



SciDAC Institute for Ultrascale Visualization

Final Report

Institute for Ultrascale Visualization

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Abstract

The SciDAC Institute for Ultrascale Visualization brought together leading experts from visualization, high-performance computing, and science application areas to make advanced visualization solutions for SciDAC scientists and the broader community. Over the five-year project, the Institute introduced many new enabling visualization techniques, which have significantly enhanced scientists' ability to validate their simulations, interpret their data, and communicate with others about their work and findings. This Institute project involved a large number of junior and student researchers, who received the opportunities to work on some of the most challenging science applications and gain access to the most powerful high-performance computing facilities in the world. They were readily trained and prepared for facing the greater challenges presented by extreme-scale computing. The Institute's outreach efforts, through publications, workshops and tutorials, successfully disseminated the new knowledge and technologies to the SciDAC and the broader scientific communities. The scientific findings and experience of the Institute team helped plan the SciDAC3 program.

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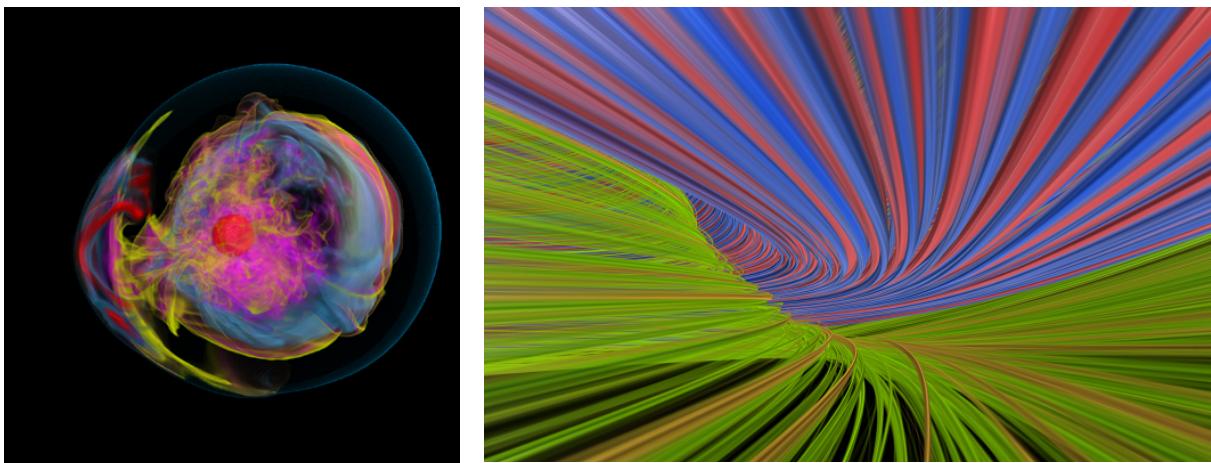
Executive Summary

Understanding the science behind extreme-scale simulations and high-throughput experiments requires extracting meaning from data sets of hundreds of terabytes or more. Visualization is the most plausible path to understanding data at this scale, but current visualization approaches were not designed with this scale in mind. This technology must be readily accessible by application scientists, portable to the wide variety of high performance computing (HPC) systems in use, and scalable to allow for timely generation of results. Fundamental advances in a variety of areas related to scientific visualization are necessary in order to effectively analyze data sets of this size.

The Institute for Ultrascale Visualization (UltraVis), a five-year research and outreach effort funded by the U.S. Department of Energy (DOE) SciDAC program, took the mission to advance and promote visualization technologies to enable knowledge discovery at peta- and exascale. The Institute involved investigators from both universities and DOE laboratories. The PIs targeted several major data analysis and visualization challenges facing SciDAC scientists, including architectures for parallel visualization, fundamental algorithms in areas such as vector field and in situ visualization, and novel techniques through which scientists might better explore the results of their labor. Through internal collaborations, the PIs in the Institute were able to tackle these complex challenges much more effectively than they could on their own, and through the Institute they were better able to interact with the SciDAC community.

Working together with other SciDAC Institutes, CETs, and application projects, the Institute made substantial research accomplishments. Likewise, through outreach activities the UltraVis Institute provided leadership in research community efforts focusing on extreme-scale visualization. These activities included hosting specialized workshops and panels at leading conferences to stimulate widespread participation.

This report mainly highlights the research accomplishments, collaborations, and outreach activities of the Institute from September 2006 to December 2011. Notably, several of the Institute projects led to visualization solutions and tools that enable SciDAC scientists to better validate their simulations, to uncover previously unseen patterns and relationships in their data, and to see their data in new inspiring ways. Institute members were able to identify critical gaps in current visualization technologies and tackle some of the most pressing issues. The Institute produced over 200 technical papers and played a major role in key activities in the fields of visualization and high-performance computing. These successes, both in research and in collaboration, set a sound foundation for SciDAC3 and the following development of extreme-scale scientific visualization technologies.



Visualization of data from a supernova simulation (Left) and a fusion simulation (Right)

Major Accomplishments

The accomplishments of the Institute for Ultrascale Visualization are best seen in three primary areas:

1. Research innovations and enabling technologies
2. Training new leaders and next generation visualization researchers
3. Outreach

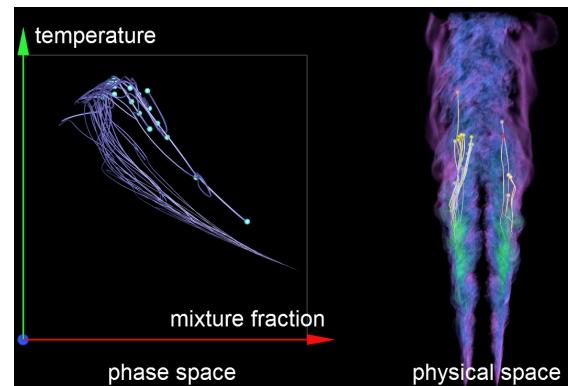
This report highlights the most important accomplishments.

1. Research Innovation and Enabling Technologies

In Situ Visualization. The most significant accomplishment of this Institute project, under the leadership of Professor Kwan-Liu Ma, is the development, demonstration, and promotion of in situ data visualization and analysis methods [38,41,52,58,59,70,94,173]. By the end of this Institute project, researchers in both the scientific simulation and visualization communities were convinced that the in situ approach is the most promising solution for extreme-scale scientific data visualization, analysis, and discovery. Consequently, in the following SciDAC3 program, the development and deployment of in situ data reduction, visualization, and analysis technologies become the primary effort in order to timely address the upcoming exascale challenges.

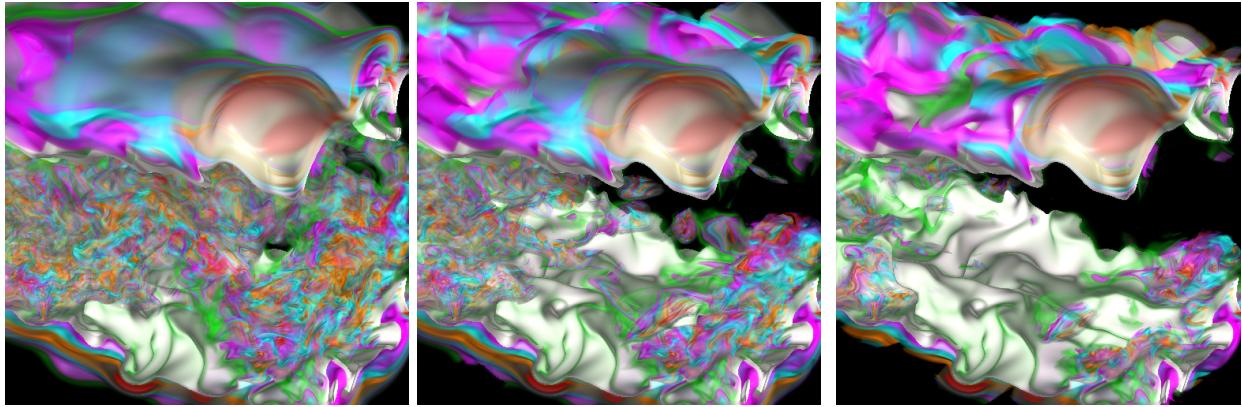
New visualization technologies and Enabling Visualization. As a result of close collaborations between application scientists and visualization researchers, many new concepts and techniques were introduced and evaluated over the course of this project. While these research efforts led to a large number of publications, more importantly some of the research results either spurred new research areas or were converted into usable software tools. For example, in situ visualization is one that has drawn new attention leading to a dozen new publications produced by researchers outside the Institute team. The Visualization by Proxy (aka. Exploration Image) design is a particularly promising one, which makes in situ visualization much more appealing to simulation scientists.

The Institute team has also introduced many new visualization techniques for studying time-varying 3D flow data including scalar fields, vector fields, and particles. Several of these techniques have been incorporated into open-source or commercial visualization toolkits such as Paraview, VisIt, and FieldView, which have been routinely used by many simulation scientists. They allow the scientists to see their data in new ways and with greater clarity, facilitating correct interpretation and effective communication. Consequently, these new visualization capabilities enable scientists to more easily and thoroughly validate their simulation, more effectively communicate their work and findings with others, and possibly discover previous unknowns. The first example is a dual space visualization technique allowing scientists to study joint particle/field data in both phase space and physical space of the data. The visual correspondences established help scientists to better understand the complex, dynamic behaviors of the model turbulent flow. The image on the right shows such dual-space visualization.

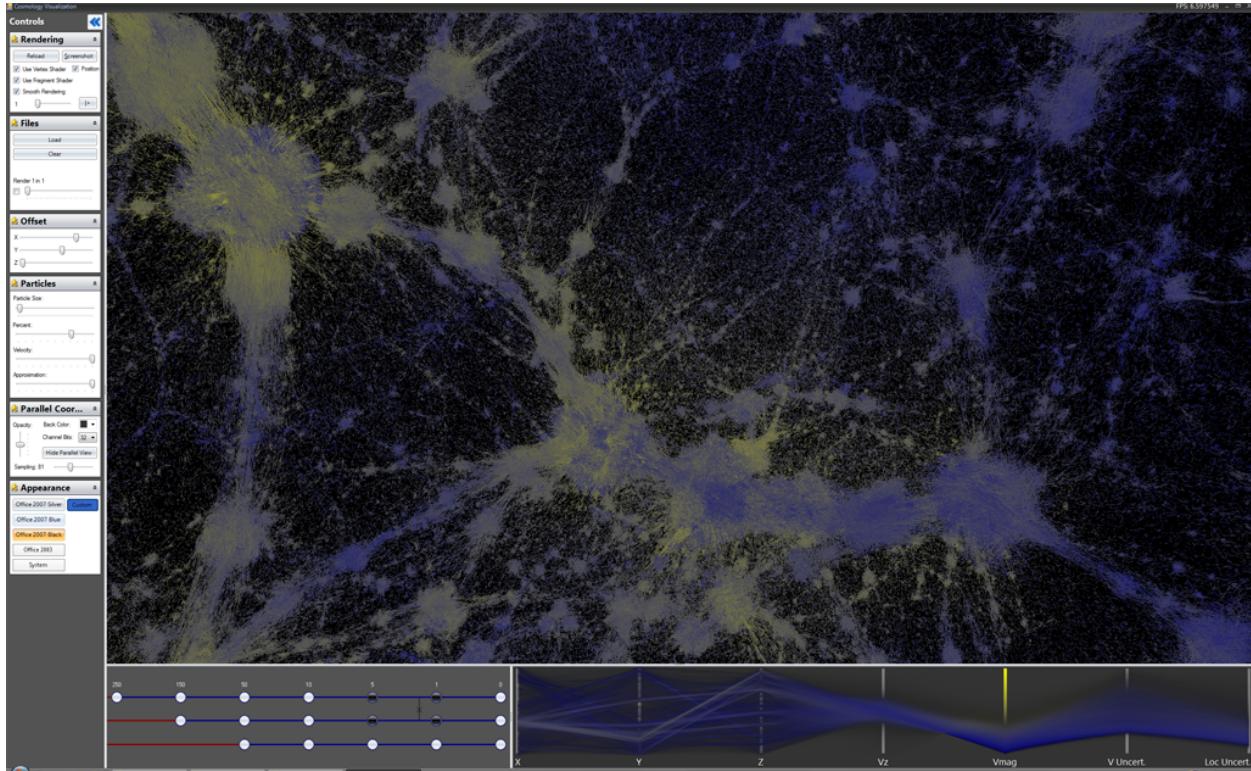


The second example is a visualization technique based on distance field applied to petascale combustion simulations. It can not only substantially reduce the data but also allow the scientists to zoom in and see for the first time the interaction of small turbulent eddies with

the preheat layer of a turbulent flame, a region that was previously obscured by the multi-scale nature of turbulence. The images below, from left to right, reveal the turbulent eddies according to their distance to the flame surface of interest.



The third example is the comparative visualization method and interface designed for cosmological simulation scientists, who have the need to visualize hundred millions of simulated cosmological particles and show how each varied across time and simulation run. The resulting visualization system allows the scientists compare a pair of simulations progressing over time. The image below shows the interface of this interactive, comparative visualization system. The approximated datasets present a more interesting challenge, as scientists wanted to examine how the differences developed over time. Most cosmologists assumed that they coalesce. However, our collaborators found that each particle's position and velocity varies more as time progresses. In other words the simulations diverge.



2. Training New Leaders & Next Generation Visualization Researchers

This Institute project provided all participants access to unique scientific applications and state-of-the-art high-performance computing facilities, and thus tremendous research opportunities. Each year, besides postdoctoral researchers, more than twenty student researchers were engaged in various projects. These students got the chance to work on the most challenging problems identified by the PI and collaborating scientists. Some of these students had access to the most powerful supercomputers in the world for their projects, and also obtained valuable internships at DOE national laboratories to work directly with the application scientists.

Through training many students and postdoctoral researchers, this project produced new leaders in the field of large-scale data visualization and analysis. Four of them are notably mentioned here:

- Tom Peterka is presently an assistant computer scientist at the Argonne National Laboratory (ANL), Fellow of the University of Chicago Computation Institute, and adjunct assistant professor at the University of Illinois at Chicago. His effort with the Institute has led to software products including the Radix-k compositing library, DIY, and Tess. He is currently a project lead at ANL, a participant of SciDAC3 SDAV project, and collaborating widely with application scientists and university researchers.
- Chaoli Wang (<http://www3.nd.edu/~cwang11>) is an associate professor of computer science and engineering at the Notre Dame University. He was extremely productive as a postdoctoral researcher at UC Davis, and became an assistant professor at Michigan Technological University in 2009. He joined Notre Dame University in 2014 and received the NSF CAREER award in the same year.
- Jon Woodring is presently a research scientist at the Los Alamos National Laboratory (LANL). He had several summer internships at LANL, received his PhD in 2009, and immediately joined LANL, where he is currently a project lead and also participating in the CESAR Co-Design project.
- Hongfeng Yu (<http://vis.unl.edu/~yu/>) is an assistant professor of computer science and engineering at the University of Nebraska-Lincoln (UNL). He got his PhD from UC Davis in 2008, and then worked as a postdoctoral researcher with the combustion simulation group at the Sandia National Laboratories before joining UNL. He is presently participating in the ExaCT Co-Design project.

Several PIs of this project were in the early stages of their career. The unique resources made available through this project helped them build their profession career. They were able to establish strong connections to several large-scale scientific investigations, leading to long-term collaborative relationships. Some have become leaders in several of the following projects sponsored by DOE, including the SciDAC3 projects and ASCR basic research projects. Professors Jian Huang, John Owens, and Han-Wei Shen have all been promoted to full professors. Dr. Kenneth Moreland is presently participating in the SciDAC3 SDAV project, and also the lead PI for the XVis project, which consolidates three previous massively parallel visualization projects of DOE. Dr. Robert Ross is also participating in SciDAC3 SDAV project, and as the project lead for several other projects at the Argonne National Laboratory.

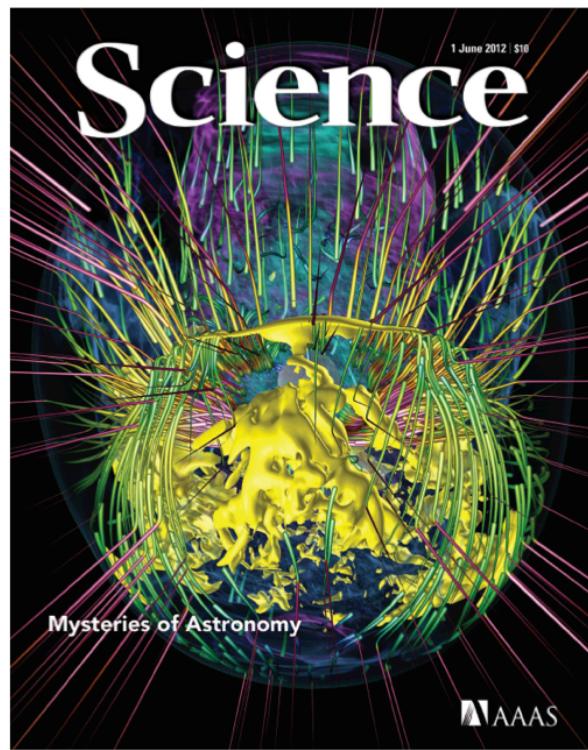
Senior people on this project continue their impact and contributions, and received significant recognitions from the respective communities. The lead PI, Professor Kwan-Liu Ma, presently participating in the SciDAC3 SDAV project and ASCR XVis project, was elected IEEE Fellow in 2012 and received the IEEE Visualization Technical Achievement award, the highest honor from his research community with the Technical Achievement Award, in 2013. Professor Nelson Max received the most prestigious recognition, the Steven A. Cons Award, from the ACM SIGGRAPH in 2007, and was elected ACM Fellow in 2011. Professor Deborah Silver has since continued her collaborations with DOE scientists. Professor Giulia Gallis is currently chair of the Extreme Physics and Chemistry of Carbon Directorate of the Deep Carbon Observatory.

3. Outreach

The outreach efforts by the Institute were very well received by the community. The most visible Institute outreach activities were the large number of workshops and tutorials organized by the Institute PIs. These activities brought a very efficient way to communicate with a large number of interested parties about new visualization technologies, applications, and requirements. For example, the Ultrascale Visualization Workshop has been held with the annual ACM/IEEE Supercomputing Conference for nine consecutive years (2006-2014). These workshops provided perfect venues for dialogue between visual analysis experts and computational scientists. In addition, over twenty tutorials on topics from large-scale data visualization and analysis, high-performance graphics/visualization, and data management were organized and taught by the Institute PIs at the annual Supercomputing Conferences, the annual SIAM Conferences on Parallel Processing for Scientific Computing, the IEEE Visualization Conferences, and the ACM SIGGRAPH Conferences.



Through goal-oriented collaborations, the institute PIs were able to target the most challenging and representative visualization applications in the Department of Energy, and the research results and findings have benefited the SciDAC community at large and beyond. The impact of the research results has been significant with the large number of conference presentations and journal publications, which helped direct the research community to those most essential and promising areas. Furthermore, the software tools and libraries made available by the Institute have helped accelerate the adoption and creation of new visualization technologies. The image on the right is the cover of the June 2012 issue of *Science*, which exhibits astonishing visualization of supernova simulation created by the Institute. Demonstrations of advanced visualization for some of the most challenging science applications as such have made scientists rethink about their overall research process and scientific discovery at extreme scale. As we can see, now visualization researchers are closely engaged in several of the major science teams. The value of visualization is highly recognized.



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