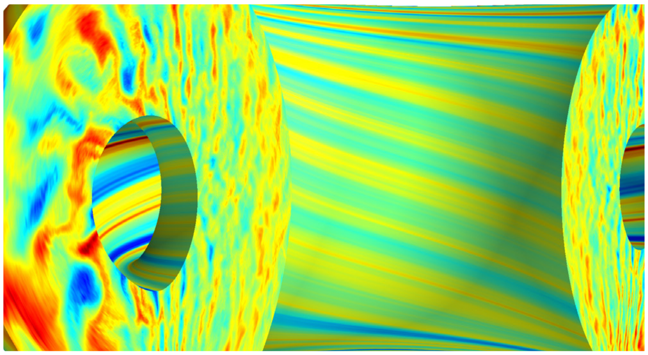
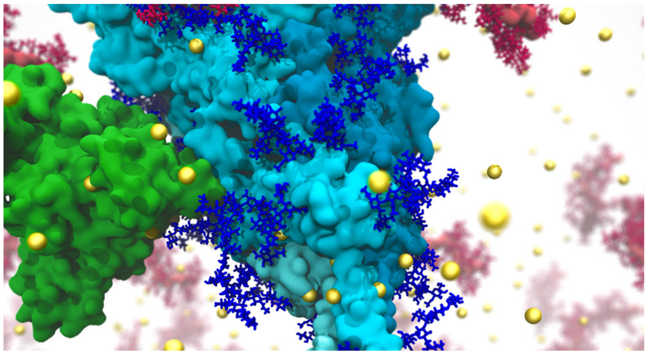
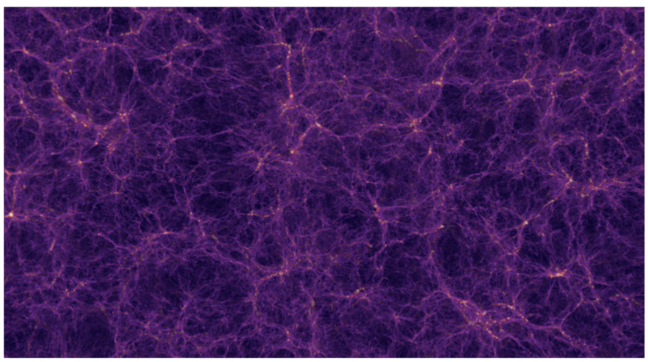
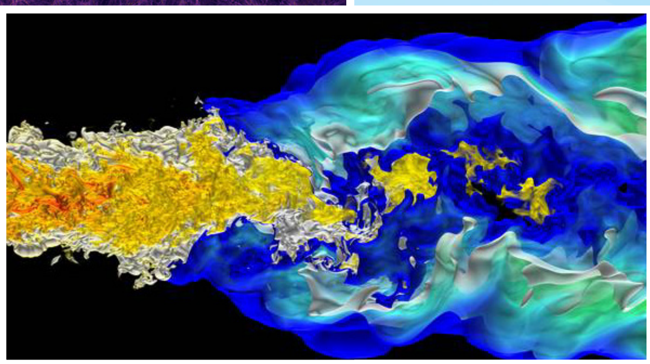
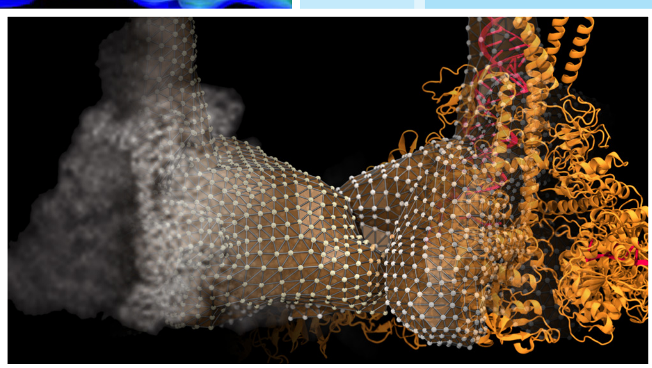






Basic Research Needs for Visualization for Scientific Discovery, Decision-Making, and Communication





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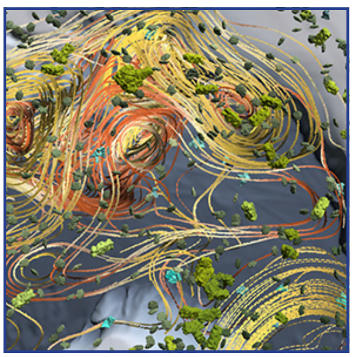
Visualization–the use of visual elements to explore data, form hypotheses, or convey conclusions–is an integral part of the scientific process. Starting from an initial exploration of new data to illustrating outcomes to the general public, visualization is one of the most intuitive and powerful modes of communication. With the explosion of new data sources and types, unprecedented volumes of data, and new technologies, such as virtual reality and AI, visualization has become increasingly essential but also ever more challenging.

Department of Energy's (DOE) Office of Advanced Scientific Computing Research (ASCR) sponsored a Basic Research Needs workshop in January 2022 to understand the major opportunities and grand challenges in visualization tools and technologies for scientific computing, with a special focus on DOE-relevant applications and goals. The workshop identified five priority research directions (PRDs) for visualization to support scientific discovery, decision-making, and communication.

1) Advancing Theory and Techniques for Visualization to Support the Analysis and Understanding of Complex Scientific Data

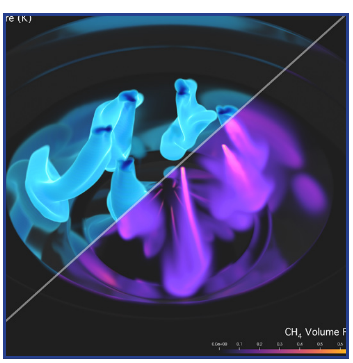
Key Question: *What are the most informative, reliable, and intuitive visualizations of complex data?*



New techniques and corresponding theory are needed to develop novel representations, algorithms, and systems to promote scientific understanding of the many different data types of interest to DOE. Many of the common scientific visualization techniques focus on 2D or 3D scalar fields. However, most of the data collected today has much more complex encoding, either because at each location multiple values (multivariate) or even multiple data types (multimodal) may exist, or because data is defined non-spatially, i.e., in high dimensions, in graphs, etc. Furthermore, abstract information about the behavior of a complex system or about the inherent uncertainty of a decision could be more accessible through intuitive visualizations.

2) Introducing Interoperable and Adaptable Visualization to Support Diverse Scientific Workflows Across All Scales

Key Question: *How do we design, develop, and deploy portable visualization tools to support different use cases across different resources and diverse audiences?*



New visualization approaches are required to leverage as much common infrastructure as possible, maintain data provenance and uncertainty information, and span the needs of multiple scientific communities while taking advantage of the unique resources and opportunities of the specific application. The need for informative visualizations is near universal, covering a plethora of scientific domains and systems ranging from embedded sensors to high-performance computing resources, rare and expensive data, and petabyte-sized collections. Developing bespoke solutions for every unique combination is infeasible.

3) Harnessing Technology Innovations to Accelerate Science through Visualization

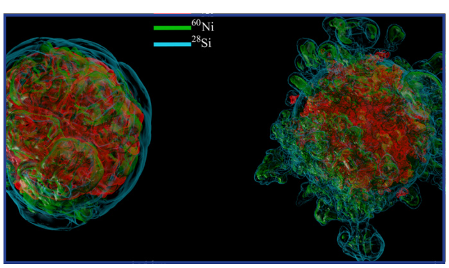
Key Question: *How can visualization best utilize new technology and most effectively exploit future computational hardware?*

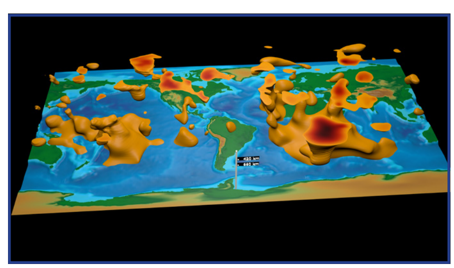
New techniques are needed to take advantage of novel displays, interfaces, and collaboration tools while exploiting state-of-the-art computing architectures. Rapidly evolving technology is creating tremendous opportunities for new visualization and collaboration paradigms with novel displays, virtual reality, haptic interfaces, and more. However, realizing this potential to develop immersive yet intuitive environments or enable real-time, remote collaborations will require techniques and frameworks significantly beyond the current state of the art. Furthermore, visualization must effectively exploit diverse and disruptive computing modalities, including exascale platforms, cloud, sensors, and mobile chips, each of which may enable unprecedented visualization solutions if they can be integrated effectively into portable tools.

4) Improving Equity in Accessing and Engaging with Scientific Data and Processes

Key Question: *How can visualization help communicate scientific data and processes while promoting equitable access to the vast amounts of information created, curated, and analyzed by DOE scientists?*

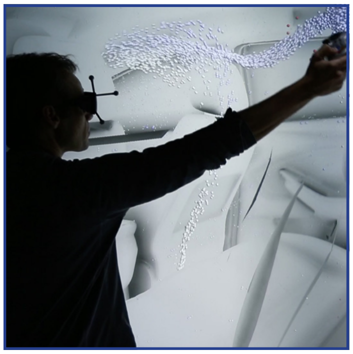
New approaches to visual communication are needed to significantly accelerate team science, integrate all stakeholders–from policy makers to the general public– and change the scientific discourse. Visualization is one of the most powerful ways to communicate complex ideas, concepts, and decisions across domains, educational backgrounds, or cultures. Distinct from the goal of providing new insights to subject matter experts, visual communication requires a new focus on accessibility, transparency, and trustworthiness to promote engagement and understanding.





5) Developing Intelligent Approaches for Adaptive, Context-Aware Visualization of Scientific Data and AI

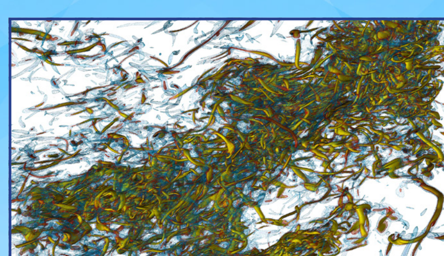
Key Question: *What novel approaches leveraging perceptual and cognitive principles can be developed to enable intelligent design and evaluation of next-generation visualization tools?*

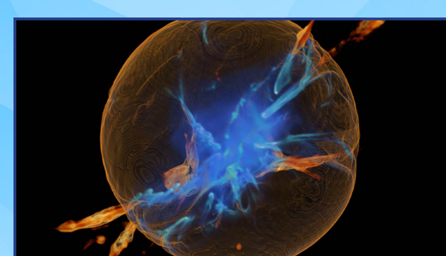


Visualizations are designed to be consumed by humans. Understanding how individuals may interpret visual content differently depending on the application context and intended use is a key challenge for designing new tools and techniques. Recent advances in our understanding of perceptual learning and reasoning processes are crucial in developing general-purpose, intelligent visualization tools that are readily customizable to meet the evolving needs of the users (e.g., scientists, general public) and the task at hand (e.g., hypothesis generation, decision support, scientific information dissemination). Furthermore, as data and visualization become more embedded in scientific exploration and systemic decision-making processes, it is important that visualization tools are properly validated to ensure broad and lasting impact. There exists a growing need for human-centric design and evaluation methodologies, particularly those that properly account for minority viewpoints. Technical advances are needed across multiple fronts: (i) development of mathematical models of perception and cognition to drive the development and adaptation of next-generation visualization tools and serve as surrogates for large-scale visualization evaluation studies, (ii) methods to enable dynamic personalization of visualization tools to address the needs of individual users for scientific discovery and effective utilization, and (iii) development of robust, scalable, and unbiased evaluation methods and metrics for visualization tools.

Summary

Visualization is integral to scientific discovery but is also key to communicating results and supporting strategic planning. As such, visualization technology can have a significant impact across the DOE. To address future opportunities and challenges, a Basic Research Needs workshop has identified five PRDs. The first three PRDs describe interconnected research themes addressing the need for new techniques to deal with complex data, uncertainty, and interpretability (PRD 1); the need for scalable and interoperable software stacks (PRD 2); and the challenges and opportunities inherent in new technologies, such as, virtual reality, cloud, or exascale computing (PRD 3). The remaining two PRDs describe foundational research themes that recognize the potential of visualizations to provide equitable access to information and to strengthen the scientific discourse (PRD 4) and (PRD 5) and the need to consider human factors when designing visualizations (PRD 5). Collectively, these PRDs form the pillars for a coherent, long-term research and development strategy in Visualization for Scientific Discovery, Decision Making, and Communication in the context of the Office of Science's mission scope. These research opportunities are summarized in the following pages, with more details available at: https://doi.org/10.2172/1845709.





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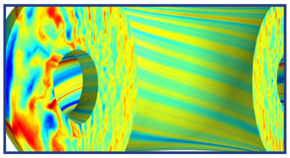
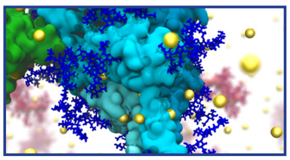
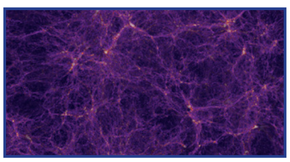


A visualization of deuterium-tritium density fluctuations in a tokamak driven by turbulence. Areas of red are representative of high density and areas of blue are representative of low density. Credit: Emily Belli, General Atomics

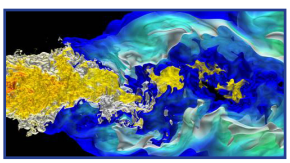
Children from the Sun Valley Youth Center, experience a 3D visualization as they take part in the Head to Heart program. Credit: Dennis Schroeder, National Renewable Energy Laboratory



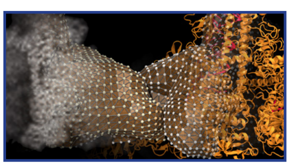
Visualization of the the SARS-CoV-2 virus' spike protein (cyan) surrounded by mucus molecules (red) and calcium ions (yellow). Image Credit: Created by Lorenzo Casalino, Amaro Lab, UC San Diego, for the #COVIDisAirborne Team including DOE Laboratories (Shantenu Jha, et. al.)



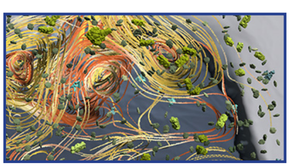
An image of the distribution of matter in the universe generated by a Mira simulation run modeling 1.1 trillion particles. Credit: Katrin Heitmann, et al., Argonne National Laboratory



Direct numerical simulation reveals turbulent combustion of direct-injection processes in internal-combustion engines and provides an essential component for development of high-efficiency, low-emissions vehicles. Credit: Jacqueline Chen, Sandia National Laboratories



To study the SARS-CoV-2 replication transcription complex, researchers built an integrated workflow that models the experimental Cryo-EM volumetric data as a finite element mesh. Credit: Defne Gorgun, Anda Trifan, Arvind Ramanathan, Argonne National Laboratory

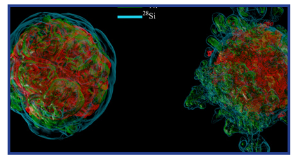


An Energy Exascale Earth System Model (E3SM) visualization of currents and nitrates in the Gulf of Mexico. Credit: Los Alamos National Laboratory

Predictive simulations of the complex incylinder processes of internal combustion engines that are being used to improve performance and decrease pollutant emissions.
Credit: Kenny Gruchalla,
National Renewable Energy Laboratory

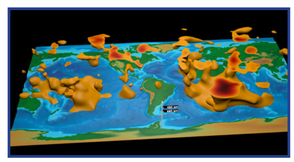
An image representing future technologies. Credit: Adobe Stock

An audience at the Adler Planetarium in Chicago being immersed in a visualization of the Kuiper Belt. Credit: AdlerPlanetarium.org



A 3D simulation developed using Summit reveal the early formations of nickel fingers or bullets, surrounded by a shell of silicon, that will be expelled from a star's core during a supernova. Credit: Michael Sandoval, et al., Oak Ridge National Laboratory

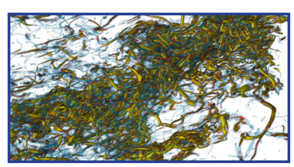
A visualization of laser ablation depicting nanoparticle generation. Credit: Benjamin Hernandez, Oak Ridge National Laboratory



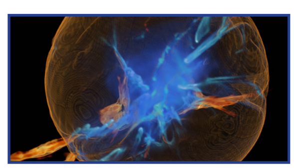
A visualization imaging the interior of the Earth with adjoint tomography. Credit: David Pugmire, Oak Ridge National Laboratory; Jeroen Tromp, Princeton University

An engineer interactively exploring complex airflow inside an electric vehicle cabin by directly seeding particles in the flow. Credit: John De La Rosa, National Renewable Energy Laboratory

An artist's representation of two protons colliding. Protons contain quarks and gluons. Computer calculations help scientists understand how quarks and gluons define protons and neutrons. Credit: Andy Sproles, Oak Ridge National Laboratory



An illustration of intricate flow structures in turbulence from a large simulation performed using 1,024 nodes on Summit. Credit: David Pugmire and Mike Matheson, Oak Ridge National Laboratory



3D volume renderings of temperature in the wake of the supernova shock wave reveal this seething, turbulent environment in unprecedented detail. Credit: Joseph Smidt, Brandon Wiggins, Francesca Samsel, Texas Advanced Computing Center