Community petascale project for accelerator science and simulation: Advancing computational science for future accelerators and accelerator technologies[†]

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Abstract. The design and performance optimization of particle accelerators are essential for the success of the DOE scientific program in the next decade. Particle accelerators are very complex systems whose accurate description involves a large number of degrees of freedom and requires the inclusion of many physics processes. Building on the success of the SciDAC-1 Accelerator Science and Technology project, the SciDAC-2 Community Petascale Project for Accelerator Science and Simulation (ComPASS) is developing a comprehensive set of interoperable components for beam dynamics, electromagnetics, electron cooling, and laser/plasma acceleration modelling. ComPASS is providing accelerator scientists the tools required to enable the necessary accelerator simulation paradigm shift from high-fidelity single physics process modeling (covered under SciDAC1) to high-fidelity multiphysics modeling. Our computational frameworks have been used to model the behavior of a large number of accelerators and accelerator R&D experiments, assisting both their design and performance optimization. As parallel computational applications, the ComPASS codes have been shown to make effective use of thousands of processors.

1. Introduction

Particle accelerators are critical to scientific discovery in the DOE program in America and indeed the world [1]. Of the twenty-eight facilities listed in the DOE report "Facilities for the Future of Science: A Twenty-Year Outlook," fourteen involve accelerators. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time and for enabling research in aspects of materials science, chemistry, geosciences, and bioscience.

The High Energy Physics (HEP) program uses accelerators to answer fundamental questions about nature such as the origin of mass and the asymmetry between matter and antimatter and to search for new particles, new symmetries, and possible extra dimensions of space. In the DOE 15-year plan [2] for HEP, the first two action items call for full support of the program of the Large Hadron Collider (LHC) at CERN and for the establishment of leadership in the R&D effort to design and build the proposed International Linear Collider (ILC) on U.S. soil. Even with the current HEP budget difficulties, the recent report of the Particle Physics Project Prioritization Panel (P5) [3] emphasizes in its recommendations the need to maintain leadership in both the energy and the intensity frontier of accelerator science. At the same time, it is imperative to maximize the physics reach of the ongoing DOE/HEP program, and that involves the performance optimization of the Fermilab Tevatron. Furthermore, DOE/HEP is supporting a world-class R&D program to develop new accelerator technologies including laser wakefield and plasma wakefield accelerators, as well as other types of advanced accelerator concepts.

The Nuclear Physics (NP) program uses accelerators to study the properties of nuclear matter and the structure of the nucleus, understand the mechanism of quark confinement, and create and study a heretofore-unknown state of nuclear matter, the quark-gluon plasma. The flagship NP accelerators are CEBAF at Jefferson Lab and RHIC at Brookhaven National Laboratory (BNL). The worldwide nuclear physics community has identified [4] the construction of a polarized electron-ion collider as a long-term objective in the ongoing effort to understand and answer questions in these areas. DOE/NP is considering two approaches for such a facility: e-RHIC [5] and ELIC [6]. DOE/NP is also considering a proposed rare isotope facility that will permit studies of nuclei far from stability that promise to radically improve our understanding of atomic nuclei.

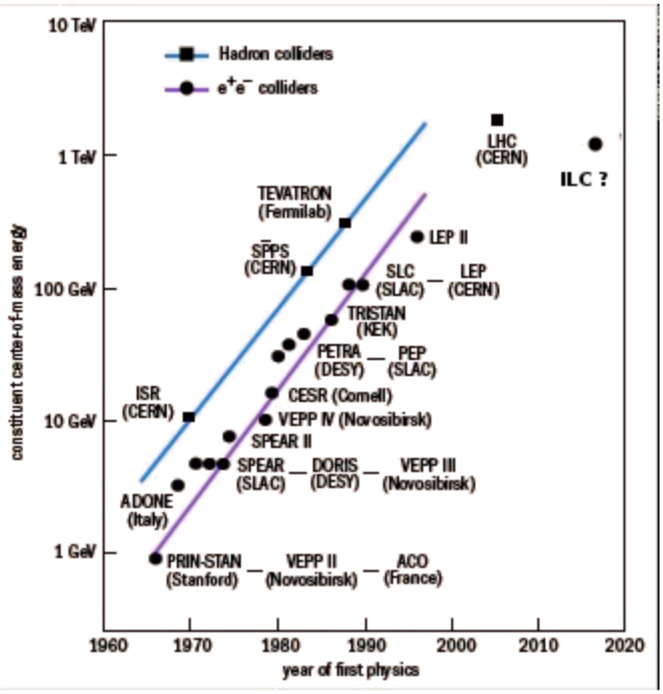

Figure 1. Livingston plot showing the center of mass energy of particle accelerators (lepton and hadron colliders) versus time. In the case of the hadron machines, energies have been adjusted to account for quark and gluon constituents.

The flagship accelerator facilities for the Basic Energy Sciences (BES) program are its spallation neutron sources (SNS, LANSCE) and its synchrotron light sources (ALS, APS, NSLS, SSRL). Over the past decade, the light-source community consensus has been that short-wavelength, free-electron lasers (FELs) will form the basis for the so-called fourth-generation light sources. DOE/BES is building the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center, which will operate with ultra-short x-ray pulses to shed light on ultra-fast processes in chemistry and biology.

LCLS will also further our understanding of the arrangement of atoms in inorganic and organic materials, thus enabling the development of new materials and molecules with desirable properties.

The discussion above clearly shows that accelerators are the primary instruments for scientific discovery at the forefront of basic physics research across all programs of the Office of Science. In order to maintain this forefront position over the past forty years, accelerators have become bigger and much more expensive, with ever-increasing demands for higher energy and intensity (see figure 1), increased complexity, and tighter operational tolerances. The design, cost optimization, and successful operation of modern accelerators require the optimization of many parameters and the understanding and control of many physics processes. In addition, the preceding discussion also shows that the different areas of scientific research have different requirements for the type of particle accelerator that is needed to enable each research activity. Although the basic concepts that guide the design and operation of the different types of particle accelerators are similar, the technologies involved and the critical design and operational parameters vary depending on the application, thus increasing the necessary complexity of high-fidelity modeling tools. The same plurality exists in accelerators used for industrial or medical applications. A representative list of particle accelerator applications in the applied sciences, based on different types of particle beams and accelerator technologies, is shown in table 1. Advances in accelerator technology and careful design have resulted in a more than order of magnitude reduction in the size of accelerators used for medical applications (see figure 2). Advances in accelerator technology triggered by basic research R&D (dielectrics, laser wakefield accelerators) are already discussed as candidates for the next generation of medical accelerators [7].

Table 1. Representative list of accelerator utilization in the applied sciences.

Field	**Accelerator type**	**Topics of study**
Atomic physics	Low energy ion beams	Atomic collision processes, study of excited states, electron-ion collisions, electronic stopping power in solids
Condensed matter physics	Synchrotron radiation sources	X-ray studies of crystal structure
	Spallation neutron sources	Neutron scattering studies of metals and crystals, liquids, and amorphous materials
Material science	Ion beams	Proton and X-ray activation analysis of materials; X-ray emission studies; accelerator mass spectrometry
Chemistry and Biology	Synchrotron radiation sources	Chemical bonding studies: dynamics and kinetics; protein and virus crystallography; biological dynamics
Medicine	Proton, electron, and neutron beams	Radiation therapy

Under SciDAC-1, the Accelerator Science and Technology (AST) project produced a powerful suite of parallel simulation tools representing a paradigm shift in computational accelerator science. Using AST codes, simulations that used to take weeks or more now take hours, and simulations once thought impossible are now performed routinely. These codes were applied to major DOE accelerator facilities and future accelerator projects including the Tevatron, PEP-II, LHC, RHIC, NLC, ILC design, SNS, and LCLS [8]. They were also applied to advanced concepts such as plasma-based accelerators, where they played a key role in understanding the physics of doubling the energy of a 42 GeV beam at SLAC and of low-energy-spread beam production in laser wakefield accelerators [9].

Under SciDAC-2, the Community Petascale Project for Accelerator Science and Simulation (ComPASS), the successor of AST, recognizing the increased complexity, precision, and beam intensity requirements of next-generation particle accelerators, changes again the focus of accelerator high-performance simulation software. Our accelerator simulation paradigm is shifting from single-machine, single-component simulations to end-to-end (multistage or complete system), multiphysics simulations. Building on the foundation laid under SciDAC-1, ComPASS is extending terascale capabilities to the petascale and is adding new capabilities in order to deliver a comprehensive, fully integrated accelerator simulation environment. The ComPASS vision is to create a *virtual accelerator modeling* environment for the realistic, inclusive simulation of all relevant beam dynamics effects (single and multi-particle dynamics, realistic geometry and parameters), and a *virtual prototyping* environment for realistic simulation of all relevant accelerator component effects (thermal, mechanical, and electromagnetic properties with accurate geometry description). The ComPASS accelerator modeling applications, discussed in Section 3, target important problems in nearly every accelerator laboratory in the country. The success of these applications depends on the success of the collaboration of ComPASS researchers with accelerator scientists from these laboratories. In addition, the success of the development of the necessary infrastructure that will enable the integration of the high-end capabilities we are building depends on the successful collaboration with ASCR researchers. This collaboration helps ensure that our accelerator tools development uses the most appropriate algorithms and computer science technology for petascale platforms.

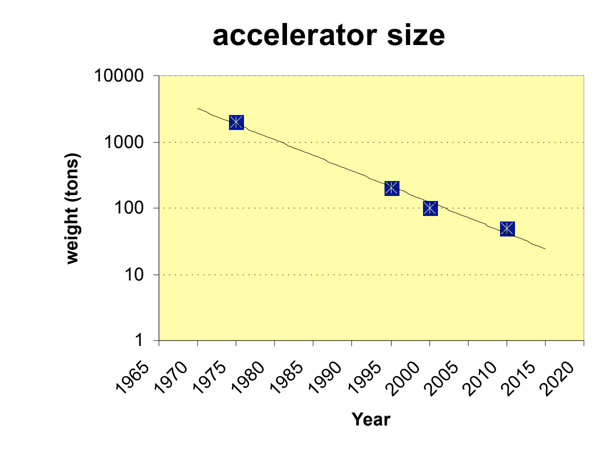

Figure 2. Advances in accelerator technology have resulted in more than order of magnitude reduction in the size of cyclotrons used for medical applications.

2. The ComPASS program

Accelerators rely on electromagnetic fields to provide particle acceleration, and they typically use magnetic fields to guide (bend and focus) the particle beams. Radiofrequency cavities (for acceleration), dipole magnets (for bending), and quadrupole magnets (for focusing) are the most commonly used beamline elements in accelerators. In addition, many more systems are necessary for the operation of a modern accelerator, such as high-order multipoles (to control the nonlinear behavior of the particles), devices for diagnostics (such as beam position monitors), feedback systems, and control systems. A modern accelerator operates like a modern airplane: it requires active damping or it is going to crash! The behavior of the particle beams (the *beam dynamics*) is affected not only by the interaction of the particles with the accelerator elements but also by the interaction of particle ensembles with each other, either via their own fields or via fields created by other particle ensembles.

These collective, multiparticle effects in many cases are the limiting performance factor for particle accelerators. All the effects described above combine with operational effects such as misalignments of accelerator components to make the design and operation of an accelerator a very challenging problem. Moreover, the quest for higher and higher energies and particle beam intensities requires continuous R&D for new accelerator techniques and technologies.

~~2.2.~~ 2.1. ComPASS computational tools development

Given the size, cost, and complexity of modern accelerators, the research to improve their design and performance becomes as challenging as the basic research and applications they enable. High-fidelity numerical modeling is essential to ensure cost effectiveness and performance optimization. The ComPASS program for computational accelerator physics development is organized so it mirrors the structure of the different accelerator science and technology R&D areas. From the discussion in the previous section, we see that the main ingredients required to compose an accelerator model are tools for electromagnetic field calculations, beam dynamics simulations, and tools that support new accelerator technology R&D. Thus, the main thrust areas of this project are threefold:

- Beam dynamics (BD): Development and applications of tools that model the evolution of beams through beam optics systems, including self-forces and other forces of interaction. A particularly interesting area of BD development is electron cooling (EC), where the beam phase-space is controlled by using the dynamical friction from relativistic copropagating electron beams.
- Advanced acceleration (AA): Development and application of tools that guide the R&D efforts for the realization of new high-gradient acceleration techniques such as plasma or laser wakefield accelerators.
- Electromagnetics (EM): Development and application of tools that model the electromagnetic fields in geometrically complex accelerating cavities and other accelerator components, in order to maximize acceleration while minimizing beam quality degrading effects. Such effects include wakefields, which are generated by a particle bunch as it passes a perturbation in an accelerator structure and can reinteract with the charged particle beam, multipactoring, that is, resonant electron multiplication that builds up an electron avalanche, leading to remarkable power losses and heating of the walls, and so forth.

Of course, these areas are not independent: the dynamics of a particle beam is affected by wakefields that require electromagnetic computations; particle-in-cell methods are common to beam propagation in cavities and advanced acceleration; electron cooling is needed for heavy ion beams because of emittance growth due to intrabeam scattering and beam-beam interactions. Hence, the code development in the three ComPASS areas aims to provide integrated simulation capabilities. This is accomplished by the project's enabling computer science activities in the area of component technologies, such as development of common component interfaces, code refactorization, and development of quality-of-service infrastructure software for our frameworks. In addition, activities in computer science and applied mathematics are common to all areas of development. These activities aim to improve the performance of our simulations and our analysis tools, such as solver development, optimization, and research on new or improved algorithms, data handling, and visualization.

2.2. ComPASS computational tools development

The accelerator modeling codes developed under ComPASS, together with their major applications, are described in the following list:

- Impact-T: A beam dynamics parallel particle tracking code that uses time as the independent variable. This code aims to accurately model low energy beams with large energy spreads, assumes a quasi-static model for the beam, and includes a self-consistent model of space-charge (the effects of the charge of the beam on itself). Applications include modeling of the Advanced Light Source streak camera, Advanced Photon Source upgrade, LCLS injector, the

Fermilab A0 experiment, and photoinjectors at BNL, UCLA, and Cornell, the UW-Madison FEL, PSI FEL, SPARC/X, and Fermi/Electra.

- Impact-Z: Beam dynamics simulation in rf linacs using path length as the independent variable. The Impact family of codes (Z and T) share a variety of Poisson solvers, either spectral based or convolution based. Applications for Impact-Z include Berkeley FEL studies, LEDA Halo experiment, ILC damping ring modeling, SNS, RIKEN cyclotron injector, and RIA driver, and JPARC, GSI, CERN SPL, and CSNS linac simulations. The Impact family of codes have been ported to Cray XT4, IBM SP4, and Blue Gene machines.
- MaryLie/IMPACT (ML/I): Beam dynamics framework focusing on ring problems involving high-order optics and space charge, realistic magnetic field profiles, realistic cavity simulations, fitting and optimization. Applications include RHIC upgrade.
- BeamBeam3D: A comprehensive code for modeling beam-beam effects in colliders using a variety of models including strong-strong and weak-strong models, short-range and long-range beam-beam interactions, crab crossing, multiple bunches, multiple interaction points, and impedance effects. Applications include the Fermilab Tevatron, KEKB, RHIC, and the LHC. BeamBeam3D has been ported to desktop MPI PC clusters, Cray XT4, and IBM SP3, SP4, and BG/L machines.
- PLIBB/ Nimzovich: A general-purpose parallel tracking framework for beam-beam simulations. Applications include RHIC wire compensation beam-beam experiments. The code has been used on the NERSC supercomputers.
- Synergia2: An extensible framework for beam dynamics. It is driven by Python, so it can be configured at run time, allowing for arbitrarily complex simulations. The framework includes nonlinear single-particle physics, beam generation and diagnostics, and collective effects modules. The collective effects modules include extensive support for space-charge calculations for a variety of geometries and boundary conditions. These calculations are available both through native Synergia solvers and through an interface to IMPACT. Application focus: Fermilab booster, ILC Damping Ring and Ring to Main Linac accelerator design, and modelling of Fermilab A0 photo injector experiments. The framework is optimized for massively parallel computations utilizing MPI. It is currently ported on desktop PC MPI clusters and Unix supercomputers supporting shared libraries (IBM SP3 and SP4).
- Elegant: Beam dynamics framework with focus on electron beams. Applications include FEL driver linac and energy recovery linac design. The parallel version of elegant is currently developed under ComPASS.
- VORPAL: A framework that can be configured in different ways at run time to solve a variety of problems. It provides models for neutral gases and plasmas interacting with electromagnetic fields and with each other through collisions. Applications include Laser Wake Field Accelerators (LWFA), EM cavity calculations (ILC, JLab), electron cooling (BNL), electron gun modelling and multipactoring (JLab), and modelling and analysis of electron cloud measurements. VORPAL is running in production on Bassi, Franklin, and Jacquard at NERSC and has been ported to Blue Gene.
- UPIC: A flexible framework for rapid construction of parallel particle-in-cell (PIC) applications. It supports electrostatic, darwin, and EM solvers. Applications focus: QuickPIC, which is based entirely on the UPIC framework and IMPACT solvers. UPIC is strictly Fortran90 compliant, with no dependencies other than MPI and pthreads, so it can be ported to any platform.
- Osiris: Fully explicit PIC code with ionization and coulomb collision packages. Applications of Osiris focus on LWFA and PWFA design and experiment modeling. Osiris runs on all the NERSC machines at LBNL, the ATLAS machine at LLNL, and on os-10 clusters.
- QuickPIC: A quasi-static PIC code based on the UPIC framework. Applications include LWFA and PWFA design and experiment modeling and e-cloud modeling for LHC, ILC, and

Fermilab Main Injector applications. QuickPIC is used on the NERSC machines and the UCLA OSX-based cluster.

- Omega3P: Frequency domain eigensolver for cavity mode and damping calculations. Applications include simulations of the ILC cryomodule, LHC crab cavity and collimator, X-band high gradient structure, JLab 12-GeV upgrade superconducting cavity, the BNL RHIC cavity, and the SNS superconducting cavity. The code runs on NERSC and NCCS supercomputers.
- S3P: Frequency domain scattering parameter calculations. S3P was used for ILC superconducting cavity coupler calculations. The code runs on NERSC supercomputers.
- Track3P: Particle tracking for simulation of dark current and multipacting. Applications include modelling the coupler of the ILC superconducting cavity, the SNS superconducting cavity, and BNL RHIC cavity calculations. Track3P runs on NERSC and NCCS supercomputers.
- T3P: Time domain solver for wakefield computations with beam excitation. Applications include the ILC cryomodule and Damping Ring components, CLIC PETS structure, MIT photonic band gap structure. T3P is ported on NERSC and NCCS supercomputers.
- Gun3P: Space-charge trajectory code for beam formation and beam transport. Applications: ILC sheet beam klystron gun. Gun3P runs on NERSC supercomputers.
- Pic3P: Self-consistent particle-in-cell code for rf gun and klystron simulations. Applications include the LCLS rf gun. Pic3P runs on the NERSC supercomputers.
- TEM3P: Framework for integrated electromagnetic, thermal and mechanical analysis for rf cavity design. The framework uses solvers from the 3P family of codes described above. Applications include the LCLS rf gun design. The framework runs on the NERSC supercomputers.
- V3D: Visualization utilities for meshes, field, and particles on unstructured meshes. These utilities are used with the 3P family of codes described above.

Detailed descriptions of the ComPASS codes and their applications can be found in [10] for electromagnetics [11] for advanced acceleration and [12] for beam dynamics. The high-performance-computing (HPC) capabilities of most of these codes were developed under the AST SciDAC project, each targeting specific areas of computational accelerator physics applications, with emphasis on the performance and high fidelity of the calculation. The above list shows not only the wide spectrum of capabilities developed under the SciDAC accelerator modeling project, but also the complexity of the field of computational accelerator physics. Under ComPASS, the emphasis is shifting toward developing the necessary infrastructure for integrating these capabilities into accelerator simulation frameworks, allowing for multi-physics, multi-scale simulations. These activities are in addition to the continuing effort for code and algorithm performance improvements and optimization on the newer HPC platforms.

~~2.2.1.~~ 2.3 *Enabling technologies*

Software infrastructure for multiphysics accelerator modeling is a central part of ComPASS. Our approach is to develop application components using existing mature physics or algorithmic implementations as the core of each component. In this discussion, “component” is defined as a portion of software implementation that can be added or removed from multiple applications. The most serious challenge in developing simulation components is the definition of their interfaces: the components need to be objects that can be used for multiple implementations of different ComPASS simulations. Thus, the interface

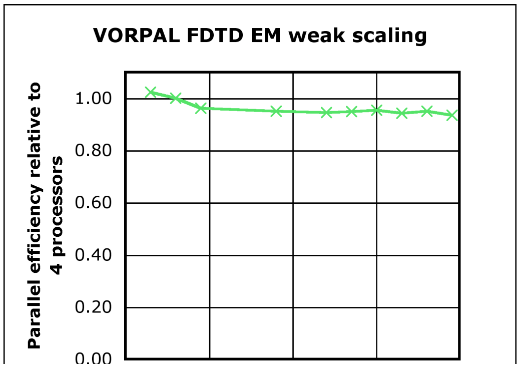

Figure 3. Weak scaling of VORPAL for an 803 domain size relative to a computation on 4 processors. VORPAL is achieving

definition has to be independent of any details from any particular application implementation, including the parallelization (data distribution) schemes. Our approach builds on AST and ComPASS work on the Synergia2 [13] and MaryLie/IMPACT [14] beam dynamics frameworks and the UPIC framework and is extending to other areas of the project with work such as the TEMP3P electromagnetic simulation framework. Figure 4 shows a schematic of the Synergia2 framework, with the physics components and software infrastructure dependencies.

Use of advanced mathematical techniques, scalable numerical algorithms, and computational tools are also major components of the ComPASS activities. For example, through implementation in VORPAL, SciDAC has supplied the first massively parallel implementation of FDTD electromagnetic computations (see figure 3). While many of the mathematical and computational tools we employ are relatively mature, we need to enhance their capabilities to meet the petascale computational challenges of SciDAC-2. In addition, we need to explore the benefits of employing new techniques and algorithms, and we need to port the new and old implementations to the new petascale capable hardware that is or will be available in the SciDAC-2 era.

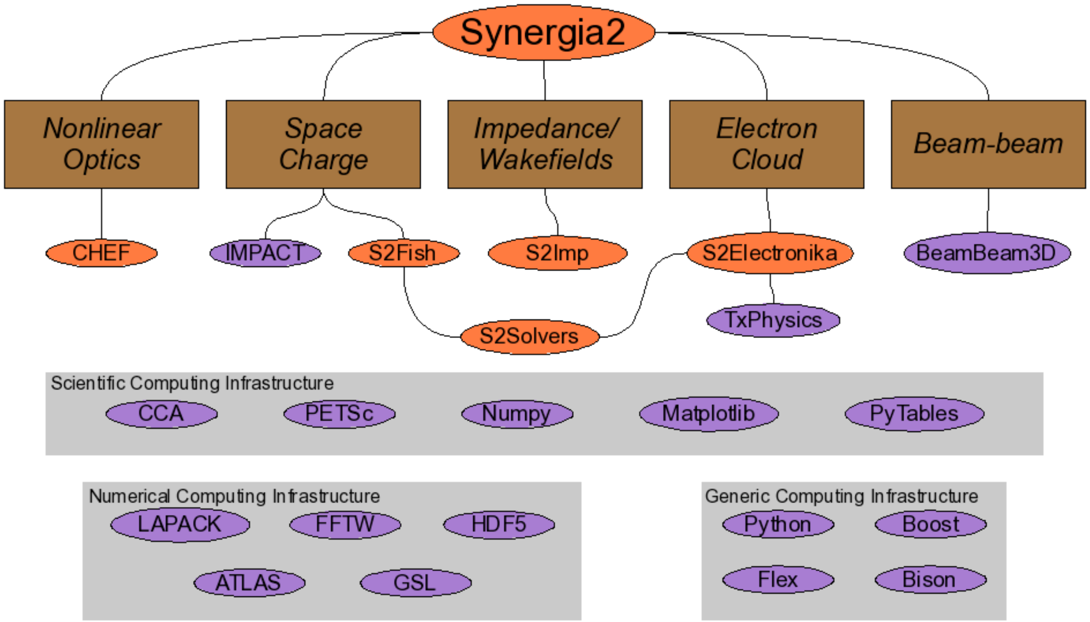

Figure 4. Componentization of the Synergia2 infrastructure. The Synergia2 framework includes many beam dynamics physics modules, both native to Synergia (orange) and reused modules from other ComPASS beam dynamics codes (magenta).

Shown below is a list that summarizes the necessary enabling technology activities for the success of the ComPASS program. Note that not all of the listed activities are funded under the ComPASS project, so collaboration and coordination with the SciDAC Centers for Enabling Technologies and SciDAC Institutes is essential.

- Development of scalable parallel eigensolvers, in collaboration with Terascale Optimal PDE Simulation (TOPS) [15]. The success of this activity is essential to enable simulation of complete systems of rf cavities with many millions of degrees of freedom.
- Domain-specific scalable linear solvers development, in collaboration with TOPS. This is another essential activity for detailed modeling of large electromagnetic systems.
- Development of meshing technology for electromagnetic calculations to enable shape adaptation procedure that is essential for the optimal (cost effective) design of rf cavities. This work relies on collaboration with the Interoperable Technologies for Advanced Petascale Simulations (ITAPS) project [16] and TOPS.

- Development of new Poisson solvers that will perform and scale well on petascale platforms, in collaboration with TOPS. Fast and scalable Poisson solvers are essential for petascale applications involving particles in a mean field treatment of space charge.
- Parallel adaptive refinement for finite elements, to improve solution accuracy and reduce computational cost, in collaboration with ITAPS and the Combinatorial Scientific Computing and Petascale Simulations (CSCAPES) project [17].
- Utilization of remote and interactive visualization tools to enable remote collaboration and analysis of large, complex data sets; in collaboration with the Institute for Ultrascale Visualization (ISUV) [18].
- Deployment of performance analysis and optimization tools for ComPASS codes and applications to maximize performance on petascale platforms; work in collaboration with PERI [19].
- Development of embedded boundary methods for PIC simulations of electromagnetic structures, to reduce memory requirement for simulation utilizing a finite differences approach; in collaboration with ITAPS.
- Enhancement of the UPIC framework, to include mesh refinement and optimized preconditioning in reduced PIC and spectral method-based dispersionless solvers. This activity benefits from interactions with the Applied PDE Center (APDEC) [20], TOPS, and PERI.
- Development of "computational quality-of-service" infrastructure for beam dynamics modelling applications. This activity includes the development of interoperable components using the Common Component Architecture (CCA) [21] approach and infrastructure for their effective utilization in accelerator modelling frameworks; work is in collaboration with TASCS [22], TOPS, and the Performance Engineering Research Institute (PERI).
- Development of high-performance parallel data management and analysis tools for beam dynamics modelling, to provide common parallel particle data representation and utilities necessary for analysis of massive data sets; in collaboration with the Visualization and Analytics Center for Enabling Technologies (VACET) [23].
- Implementation of effective load balancing for particle-field simulations, to improve performance of rf gun simulations and PIC applications in general. This activity depends on collaborating with ITAPS and CSCAPES.

3. Applications

The applications of the new capabilities developed under ComPASS aim to tackle the most computationally challenging problems of near-, medium-, and long-term priorities of HEP, NP, and BES, with the objectives of assisting design and cost optimization and helping improve machine performance. As we discussed in Section 1, the HEP priorities include support for the Fermilab Tevatron and CERN LHC programs, continuation of R&D for a lepton collider (such as the ILC, with exact specifications depending on the LHC results), and support of the high-intensity frontier program at Fermilab (Project-X). The ONP future program focuses on the design of an electron-ion collider to explore the quantum-chromodynamics frontier, and a rare isotope accelerator, to shed light to the laws governing the creation of the elements. The future plans for a large BES facility focus on LCLS, the fourth-generation light source at SLAC. Using these priorities as guidelines for the ComPASS application development program, our activities focus on the following problems: large-scale electromagnetic modeling of an ILC-like rf unit, with realistic cavity shapes and misalignments; assessment of the impact of wakefields on beam dynamics; multiphysics, multibunch modeling of ILC Damping Ring beam dynamics; and Project-X Accumulator and Main Injector rings. We also focus on design optimization of accelerator components with complicated geometries, such as the hybrid rare isotope accelerator rfQ and the ILC crab cavity, which includes couplers with very fine features. For the LHC and LHC upgrade R&D projects (LARP) we focus on beam-beam and electron-cloud simulations to help understand and optimize machine performance. For the Tevatron we focus on multi-bunch beam-beam and impedance effects using exact geometry to help understand the antiproton current limitations. For the RHIC II proposal, the e-RHIC concept design, the CEBAF upgrade proposal and the ELIC concept design, we focus on three areas: (1) electromagnetic simulation of superconducting rf cavities, with and without self-consistent beam treatment, (2) multiphysics beam dynamics simulations with emphasis on nonlinearities, beam-beam effects, and intrabeam scattering, and (3) electron cooling physics, aiming to quantitatively understand the dynamical friction force on ions moving through electron distributions in the presence of strong external fields. In the area of accelerator based x-ray light sources ComPASS tools are applied to help understand and predict limits on beam brightness, coherent and incoherent undulator radiation, emittance preservation, and microbunching [10, 12]. In addition, ComPASS is assisting the development of advanced accelerator concepts [11]. These technologies have already demonstrated gradients and focusing forces more than 1000 times greater than conventional technology. Under SciDAC-2, we aim to provide real-time or near-real-time feedback between simulation and advanced accelerator experiments.

3.1. ComPASS application example

In the past few years, the Fermilab Tevatron Run II collider program has delivered unprecedented levels of luminosity (see figure 5) to the collider detectors, producing a plethora of interesting new results and closing in on the discovery of the Higgs boson, the particle that in the Standard Model of particle physics is conjectured to be responsible for the creation of mass. This great performance was achieved as a result of the implementation of a three-part upgrade strategy, which focused on increasing the antiproton production rate, providing a third stage of antiproton cooling (concentrating the beam) with the Recycler storage ring, and increasing the transfer efficiency of antiprotons to the Tevatron (a schematic of the Fermilab accelerator complex is shown in figure 5)

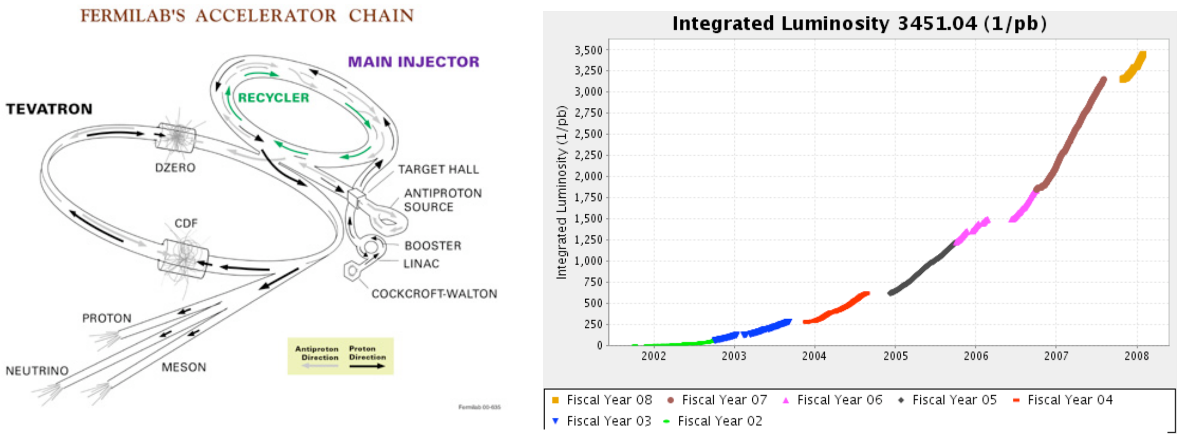

Figure 5. Schematic of the Fermilab accelerator complex (left); Tevatron integrated luminosity versus fiscal year (right).

There were five main areas of improvement:

- *Antiproton production—* antiproton creation and collection rates were increased, decreasing the time it takes to stack them in Fermilab's Accumulator ring. Furthermore, the rate at which those antiprotons are transferred out of the Accumulator was increased. Storing fewer antiprotons in the Accumulator increased efficiency.
- *Slip-stacking protons—* implemented slip-stacking, which effectively doubled the number of protons that the Main Injector ring delivers to the antiproton-producing target. Protons travel

around the Main Injector ring in small bunches. Slip-stacking allows extra bunches of protons to be slipped in beside bunches already circulating the Main Injector.

- *Recycler e-cooling* — used the Recycler ring to "cool" antiproton beams using electron cooling thus creating denser antiproton bunches. Fermilab was the first lab to use electron cooling at high energy.
- *Tevatron beam position monitors* — upgraded the electronics and software for the 240 beam position monitors (BPMs) in the Tevatron, which help prevent the beam drifting too close to a wall and causing losses.
- *Controlling collisions* — controlled premature ("parasitic" or "long range") collisions in the Tevatron waste antiprotons and reduced luminosity at the detectors (see figure 6). Electrostatic separators create an electric field that pulls the protons and antiprotons in opposite directions toward the outside of the beam pipe as they orbit. When Run II began, parasitic collisions claimed 30 to 35 percent of the antiprotons in the beams. With new separators, losses to parasitic collisions have fallen to less than 3 percent.

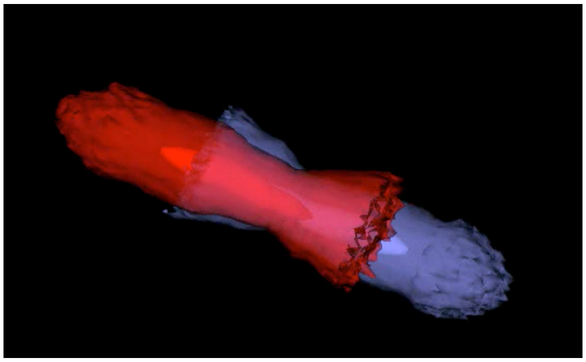

Figure 6. Beam-beam effects for a proton-antiproton head on collision. The bunch charge is 400 times larger than the charge currently used at the Tevatron, to maximize the effect.

The ComPASS code BeamBeam3D was used to perform multi-bunch (thirty six proton on thirty six antiproton bunches) Tevatron simulations in an attempt to explain emittance growth patterns in the presence of kicker misfiring. The 4D, transverse phase space,

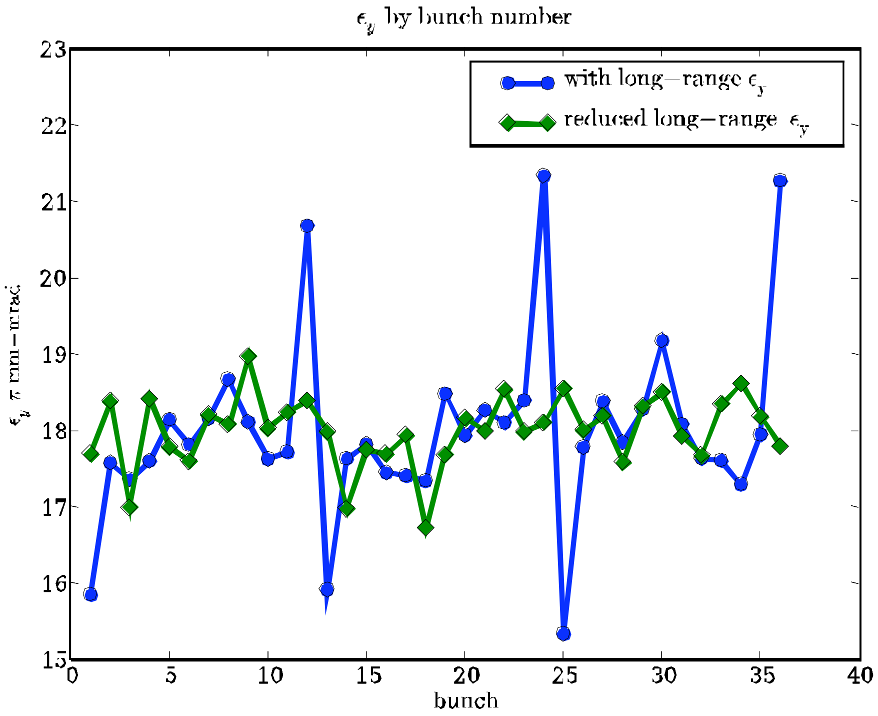

Figure 7. The simulated transverse phase space emittance of the thirty-six proton bunches for the full effect (blue line) and with reduced long-range effects (green line), versus bunch number.

emittance growth of the thirty-six proton bunches is shown in figure 7 as the blue line. This simulation run includes beam-beam interactions at the CDF and D0 detector collision points and one long-range interaction point upstream and downstream of each (these are the most significant points), as well as impedance effects. Beam-beam effects are caused by the two beams interacting with each other through their charge (see figure 6 for an illustration of the effect). Impedance effects are caused by the electromagnetic wake generated by preceding beam bunches interacting with the accelerator chamber. The Tevatron lattice in the simulation was built from analysis of experimental measurements of lattice functions. The three-fold symmetry of the Tevatron filling pattern is evident as is the different behavior of the head bunch of each train: bunches 1, 13, and 25. The first bunch of the train suffers only one parasitic collision around the location of the head-on collision point because there is no preceding bunch from the opposing beam. When the separation of the two beams is artificially increased in the simulation, we obtain the green curve for emittance (Figure 7), which shows no bunch dependence. Figure 8 shows the measured proton intensity loss rate from a Tevatron store [24]. The losses vary significantly along a bunch train, in a systematic fashion that follows the same pattern we see in the simulation with the realistic long-range effects: the losses are lower for bunches at the start of each train and larger near the end of each train. Since beam emittance is indeed a "figure of merit," where a lower value denotes a higher-quality beam, the simulation is describing very well the loss pattern.

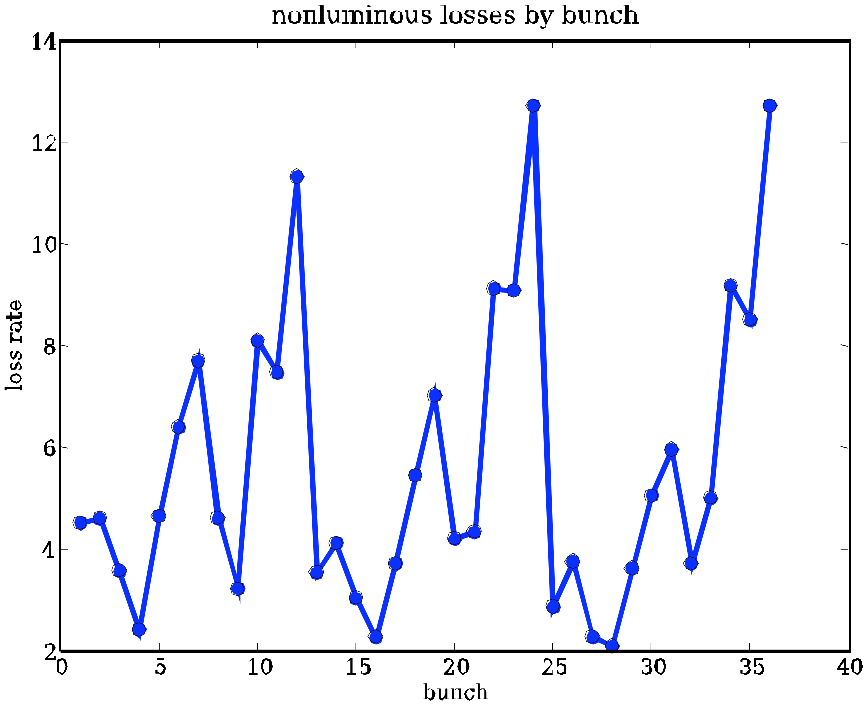

Figure 8. The measured loss rate of the thirty-six proton bunches from a Tevaton store versus bunch number.

3.2. *Future Work with ComPASS*

It is clear that although the simulations are impressive, the contribution of the ComPASS studies to the Tevatron improvements is a small part of the overall effort. On the other hand, four out of five of the necessary actions for the improved performance could have benefited from studies or designs using ComPASS code capabilities that exist today. The ComPASS vision focuses on using ComPASS codes in a unified simulation environment when a performance improvement problem, such as the Tevatron in the early days of Run II, needs to be tackled. In 2003, AST codes were under development for some of the studies necessary for the Tevatron improvement. Today, the ComPASS code suite is capable of addressing them successfully, and under the ComPASS modelling paradigm, our objective is to be able to perform these studies in the same integrated simulation environment.

4. Summary

The SciDAC Community Petascale Project for Accelerator Science and Simulation (ComPASS) is in the first year of executing its plan to develop the next-generation HPC accelerator modeling tools. ComPASS aims to develop an integrated simulation environment that will utilize existing and new accelerator physics modules with petascale capabilities, by employing modern computing and solver technologies. The ComPASS vision is to deliver to accelerator scientists a virtual ccelerator and virtual prototyping modeling environment, with the necessary multiphysics, multiscale capabilities. The plan for this development includes delivering accelerator modeling applications appropriate for each stage of the ComPASS software evolution. Such applications are already being used to address challenging problems in accelerator design and optimization [10, 11, 12].

The ComPASS organization for software development and applications accounts for the natural domain areas (beam dynamics, electromagnetics, and advanced acceleration), and all areas depend on the enabling technologies activities, such as solvers and component technology, to deliver the desired performance and integrated simulation environment.

The ComPASS applications focus on computationally challenging problems important for design or performance optimization to all major HEP, NP, and BES accelerator facilities. With the cost and complexity of particle accelerators rising, the use of computation to optimize their designs and find improved operating regimes becomes essential, potentially leading to significant cost savings with modest investment.

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References

[1] Abraham S, 2003 Spencer Abraham announces Department of Energy 20-year science facility plan, text available at http://www.er.doe.gov/Sub/Newsroom/News_Releases/DOE-SC/2003/Energy%2020-Year%20Science20Facility%20Plan.htm

[2] NRC Committee on Elementary Particle Physics in the 21st Century 2006 Revealing the hidden nature of space and time: charting the course for elementary particle physics (The National Academies Press)

[3] US Particle Physics: Scientific Opportunities A Strategic Plan for the Next Ten Years, http://www.er.doe.gov/hep/HEPAP/reports/P5_Report%2006022008.pdf .

[4] Deshpande A, Milner R, Venugopalan R and Vogelsang W 2000 *Ann. Rev. of Nuclear and Particle Science* **55:**0506148

[5] e-RHIC website, http://www.bnl.gov/cad/eRHIC/

[6] ELIC website, http://casa.jlab.org/research/elic/elic.shtml

[7] Burr F H 2007 HST.187 Course (Massachusetts General Hospital, Harvard Medical School, Proton Therapy Center)

[8] Ko K, *et al*. 2005 Impact of SciDAC on accelerator projects across the Office of Science through electromagnetic modeling *Proc. SciDAC Conf.* (San Francisco, CA); see also Ryne R 2006 J. *Phys.: Conf. Ser.* **46:**171; Spentzouris P 2006 Accelerator modeling under SciDAC: meeting the challenges of next-generation accelerator design, analysis, and optimization (9th Intern. Comp. Accel. Physics Conf.) http://bel.gsi.de/icap2006/PAPERS/THMPMP03.PDF; and Qiang J,Lidia S, Ryne R and Limborg-Deprey C 2006 *Phys. Rev. ST/AB* **9:**044204 (2006)

[9] Blumenfeld I, *et al*. 2008 Energy doubling of 42 GeV electrons in a metre scale plasma wakefield accelerator *Nature* (to appear); see also Geddess C G R, *et al*. 2004 *Nature* **431:**538 and Mangles S, *et al*. 2004 *Nature* **431:**535

~~[11]~~[10] Ng C 2008 Design and optimization of large accelerator systems through high-fidelity electromagnetic simulations *Proc. SciDAC 2008*

[11] Geddes C 2008 Computational studies and optimization of wakefield accelerators *Proc. SciDAC 2008*

[12] Qiang J 2008 SciDAC advances in beam dynamics simulation: From light sources to colliders *Proc. SciDAC 2008*

[13] Amundson J, *et al*. 2006 Synergia: An accelerator modeling tool with 3-D space charge *J. Comp. Phys.* **211:**229–248; see also Amundson J, *et al*. 2008 Multi-Scale, Multi-Physics Beam Dynamics Framework Design and Applications *Proc. SciDAC 2008*

[14] Ryne R 2006 MaryLie/IMPACT: A Parallel Beam Dynamics Code with Space Charge, http://scidac.nersc.gov/accelerator/marylielayer.html

[15] Keyes D 2007 Towards Optimal Petascale Simulations (TOPS) http://www.scidac.gov/math/TOPS.html

[16] Diachin L 2007 Interoperable Technologies for Advanced Petascale Simulations (ITAPS) www.itaps-scidac.org

[17] Pothen A 2007 Combinatorial Scientific Computing and Petascale Simulations (CSCAPES) http://www.scidac.gov/math/CSCAPES.html

[18] Ma K-L 2007 Institute for Ultrascale Visualization http://www.scidac.gov/viz/ultraviz.html

[19] Lucas R 2007 Performance Engineering Research Institute http://www.peri-scidac.org

[20] Colella P 2007 Applied Partial Differential Equations Center (APDEC) http://www.scidac.gov/math/APDEC.html

[21] Bernholdt D, *et al.* 2006 A Component Architecture for High-Performance Scientific Computing Int J High Performance Computing Applications 20 163–202

[22] Bernholdt 2007 Center for Technology for Advanced Scientific Component Software (TASCS) http://www.scidac.gov/compsci/TASCS.html

[23] Bethel E 2007 Visualization and Analytics Center for Enabling Technologies (VACET) www.vacet.org

[24] Shiltsev V, *et al.* 2005 *Phys. Rev. ST Accel. Beams* **8:**101001