon whom the action later focuses.

C. The Writer’s dilemma and the visual dilemma

The compromise between accuracy and comprehensibility brought a number of difficult design challenges. First, relevant size scales are smaller than the wavelength of visible light; therefore, intuitive meanings of color and opacity become in-applicable. Second, scene complexity of a cellular environment is overwhelming, especially for a child who gets only a brief exposure to it. Third, the processes depicted span a vast variety of time scales (femtoseconds to milliseconds, as discussed in Sec. II). A simple linear scaling of time would have implied that some processes appear at standstill, while others become blurs. Fourth, the primary processes involved in the interaction of light with biological matter are quantum mechanical, which human perception has not evolved to process. Any accurate depiction of probability dynamics, as would be customary for a scientific presentation involving quantum processes, would be incomprehensible to a lay audience.

Creating an accessible narrative for an 8 year old in the face of these challenges, requires careful simplification of the story, while still retaining the underlying structural model as a basis for the visualization. For example, picosecond scale excitation transfer steps are depicted alongside millisecond scale charge diffusion steps. However, a qualitative ordering of event speeds is employed so that fast events do appear faster to the viewer, though not commensurately with their actual time scales. The chromatophore and its host cell are depicted in terms of protein

scaffolds only, where lipids are abstracted as transparent membranes. Charge carrier molecules (quinol/quinone) are visualized as glowing point particles instead of molecular models, and their dynamics is abstracted as a semi-directed flow instead of stochastic diffusion [7]. The protein responsible for ATP synthesis (ATP synthase) is animated as a ‘turnstile’ undergoing a directed, cohesive motion, instead of a complex stochastic machine [12]. Components of the ATP synthase and its interaction partners (protons, ADP/ATP) were synchronized to guide the perception of the viewer to the culmination of the story in the form of ATP release, powering life, at last.

D. Choreography of elements in the fulldome environment

The motion of photons, protons, quinones/quinols, and ATP/ADP molecules were meticulously choreographed so that the viewer could follow the path of energy directly through a chain of conversion steps, creating a narrative visual thread through the chromatophore. Many of the moving elements in this visualization were designed to appear random but are guided by the viewpoint of the camera.

A ‘hero’ quinol and a ‘hero’ proton were separately choreographed and given a brighter starburst appearance to guide the viewer’s eye, without being too visibly different from the surrounding elements. The ‘hero’ chromatophore was shown with transparent surfaces, allowing the viewer to see the internal structures. In a fulldome environment, the viewer is free and encouraged to look around at the action happening all around them, but their vision must be guided to a central location to where the story is evolving, including focusing one-by-one on successive steps of a multi-step process. This is done through the design of the scene as well as the motion of the camera.

IV. VISUALIZATION AND RENDERING USING HPC

The basis of the visualization presented here is the structural model of the chromatophore (Fig. 1A) [3]–[7] as well as corresponding atom selections, molecular representations, and animation scripts developed for exploratory visualizations [8], [9]. The molecular visualization software VMD [15] is unparalleled at generating visual abstractions of large biomolecular complexes and was the tool used to build the chromatophore structural models [7]. No single visualization tool provided the required range of rendering capabilities and visual effects, so several were integrated to create an effective production pipeline (Fig. 1C), starting with computational models and ending with the fulldome visualization (Fig. 1A).

A. Visualization Tools (Virtual Director, Houdini, VMD, Nuke)

VMD incorporates a built-in GPU-accelerated ray tracing engine that excels at rendering biomolecular scenes with semi-transparent surfaces [18], [19]. To meet the needs of the project, VMD was extended with special material shaders for visual effects, and direct ray tracing of full-dome images [9], [16]. VMD scripting enabled Virtual Director to assume camera control, and allowed effective interchange of scene geometry and motion effects with Houdini. VMD was the

tool of choice for portraying the ‘hero’ chromatophore as seen close up, as it efficiently renders highly-detailed biomolecular data. But not all rendering could be handled by VMD, which lacked some visual effects needed for the larger bacterial cluster environment. It was used to generate the geometric data used in other software.

The visual-effects package Houdini was a capable authoring system for constructing the larger environment—a pond, incoming photons of sunlight, and a cluster of bacteria—and for rendering the resulting computationally demanding scenes. Houdini also served as an authoring platform for choreography of dynamic elements such as electronic excitations, protons, ATP molecules and so on.

B. Previsualization and camera choreography

Virtual Director [20] software provided fluid cinematic camera path design (Fig. 2G) in a pre-visualized version of the scene. It is our preferred tool for camera design, supporting recording and editing of tours performed with an intuitive six-degree-of-freedom input device.

The pre-visualization of the scene included a simplified static chromatophore model that was exported from VMD into meshes which Virtual Director could display at interactive rates. Choreographed phosphate/ADP/ATP elements from Houdini were incorporated as animated glyphs, providing an interactive representation of the scene for camera design. Further, using VMD scripting, a live connection was made from a running Virtual Director instance to a running VMD session. Interactive camera motion in Virtual Director promptly updated the fully-detailed VMD view (Fig. 2H).

The motion of the camera in an immersive fulldome theater can create a visceral impact on viewers, which can be used to create engagement and excitement, but risks motion sickness if not employed well. The camera’s path is key to constructing the visualization narrative, guiding the viewer’s attention throughout the scene from macroscopic to atomic scale. The camera treatment here was performed in two sections with different spatial scales: the flight through the bacterial cell colony and the flight through the ‘hero’ chromatophore. The two performances were merged and blended to create a seamless, immersive journey that allows the viewers to maintain a sense of scale. The measured pacing and smooth motion of the camera enable the viewer to focus on the unfolding story.

For the camera performance, we approach and fly over the chromatophore, looking down on it as if it were a planet landscape, capturing a photon beam like lightning. We follow the excitation to the reaction center and then descend, bringing the audience inside the chromatophore to follow the ‘hero’ proton toward the towering ATP synthase. The audience rises up to see the complex, transforming machinery of the ATP production process and then finally the camera pulls away to have a grand view of the of the chromatophore environment.

C. Model construction in Houdini

Electronic excitations were choreographed in Houdini using a random walk representing transfers between neighboring

light harvesting proteins in resemblance of excitation transfer kinetics [3]. This random walk ends with arrival at a ‘hero’ light harvesting protein (LH1), followed by a jump inward to the so-called ‘special pair’ of chlorophyll molecules at the reaction center.

The proton-transporting quinol molecules traverse between membrane proteins in apparent stochasticity, with docking positions determined from the chromatophore structure [6]. Protons were choreographed as five separate populations, with synchronized arrival/departure times at constituent proteins, and discarded when not visible on screen.

Houdini was further used to build the wider environment: a pond, incoming photons of sunlight, and a cluster of bacteria. Each bacterium comprised a volumetrically-rendered membrane and many copies of the chromatophore model. Chromatophores were packed into each membrane in a perturbed hexagonal grid, to approximate the packing of organelles seen in electron microscopy images. The ‘hero’ chromatophore was placed near the outer edge of a bacterium, such that the camera move approach could see the featured chromatophore clearly. This placement facilitated a dissolve from a Houdini rendered chromatophore to the VMD ‘hero’ render, and also enabled unobstructed lighting of the ‘hero’, since internal chromatophores were dimmed by ambient occlusion shading.

D. Exporting geometry for Houdini and reading into VMD

Dynamic elements designed using Houdini were exported as tables of particles for each animation frame, describing their configuration—position, orientation, brightness, unique id, ‘hero’ status. A VMD driver script created and destroyed corresponding VMD scene geometry elements as needed for each frame.

Electronic excitations within the chromatophore were embedded as transparent surfaces rendered by VMD. VMD was adapted so that the visualization team could add a *glow* shader to VMD’s shader library. The blue-glow excitation animations, as well as embedded proton and quinol elements, use this new feature.

E. Simulation/animation cross-over

Depicting ATP synthase function combined molecular dynamics simulation data [11] for the ‘mushroom’ (F_1) part, a pulsed, stepwise rotation of the ‘turnstile ring’ (F_0) part, choreography of diffusing molecules, and matching timing to give the appearance of a cohesive biological machine, as mentioned in Sec. III. No molecular dynamics simulation was available of the entire ATP synthase system, but one did exist of a related F_1 unit as it performed a complete catalytic cycle [11], so it was adapted in relationship to the F_0 unit. A synchronization was enforced between motions of the ‘turnstile’ and ‘mushroom’ to ensure a geometric match between components.

F. Rendering Layers in Blue Waters

The visualization was rendered in 14 separate layers from both VMD and Houdini as hemispherical fulldome images

in 4096×4096 resolution. A VMD batch rendering pipeline imported the Houdini-generated particle effects and followed the Virtual Director camera path, rendering the structural model as a high-quality foreground element. Five versions of the VMD scene were rendered, with various combinations of moving elements, allowing those elements’ brightnesses to be adjusted in the Nuke compositing step. Nine more layers were rendered in Houdini’s Mantra, including instanced chromatophores, particle effects, photons, and cell membranes, along with depth passes to control relative luminance levels and depth effects. Houdini scene rendering was done on the Blue Waters supercomputer with a custom dome lens shader for fulldome imagery, permitting an extended geometric complexity that could be represented in a scene—i.e., 300 1.3GB volumetric bacterial domains containing more than 500,000 900MB chromatophore surface geometries. Rendering these layers was computationally intensive—the final run taking 27,763 node-hours, with many more used in preceding iterations.

A new process was developed for rendering on Blue Waters. The Houdini standard method of doing such large-scale rendering created over 100TB of intermediate data, which was not feasible to work with. This amount was reduced to 0.5TB by selectively creating minimal packed disk primitives from the geometry and linking these to the scene description files rather than including the data directly.

G. Compositing

Rendering of layers provided flexibility in the image composite to control luminance levels of the various elements and the magnitude of depth effects across the scene. It also provided efficiency in rendering by reducing the number of iterations for some layers as well as segmenting the computational demands of rendering. The ray tracing engine in VMD was augmented to generate alpha buffers for compositing. The 14 render layers from Houdini and VMD were composited with Nuke, where the scene was made to appear integrated and under water (Fig. 2I).

V. DISCUSSION AND BROADER IMPACT

Fulldome shows typically reach millions of viewers over lifespans exceeding a decade. The visualization presented here as part of a fulldome show provides a workflow that can be employed for creating other accessible narratives that bring complex natural processes to broad audiences. A visualization that successfully engages its target audience requires: (i) choice of a problem of immediate and intuitive relevance to many—e.g., sunlight powering life on Earth—with abundant visualization-ready data on key processes; (ii) close collaboration between computational/experimental and visualization scientists, neither of whom could produce such content alone; (iii) consultation with psychology researchers, writers, and actors, as well as audience tests, since the challenges of human perception are of equal importance as technical challenges. Accessible presentations of science need to obey the rigors of a performance art in addition to the rigors of research.

But why should a scientist undertake such an ordeal, when one could instead contend with presenting to other experts only? Arguably, scientists have a responsibility exceeding that of others for performing *science outreach*. Today, data visualization has become akin to empowering people to read [1]; numerical literacy has become the new literacy upon which democratic institutions depend; and the ability to visualize information has become a basis for empathy in a society where misinformation is rampant.

Specifically, the subject of solar energy harvesting is associated directly with the prosperity of human civilization: The total energy demand of humanity (~ 15 TW) is a tiny fraction of the solar energy incident on Earth ($\sim 120,000$ TW), representing an abundant clean energy solution in the long term [10]. Energy efficiency is shown to correlate with economic, environmental, and social benefits to a society [21], whereas biological systems provide examples of high energy efficiency surpassing comparable human technologies when considered at systems-level [2]. Yet, public support for the development of such clean energy solutions remains elusive. It is the responsibility of scientists to make a case of our relevance to the public interest.

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