Accelerator Physics

Background

Particle accelerators have enabled remarkable scientific discoveries and important technological advances that span all programs within the DOE Office of Science (DOE/SC). In the High Energy Physics (HEP) and Nuclear Physics (NP) 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. The importance of accelerators to the DOE/SC mission is evident from an examination of the DOE "Facilities for the Future of Science: A Twenty-Year Outlook." Of the 28 facilities listed, 14 involve accelerators.

Particle accelerators and their associated detectors are among the largest, most complex scientific instruments in the world. The successful development of large accelerator facilities involves enormous investments in the three paradigms of scientific research: theory, experiment, and simulation. Neglecting any of these can lead to an inability to meet performance requirements, cost overruns, and ultimately, project failure. Simulation is already playing an increasingly prominent and valuable role in the theory, design and development of accelerators and their associated technologies. It is being used to understand and improve the performance of existing accelerators such as the PEP-II B-factory, the Fermilab Tevatron, the Fermilab Booster, and the Relativistic Heavy Ion Collider at Brookhaven National Laboratory. In the future, a new level of simulation will be needed as researchers push the frontiers of beam intensity, beam energy and system complexity. The three-dimensional, nonlinear, multi-scale, many-body aspects characteristic of future accelerator design problems, and the complexity and immensity of the associated computations, account for their extreme technical difficulty. But, despite the difficulty, the corresponding return to Science, and to the DOE/SC mission, is equally significant. High-end simulations, used in concert with theory and experiment, will help to ensure the success of next-generation accelerators, providing optimal design while reducing design time, cost, and risk. Used as a tool of discovery, high-end simulations are helping researchers to explore systems under extreme conditions of high energy density. It will furthermore help advance the frontiers of accelerator science and technology, leading to ultra-high gradient laser- and plasma-based accelerators that will have huge consequences in scientific research, industry and medicine.

Great progress in accelerator modeling has been made under the SciDAC Accelerator Science and Technology (AST) project. Thanks to SciDAC (and its predecessor, the DOE Grand Challenge), a new suite of parallel simulation tools has been developed and applied to important problems in accelerator design and analysis with great success, laying the groundwork for the next advancement in simulation capability. NERSC has been a key computational resource for the AST project. NERSC resources have been used to model existing machines such as the Fermilab Tevatron and Booster, the SLAC PEP-II B factory, the RHIC. NERSC resources have also been used to simulate future accelerators such as the Large Hadron Collider (now under contruction) and the International Linear Collider. They have also been used to study advanced accelerator concepts through simulations of experiments at SLAC (E-157, E-162, E-164) and experiments at Lawrence Berkeley Laboratory (l'OASIS laboratory). Though there are many examples of NERSC resources being brought to bear on important problems in accelerator science and technology, below we present four such examples.

Accelerator Modeling at NERSC: Four Examples

FNAL Booster Simulation: Under the SciDAC AST project, codes such as BeamBeam3D, IMPACT, Synergia, and MaryLie/IMPACT have been developed and used to model beam dynamics in a number of important DOE/SC accelerators and to study the physics of intense charged particle beams. In one such example, NERSC resources were used to perform simulations of the first 1000 turns (~2 ms) after injection of the Fermilab Booster, using a fully 3D space charge model. The simulation results were then compared with results from Booster experiments. See Figure 1. Members of the SciDAC AST project participated in these experiments and made significant contributions in understanding and calibrating Booster diagnostic devices. Simulation studies are now being used to help optimize the injected beam parameters to achieve a matched beam in the presence of space charge and large momentum spread.

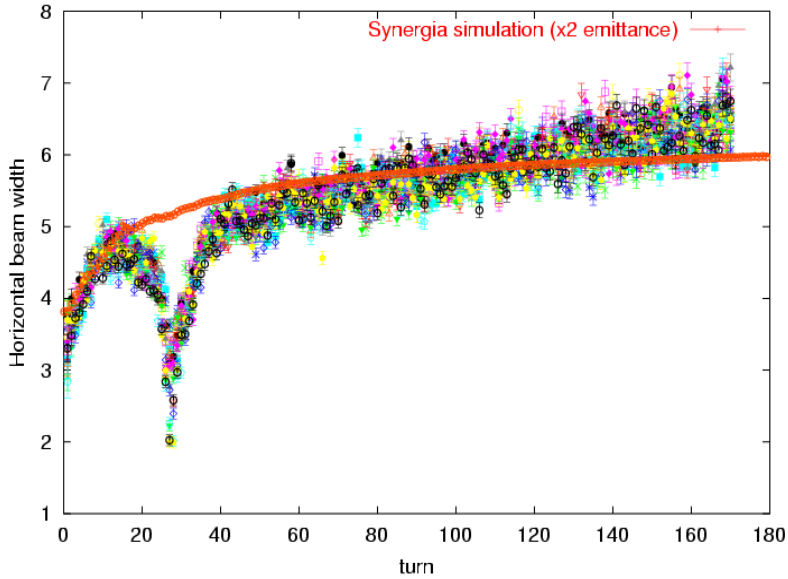

Figure 1: Comparison of FNAL Booster experimental data with results from a Synergia application. The simulation was performed for 11 turns at 440 mA of current. The simulated beam size is in good agreement with the measured size. This simulation takes into account the calibration of the ionization monitors. (The notch in the beam is due to the decay of the current of the injection orbit bump magnet, which is not included in the simulation)

Wakefield Accelerator Simulation: There is presently intense activity worldwide aimed at accelerating particles using the extremely large fields that can be produced in laser- and plasma-based systems. Previously such schemes produced beams with unacceptably large energy spread. However, recent breakthrough experiments have demonstrated acceleration of beams with just a few percent energy spread to energies of more that 100 MeV. Using NERSC resources, members of the SciDAC AST project have performed large-scale simulation using the codes OSIRIS and VORPAL to help interpret laser- and plasma-wakefield accelerator experiments and to gain insight in the acceleration mechanism. The highly nonlinear behavior of such systems in the "blowout regime" make theoretical analysis especially difficult. Fully 3D parallel particle-in-cell simulations are essential to help understand the physical processes involved, and will play a key role in the design of future wakefield accelerators to produce high quality beams accelerated to a GeV per acceleration stage. Under the SciDAC AST project, great progress has also been made in the development of reduced description models for laser/plasma simulation. One such example, QuickPIC, has been shown for some problems to provide answers as accurate as OSIRIS but with 2 to 3 orders of magnitude less computation time.

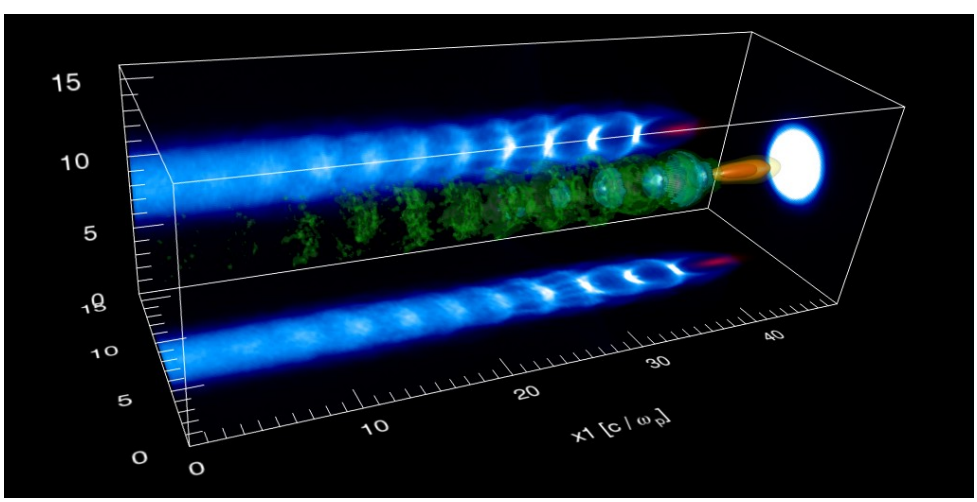

Figure 2: Results from a 3D OSIRIS simulation, performed at NERSC, of a beam with $2x10^{10}$ particles, $_r$=20 m, and $_z$ =63 m propagating through a Lithium gas cell of density $n_0=5.143\times10^{16}$ cm^{-3}. The simulation box was 512×128×128 grid cells wide, and the simulation was run for 3100 time steps. We show here a 3D plot of the electron density, showing the ionization electrons and wakefield, and also the drive electron bunch. We show both iso-surfaces and projections of this data; the drive beam is shown in red-orange-yellow colors, and background electrons are shown in blue-cyan-green colors.

Analysis of the PEP-II Interaction Region: Under the SciDAC AST project, a comprehensive suite of parallel, 3D electromagnetic modeling codes has been developed to model large, geometrically complex accelerator structures with unprecedented accuracy. These codes include Omega3P, S3P, Tau3P, T3P, and Track3P. The codes have been used to model electromagnetic structures for a number of DOE/SC projects including PEP-II, RIA, and a future linear collider. In regard to PEP-II, simulations were performed at NERSC using the codes Omega3P and Tau3P to analyze beam heating in the interaction region (IR). Initially, PEP-II was prevented from operating at higher current due to the presence of trapped modes in the IR chamber that led to excessive heating. Omega3P was used to calculate the trapped modes in the IR from crotch to crotch. Fig. 3 (Left) shows the trapped mode with the highest power loss whose frequency was close to the one measured in the experiment in the region of excessive heating. Fig. 3 (Right) is the heating power distribution centered about the interaction point which shows the heating is significantly higher on one side in agreement with what's observed. It was obtained by summing 330 modes found with Omega3P that have the highest wall loss. These results provided input on what modifications were necessary in the redesign of the IR to remedy this situation. Since the upgrade PEP-II has been able to raise the current by 15% which led to higher luminosity and physics discovery.

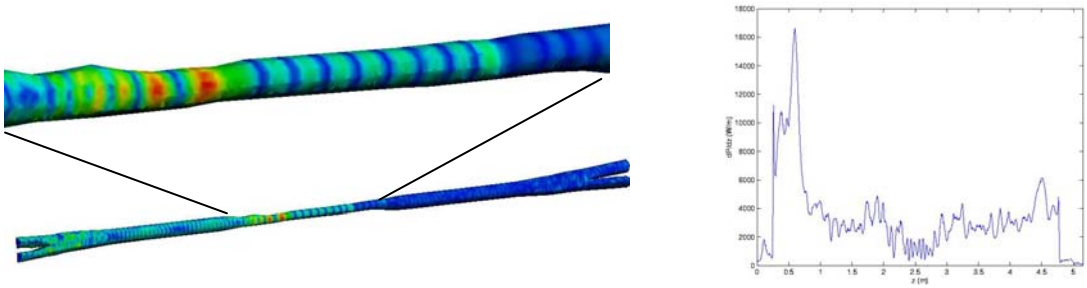

Figure 3. Left, Trapped mode with highest power loss calculated by Omega3P (5.28 GHz, 230W). Right, Power loss distribution about interaction point (17.2 kW total from 330 modes)

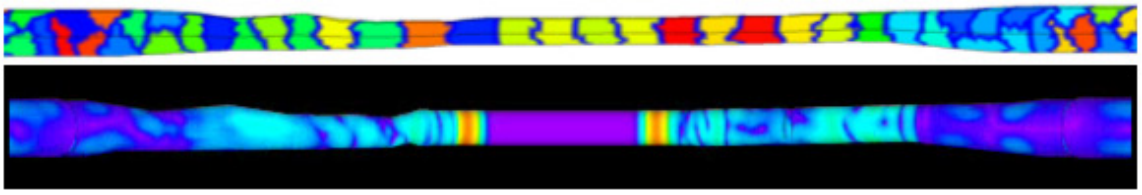

Figure 4. Top, Distributed Mesh of the IR between the crotches only. Bottom, Snapshot in time of electric field due to two colliding beams from Tau3P time-domain simulation.

Phase Space Reconstruction The applications scientists in the SciDAC AST project have close collaborations with researchers in the SciDAC ISICs and with researchers supported by the DOE/ASCR SAPP program in areas such as applied mathematics, numerical analysis, computer science, visualization, and statistics. For example, statistical methods are being developed to aid in calibration, prediction, and uncertainty quantification in beam dynamics simulations. In particular, statistical methods are being developed to reconstruct a phase space distribution from one-dimensional wire scans. This involves solving an inverse problem in the presence of a small number of data samples which themselves have intrinsic errors. One approach to this problem involves performing a large number of forward simulations that, combined with beam profile monitor data, yield an estimate of the phase space distribution function. Figure 5 shows an example of the procedure, applied to the transport of a beam with space charge in a quadrupole channel. Successful application of this procedure will make it possible to determine the phase space initial distribution in experiments, including quantitative uncertainty bounds, and help make large-scale beam dynamics simulation a tool for prediction that can be used to help improve accelerator performance.

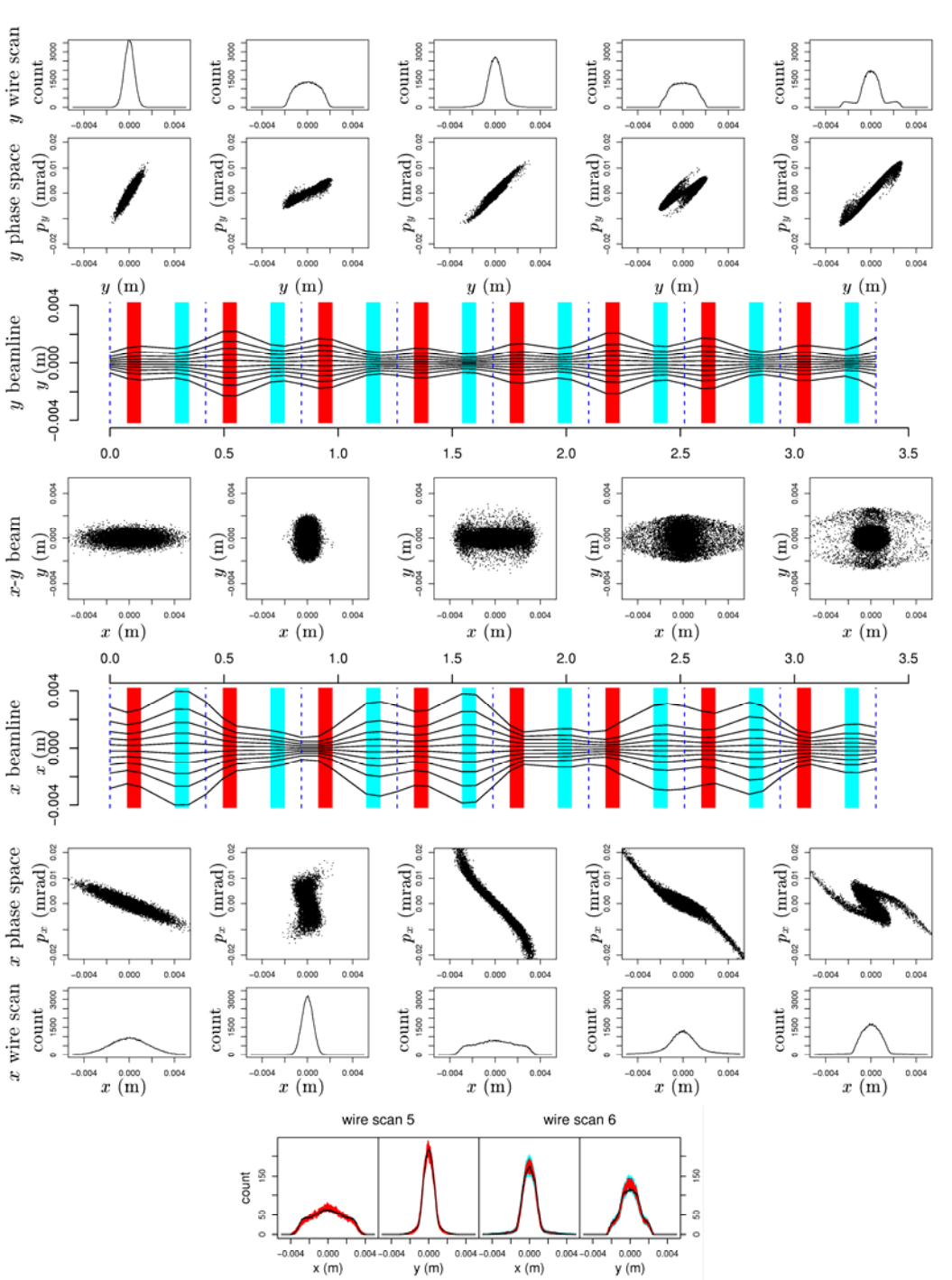

Figure 5. Simulation of a high intensity proton beam through a series of quadrupole magnets. Working with the SciDAC AST Project, statistical scientists are developing new techniques for forecasting, calibration, and uncertainty quantification]. Shown here, Bayesian techniques were used to combine 1D profile monitor data with simulations to infer the 4D beam distribution. The bottom figure shows the 90% intervals for the predicted profile at scanner #6 (shaded regions), and, for comparison, the observed data (black line). Only data from the odd numbered scanners were used to make the prediction.

Future Resource Needs of the Accelerator Community at NERSC

Currently the accelerator community receives a combined allocation of approximately 2 million processor-hours on the IBM SP3 (seaborg) at NERSC. But, already, important problems have been identified, and CPU requirements estimated, where the simulations required to solve a single problem requires the equivalent of nearly 10 million SP3 hours. These problems include, for example, the self-consistent simulation of beam-beam effects in

colliders, and a design study for a 1 GeV plasma wakefield accelerator. Given the demand in the accelerator community, the community would like to see as large an increase in CPU hours as is practical in regard to the next acquisition at NERSC. As to the type of resource, the community's codes have wide ranging needs. Problems involving unstructured grids, parallel particle-in-cell space-charge simulations, and strong-strong beam-beam simulations, involve significant interprocessor communication of varying sizes of data sets. As such, high bandwidth and low latency are both important depending on the application. Other problems, such as beam-beam simulations in the weak-strong limit, involve little communication but require significant capacity. Besides raw CPU hours, some problems, like direct Vlasov codes, require large memory, since the memory requirements scale as N^6 (for a 3D code). Given the massive number of grid points and/or particles, and the need to do visualizations and analyses, parallel I/O is also a high priority; this is especially true in regard to analyses involving the time-evolution of complex phenomena like beam/plasma interactions. Finally, the importance of algorithms cannot be over-emphasized. Already under SciDAC, the AST project has seen performance increases of over a factor of 100 through the use of optimal algorithms and software provided by the ISICs. Continued progress in the development of efficient algorithms, performed at NERSC and elsewhere, will be crucial to getting the most Science out of the next phase of NERSC resources.