Accelerating Accelerator Science

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Summary

Scientists from the SciDAC Visualization and Analytics Center for Enabling Technology (VACET) have developed new capabilities that "accelerate accelerator science" by enabling rapid scientific knowledge discovery. These new techniques leverage DOE's parallel computing platforms to: (1) reduce from hours to seconds the time required to select particles undergoing acceleration in simulation results and to track them over time; (2) automatically locate particles undergoing acceleration and to analyze them across time and space through the use of advanced machine learning techniques. These new capabilities represent a major step forward for DOE's Accelerator research programs.

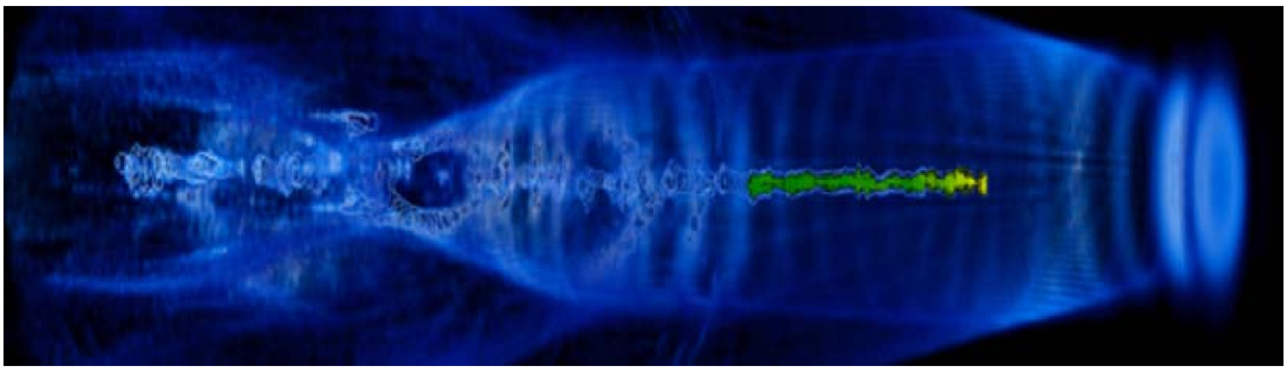

Figure 1. Petascale-class machines help accelerator scientists to model and plan experiments with better fidelity and physical accuracy then ever before possible. Output from one such simulation is shown here with the wake (blue) and beam electrons (green-yellow by energy), which show a high degree of acceleration and spatial coherency. Image, generated from VORPAL simulation results, courtesy C. Geddes, LBNL.

In laser wakefield accelerators, particles are accelerated to relativistic speeds upon being "trapped" by the electric fields of plasma density waves generated by the radiation pressure of an intense laser pulse fired into a plasma. These devices are of scientific interest because they are able to achieve very high particle energies within a relatively short amount of distance when compared to traditional electromagnetic accelerators. Advanced accelerator designs, including laser wakefield accelerators, are a component of the portfolio in the SciDAC Science Application *Community Petascale Project for Accelerator Science and Simulation (ComPASS)*.

Researchers use computer simulation to model experiments and test designs for future experimental devices. Petascale class machines enable simulation runs at unprecedented levels of spatial resolution and physical accuracy. One challenge facing this research is the sheer volume and complexity of data being produced by simulations.

The SciDAC *Visualization and Analytics Center for Enabling Technology (VACET)* has developed new technologies to accelerate discovery from LWFA simulations by working with ComPASS accelerator scientists at the L'OASIS program of LBNL (which conducts LWFA experiments, led by Wim Leemans) at at Tech-X (which also develops the VORPAL simulation framework and VizSchema data plugin). These technologies (1) reduce from hours to seconds or minutes the time required for

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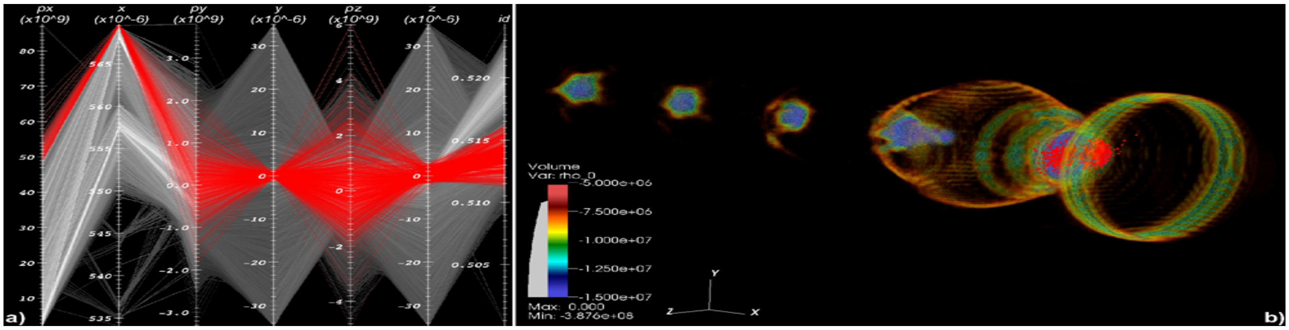

Figure 2. The interface on the left, which shows a multivariate view of particles' distribution across all simulation variables, is a vehicle for selecting particles having high acceleration and spatial coherency. All particles are shown in gray, and selected particles shown in red. This selection interface is linked with other forms of visual data exploration, so that a physical view of selected particles (right, red particles) helps the scientist to quickly gain insight into the relationship between statistical-space and physical-space features. This new capability, developed as part of VACET's research and development portfolio, is now part of widely distributed, production-quality, parallel capable visual data exploration software infrastructure (VisIt). Image, generated from VORPAL simulation results, courtesy O. Rübel et al., LBNL.

finding accelerated particles in simulation results and tracking them over time; (2) replace a manual particle search process with one that is automated and based upon state-of-the-art machine learning. Together, these two capabilities help to increase the rate and quality of scientific knowledge discovery.

Working with researchers from the SciDAC *Scientific Data Management Center*, the VACET team developed a new capability for the rapid visual exploration of very large, multivariate, time-varying datasets. Using this new technology, a scientist interactively selects subsets of data via a user interface that presents a statistical distribution (Figure 2, left) of particle information across all simulation dimensions, e.g., position, velocity, electrical charge, etc. Concurrent with exploration in statistical space, the subset is simultaneously displayed in physical space (Figure 2, right). Once a scientist finds interesting particles in one time step, the new technology will locate all those particles across all timesteps. Further investigations of this complete set of particles helps to increase scientific understanding of the processes that lead to wakefield acceleration.

These new capabilities are implemented in production-quality, parallel-capable visual data exploration software that runs on virtually all modern platforms, ranging from desktop-class machines to DOE's petascale computer systems.

To help further accelerate scientific knowledge discovery, VACET researchers developed new technology for automatically finding and tracking particles undergoing wakefield acceleration. The idea is to use machine learning technology to find accelerated particles having a high degree of spatial and phase-space coherence. Once located, the paths of these particle "bunches" can be quickly displayed and analyzed. This new capability helps to accelerate scientific knowledge discovery by replacing a manual search process with one that is automated

Both these steps represent a major new capability for accelerator scientists: before this technology, the search and tracking process consumed many hours of computer time; now, these processes take only a few seconds, even with today's largest accelerator simulation datasets, when run on DOE's parallel computing platforms.

Recent Publications

O. Rübel, Prabhat, K. Wu, H. Childs, J. Meredith, C.G.R. Geddes, E. Cormier-Michel, S. Ahern, G.H. Weber, P. Messmer, H. Hagen, B. Hamann and E.W. Bethel, "High Performance Multivariate Visual Data Exploration for Extremely Large Data." SC08, Austin TX, November, 2008. LBNL-716E.

Daniela Ushizima, Oliver Rübel, Prabhat, Gunther Weber, E. Wes Bethel, Cecilia Aragon, Cameron Geddes, Estelle Cormier-Michel, Bernd Hamann, Peter Messmer, Hans Hagen. "Automated Analysis for Detecting Beams in Laser Wakefield Simulations." 2008 Seventh International Conference on Machine Learning and Applications, Proceedings of IEEE ICMLA'08, 2008. LBNL-960E

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