Advanced Computing for 21st Century Accelerator Science and Technology

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Executive Summary

Particle accelerators have enabled remarkable scientific discoveries and important technological advances that span all programs within the Office of Science. In the High Energy and Nuclear Physics (HENP) program, experiments associated with high-energy accelerators have led to important discoveries about elementary particles and the fundamental forces of nature, quark dynamics, and nuclear structure. In the Basic Energy Sciences (BES) program, experiments with synchrotron light sources and spallation neutron sources have been crucial to advances in the materials and biological sciences. In the Fusion Energy Sciences (FES) program, great strides have been made in developing heavy-ion particle accelerators as drivers for Inertial Fusion Energy. Beyond impacts to basic and applied science, accelerators have also been proposed that address environmental, national security, and energy-related issues through projects such as the accelerator transmutation of waste, accelerator-based hydrodynamic imaging, and accelerator-driven fission energy production. In summary, accelerators play a critical role in U.S. science and technology, and are highly beneficial to the nation's health, wealth, and security.

Given the importance of particle accelerators, it is essential that the most advanced high performance simulation tools be brought to bear on the development of next-generation accelerators and new accelerator technologies. The present project will develop a comprehensive terascale Accelerator Simulation Environment (ASE) whose components will enable accelerator physicists and engineers to address a broad range of important issues in next-generation accelerators and their design. These issues, which could not be addressed without terascale resources, range from the high accuracy requirement for modeling entire accelerating structures of complex shapes with tight tolerances, to the high resolution requirement needed for simulating beam halo in high-intensity linacs, to the complexity associated with modeling the collective interaction of intense beams, lasers and plasmas. Using terascale resources and built on scalable algorithms, the software components and application codes in the ASE will be able to deliver the accuracy and resolution necessary for accelerator designs that are pushing the envelope of machine performance and system complexity. In the important area of accelerating structure design, for example, the new set of electromagnetic simulators will contain the physics needed for realistic end to end modeling so that the simulation becomes in effect a cheaper, viable and faster alternative to the expensive, time-consuming process of repeated fabrication and testing. New tools that are under development have already allowed structure designers to explore novel ideas that lead to higher acceleration gradients and lower surface fields which otherwise would have been difficult to achieve through traditional prototyping. Similarly, advanced accelerator modeling tools under development have also been used to understand and interpret beam phenomena observed in recent plasma wakefield experiments.

The creation of a new generation of accelerator simulation codes will have an impact in three areas: (1) optimizing the design of next-generation accelerators which may include, e.g., a linear collider such the Next Linear Collider (NLC), a neutrino factory, a rare isotope accelerator (RIA), a 4^{th} generation light source, and a prototype fusion driver, (2) maximizing the DOE's investment in existing accelerators by using simulation to help optimize their performance and expand their operational envelopes in machines such as PEP-II, RHIC, and the Tevatron, and (3) developing new accelerator technologies by using simulation as a tool of discovery to explore beams under conditions like those found in laser- and plasma-based accelerators. This new capability will have the most impact on the DOE's HENP programs, and has the potential to

achieve a major advance in those programs, by greatly enhancing its ability to design the next generation of high energy accelerators and high intensity drivers for HENP facilities. Terascale simulations will support important design decisions and feasibility studies, helping to reduce cost and risk, and helping to ensure that future projects are completed on schedule and within budget. The development of state-of-the-art laser/plasma simulation codes will furthermore enable accelerator scientists to explore new concepts that will advance the frontiers of accelerator science and technology.

The development of the ASE will be guided by target applications that are computationally challenging and will have maximum impact on HENP projects. These applications will serve as the test-bed for the simulators and the terascale simulation environment and they include:

- Full-scale modeling of large electromagnetic accelerating systems - the PEP-II beamline complex around the interaction region to study beam heating, the entire NLC accelerator structure to calculate wakefields, and the proposed radio frequency quadrupole (RFQ) design for RIA.
- Large-scale beam dynamics simulations for improving the performance of colliders (e.g. PEP-II, the Tevatron, and RHIC) and high intensity drivers (the FNAL booster and BNL AGS).
- Large-scale simulation of a plasma wakefield accelerator (particularly with regard to the critical issues of staging and emittance control), and simulations of laser wakefield accelerators, including particle injection, capture, and acceleration.

The project's target applications and deliverables fall into three areas: Electromagnetics (EM), Beam Dynamics (BD), and Advanced Accelerators (AA). The EM component will involve the development of three parallel solvers, Omega3P, Tau3P, and Phi3P, which are an eigenmode code, a time domain electromagnetics code, and a statics code, respectively. These codes will use unstructured grids to conform to the geometry of complex 3D structures. The BD area will involve the development of modules for treating multiple beam phenomena (such as space charge effects, high-order optical effects, beam-beam collisions, wakefields, intrabeam scattering, and ionization cooling), and their incorporation into a parallel version of the MaryLie beam dynamics code. The AA component will involve the development of the OSIRIS and XOOPIC/VORPAL codes for modeling laser- and plasma-based accelerators.

The ASE will consist of a set of parallel, portable, reusable, object-based software components that, when integrated, will enable accelerator physicists and engineers across the country to work together to solve the most challenging problems in accelerator design, analysis, and optimization. The success of the ASE will require close collaboration with computer scientists and applied mathematicians to enable the development of high-performance software components for terascale platforms. For all three areas of the ASE, new mathematical models (including reduced description models) and new algorithms will be developed to achieve high accuracy and high performance on parallel supercomputers. The successful development of all the codes will involve close collaboration with SciDAC/ISIC partners in areas such as applied mathematics and numerical algorithms (eigensolvers, linear solvers), meshing techniques (grid generation, adaptive refinement), visualization (large data sets, multi-resolution techniques), code validation, software interoperability (multiple language support, code component development), and performance optimization (load balancing and communication).