Extraordinary Tools for Extraordinary Science: The Impact of SciDAC on Accelerator Science & Technology

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Abstract. Particle accelerators are among the most complex and versatile instruments of scientific exploration. They have enabled remarkable scientific discoveries and important technological advances that span all programs within the DOE Office of Science (DOE/SC). The importance of accelerators to the DOE/SC mission is evident from an examination of the DOE document, "Facilities for the Future of Science: A Twenty-Year Outlook." Of the 28 facilities listed, 13 involve accelerators. Thanks to SciDAC, a powerful suite of parallel simulation tools has been developed that represent a paradigm shift in computational accelerator science. Simulations that used to take weeks or more now take hours, and simulations that were once thought impossible are now performed routinely. These codes have been applied to many important projects of DOE/SC including existing facilities (the Tevatron complex, the Relativistic Heavy Ion Collider), facilities under construction (the Large Hadron Collider, the Spallation Neutron Source, the Linac Coherent Light Source), and to future facilities (the International Linear Collider, the Rare Isotope Accelerator). The new codes have also been used to explore innovative approaches to charged particle acceleration. These approaches, based on the extremely intense fields that can be present in lasers and plasmas, may one day provide a path to the outermost reaches of the energy frontier. Furthermore, they could lead to compact, high-gradient accelerators that would have huge consequences for US science and technology, industry, and medicine. In this talk I will describe the new accelerator modeling capabilities developed under SciDAC, the essential role of multi-disciplinary collaboration with applied mathematicians, computer scientists, and other IT experts in developing these capabilities, and provide examples of how the codes have been used to support DOE/SC accelerator projects.

The following text is modelled on the presentation of Dr. Robert Ryne at the SciDAC 2006 conference.

1. Accelerators and the US Department of Energy

SciDAC has had a major impact on the field of accelerator science and technology. But before I elaborate on this, let me first describe why you in the audience and all American taxpayers (who foot the bill), should care about accelerators. As I will illustrate, accelerators have an immense impact on the nation’s science and technology base, and on the quality of people’s lives.

These SciDAC conferences are not only progress reports on SciDAC, they are also to some degree a celebration of computational science. In this spirit, let me take a few minutes to present what is essentially a celebration of accelerator science, and the role of the US Department of Energy in the development of accelerator technology for the nation.

One may look to the late-1920's through early-1930's as the start of the era of particle accelerators [1]. Ernest Lawrence's first cyclotron, with a diameter of 4.5 inches, accelerated hydrogen ions up to 80,000 eV. By comparison, the highest energy accelerator of the present era -- the Large Hadron Collider (LHC) at CERN set to come on line in 2008 – has a diameter of 8.3 km and will accelerate proton beams to an energy of 7 trillion eV. See Figure 1. Compared with Lawrence's first cyclotron, this corresponds to an energy increase by a factor of nearly 90 million!

Figure 1. Ernest O. Lawrence (left) built the first cyclotron (middle) in 1931. It had a diameter of 4.5" and accelerated hydrogen ions to 80 keV. The largest and highest energy accelerator of the present era, the Large Hadron Collider at CERN (right), has a diameter of 8.3 km and will accelerate counter-rating beams of protons to 7 TeV each when it comes on line in 2008.

Along with advances in particle accelerators, the advances in detectors have been equally impressive: early bubble chambers, invented by Donald Glaser, have given way to massive detectors several stories high, like the ATLAS detector at LHC (Figure 2). New particles have been observed in accelerators at the energy frontier, like the antiproton in 1955 and the W boson in 1983 (Figure 3).

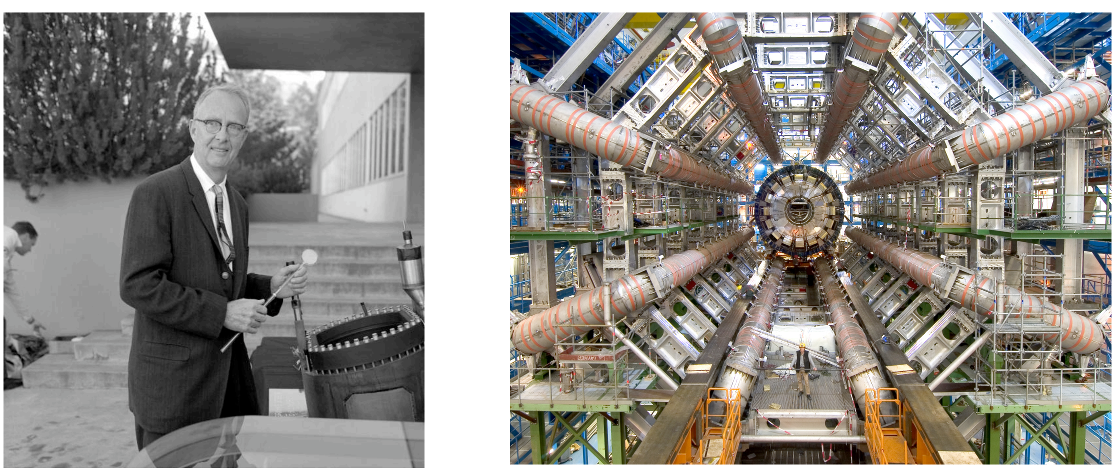

Figure 2. Left: Louis Alvarez with an early bubble chamber. Right: The ATLAS detector for the Large Hadron Collider at CERN; the scale of ATLAS is evident when compared with the person standing in the lower center of the picture.

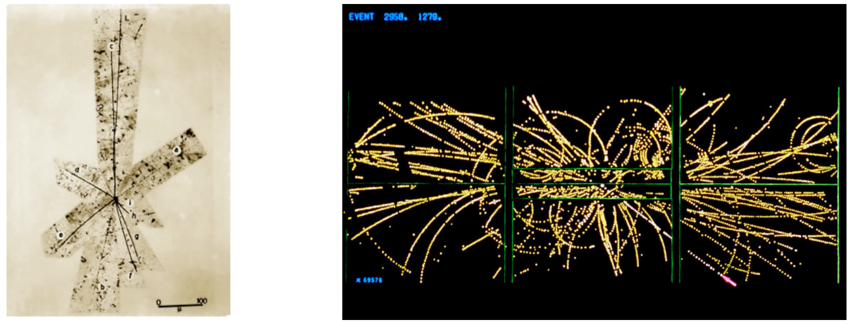

Figure 3. Left: Discovery of the antiproton in 1955 at the Berkeley Bevatron. Right: Discovery of the W particle in 1983 at CERN.

In addition to the spectacular advances in particle accelerators and detectors during the last half-century, *that which is detected and discovered* at accelerators has also changed. It is not widely appreciated outside the scientific community that, along with advances in particle physics, modern accelerators are also crucial to advances in the materials science, chemistry, the biosciences, and other fields. So, not only are accelerators responsible for unraveling the fundamental physics, forces, and particles of nature, they are also responsible for a myriad of advances and discoveries like those shown in Figure 4. These images, produced at the nation's light sources and spallation neutron sources, cover areas as wide ranging as determining the structure of ribosomes, observation of a new form of water in carbon nanotubes, determining the structure of an E. Coli membrane protein, determining protein structures associated with infections in cystic fibrosis patients, and drug design.

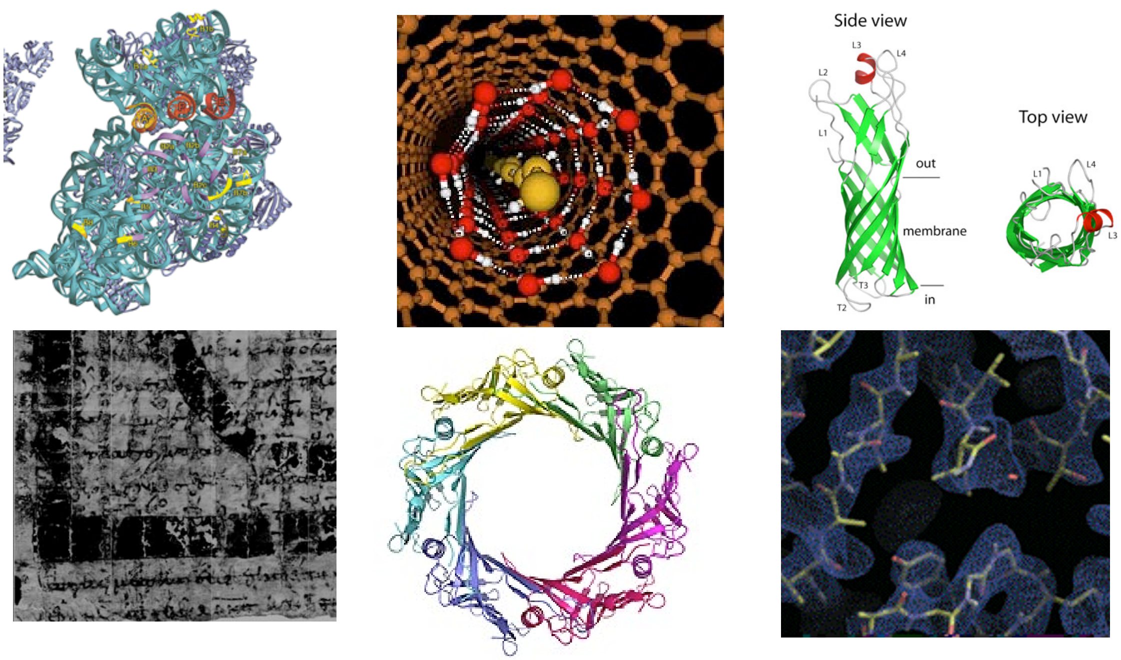

Figure 4. Originally developed for research in elementary particle physics, particle accelerators have become essential tools for basic and applied research in the biosciences, materials science, chemistry, environmental science, and other fields. This figure shows 6 examples: (1) High resolution imaging and structure determination of a ribosome complex (upper left), Advanced Light Source, LBNL. (2) Discovery of a new form of water – nanotube water (upper middle), Intense Pulsed Neutron Source, ANL. (3) Structure determination of an E. Coli membrane protein (upper right), National Synchrotron Light Source, BNL. (4) Medieval ink revealed in an X-ray fluorescence image of the Archimedes palimpsest (lower left), Stanford Synchrotron Radiation Laboratory, SLAC. (5) Structure determination of a protein involved in infection in cystric fibrosis patients (lower middle), Advanced Photon Source, ANL. (6) Hydrogen density distribution of the protein DHFR, involved in the functioning of the antitumor drug methotrexate, determined though protein crystallography (lower right), Los Alamos Neutron Scattering Center, LANL.

As is evident from the above examples, particle accelerators are among the most versatile and important tools of discovery in basic and applied research, and as such they have a huge impact on progress in US science and technology, and consequently on the US economy. In addition, accelerators have applications to national security, energy and environmental security, health and medicine. In regard to national security, accelerators are used for stockpile stewardship, e.g. in applications involving neutron and proton radiography [2]. Applications to homeland security include compact, accelerator-based neutron generators for screening sea-going cargo containers, airport containers, and for screening at border crossings. Active interrogation systems are under development to detect special nuclear materials, explosives, and other contraband [3].

In the fields of energy and environmental applications, accelerator-driven fission energy production systems have been proposed that have the potential to be both safe and environmentally friendly. Such systems would use a subcritical assembly (as opposed to a critical assembly as found in nuclear reactors), and could in principle burn a large fraction of their own byproducts thereby mitigating waste and waste disposal issues. Systems have also been proposed for the accelerator transmutation of waste, in which waste containing very long-lived radioisotopes is transmuted to shorter-lived byproducts that are much easier to store and that need to be stored for a much shorter period of time. On the topic of energy production, the US has made great strides in accelerator-based heavy ion fusion under R&D supported by the DOE Office of Fusion Energy; this research has important applications to high energy density physics research [4].

In the areas of health and medicine, it is estimated that about 10,000 cancer patients are treated every day in the United States with electron beams from linear accelerators [4]. Medical accelerators that accelerate hadrons have also been developed and are especially useful for irradiating deep-seated tumors. Accelerators are also used to produce radioisotopes for medical treatment and diagnosis. Spin-off technologies that originated with particle physics research also have an impact in the health industry and people's lives; for example, scintillator technology is now used in scinti-mammography devices used to detect breast cancer [5].

Figure 5. Left: A proton therapy device used to treat tumors. Right: A scinti-mammography device used to detect breast cancer (see reference [5]).

The importance of accelerators, and the role of the US DOE, is evident from the DOE Office of Science (DOE/SC) document on "Facilities for the Future of Science" [6]: Of the 28 facilities listed as its near, medium, and long-term priorities, *nearly half* (13) are accelerator facilities. DOE/SC (formerly called the DOE Office of Energy Research) has been the main driving force behind the nation's research and development of particle accelerators and associated accelerator technology. During the latter decades of the 20th century, the organization most responsible was the DOE/SC Office of High Energy and Nuclear Physics. Today, the Office of High Energy Physics still plays a leading role, and in addition the Office of Nuclear Physics, the Office of Basic Energy Sciences, and the Office of Fusion Energy all have vigorous accelerator R&D programs.

Currently the US DOE Office of Science operates about a dozen large accelerator facilities. The main facilities of the Office of High Energy Physics (Figure 6) include the Tevatron complex at the Fermi National Accelerator Laboratory (FNAL) and the PEP-II B-factory at the Stanford Linear Accelerator Center (SLAC).

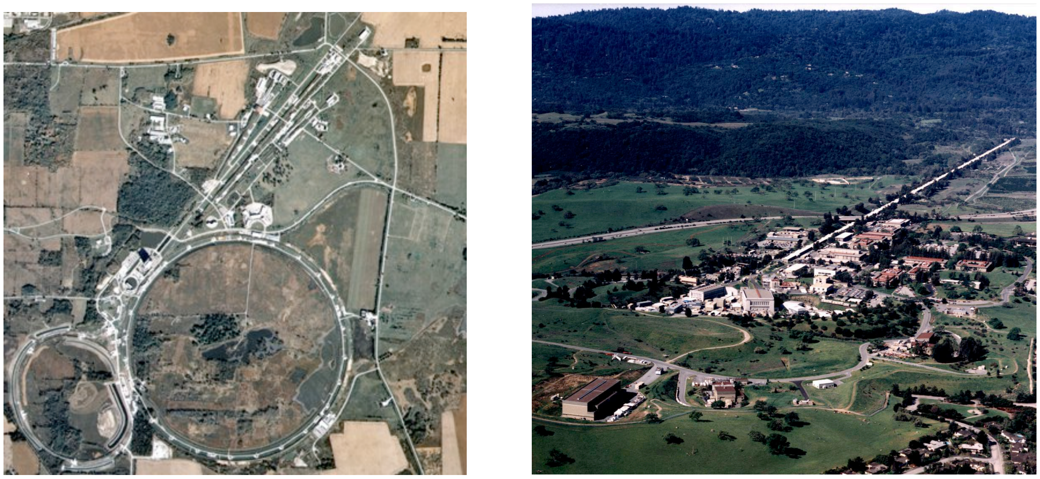

Figure 6. Aerial photos of Fermilab (left) and SLAC (right)

The major accelerator user facilities of the Office of Nuclear Physics (Figure 7) include the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL), the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility, the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory (ANL), the Holifield Radioactive Ion Beam Facility at Oak Ridge National Laboratory (ORNL).

Figure 7. Aerial photos showing RHIC (top left) and TJNAF (top right), ATLAS at ANL (lower left) and HRIBF at ORNL (lower right).

The Office of Basic Energy Sciences operates four light sources: the National Synchrotron Light Source (NSLS) at BNL, the Stanford Synchrotron Radiation Laboratory at SLAC, the Advanced Photon Source at ANL, and the Advanced Light Source at LBNL. It also operates two accelerator-based neutron sources: the Spallation Neutron Source at ORNL, and the Lujan Center at the Los Alamos Neutron Scattering Center (LANSCE) facility. See Figure 8.

Figure 8. Aerial photos the NSLS at BNL (top left), SSRL at SLAC (top right), the APS at ANL (middle left), the ALS at LBNL (middle right), the SNS at ORNL (lower left), and the Lujan Center at LANSCE/LANL (lower right).

While I have just presented a brief tour of the major US accelerator facilities, I also want to point out that there are a number of important major accelerator facilities worldwide. Furthermore, the development of large accelerator facilities is becoming an increasingly international activity, and as such the DOE Office of Science has strong collaborations with many accelerator laboratories worldwide.

It is important to note that, while the US DOE is the largest developer of accelerators and accelerator technology for the nation, other agencies also play a role. The National Science Foundation (NSF) has a very active research program involving accelerators; it operates the Cornell Electron Storage Ring (CESR), the Cornell High-Energy Synchrotron Source (CHESS) at Cornell University, the Bates Linear Accelerator Facility at MIT, the National Superconducting Cyclotron Laboratory at Michigan State University, the Indiana University Cyclotron Facility, and smaller accelerator facilities such as those at Florida State University, the University of Notre Dame, and the State University of New York at Stony Brook. Accelerators are also important to the mission of the National Nuclear Security Administration (NNSA). For example, Lawrence Livermore National Laboratory operates the Flash X-Ray (FXR) facility and Livermore Experimental Test Accelerator-II (ETA-II); Los Alamos National Laboratory operates the Dual-Axis Radiographic Hydrodynamics Test (DARHT) facility as well as other accelerator-based programs at the Los Alamos Neutron Science Center (LANSCE) including a facility for medical radioisotope production and a facility for weapons neutron research.

Given the great importance of accelerators to science and society, and given the central role that the DOE has played in their development, it is no wonder that DOE leadership has chosen to include the field of accelerator science in SciDAC. The SciDAC project, Advanced Computing for 21st Century Accelerator Science and Technology – also known as the Accelerator Science and Technology (AST) project – was initiated in 2001. Its goals are to develop and apply and advanced, comprehensive accelerator simulation environment, able to take full advantage of terascale resources, in order to solve the most important and most challenging problems in 21st century accelerator science. In the next section of this presentation I will describe some of the accomplishments of the AST project.

2. Impact of SciDAC on present and future accelerator facilities

The SciDAC AST project is a large multi-institutional, multi-disciplinary effort. It involves six national laboratories (Lawrence Berkeley National Laboratory, Stanford Linear Accelerator Center, Fermi National Accelerator Laboratory, Brookhaven National Laboratory, Los Alamos National Laboratory, Sandia National Laboratory), five universities (University of California at Los Angeles, University of California at Davis, University of Southern California, Stanford University, University of Maryland), and a small business (Tech-X Corporation). AST is sponsored by the DOE/SC Office of High Energy Physics (HEP) in collaboration with the Office of Advanced Scientific Computing Research (ASCR). Under the project, accelerator scientists are working closely with computer scientists, applied mathematicians, visualization experts, and other ASCR-supported researchers associated with the SciDAC Integrated Software Infrastructure Centers (ISICs) and researchers in ASCR's Scientific Application Partnership program. These collaborations cover many important topics including linear solvers, eigensolvers, Poisson solvers, grid technologies, adaptive mesh refinement, parallel particle-in-cell methods, parallel I/O and data handling, statistical methods for code calibration and forecasting, parallel visualization, and performance optimization.

The AST project involves 3 main thrust areas for accelerator modeling: Beam Dynamics (BD), Advanced Accelerators (AA), and Electromagnetics (EM). In each of these areas a suite of parallel 3D simulation codes has been developed and applied to a number of important problems in particle accelerator design and accelerator science. Since EM accomplishments under the AST project have been described in a separate invited talk [7], I will focus in this presentation on the BD and AA areas.

The BD and AA codes developed under the AST project are:

- BeamBeam3D: A 3D parallel PIC code for modeling beam-beam effects in colliders [8]

- IMPACT: A 3D parallel PIC code used primarily for modeling beam dynamics in electron and ion linacs [9]
- MaryLie/IMPACT: A 3D parallel PIC code combining high order magnetic optics with space-charge [10]
- OSIRIS: A fully electromagnetic 3D parallel PIC code, primarily for plasma accelerator simulation [11]
- QuickPIC: A 3D parallel PIC code for modeling plasma accelerators in the quasi-static limit and electron clouds [12]
- Synergia: A 3D parallel beam dynamics simulation framework [13]
- UPIC: A framework for parallel PIC simulation [14]
- VORPAL: A parallel framework for modeling electromagnetic fields, fluids, particles, and their interactions; here the electromagnetic 3D PIC capabilities are used for plasma accelerator modeling and time-domain electromagnetic structure modeling [15]

The impact of these codes to the accelerator community is evident both from a list of publications involving AST codes and in a list of the projects that are making use of AST codes. In regard to publications, the BD and AA codes have been used in more than 50 refereed publications since the project's inception. This includes three articles in Nature (in the AA area), 16 Physical Review Letters, and numerous articles in the Journal of Computational Physics, Computer Physics Communications, Nuclear Instruments and Methods in Physics Research A, and Physical Review Special Topics – Accelerators and Beams.

The list of facilities that are using AST codes includes nearly every major present and proposed accelerator project in the USA, several international projects, as well as several small experiments and design efforts. The list of facilities and projects includes:

- Tevatron
- LHC
- NLC
- ILC
- PEP-II
- FNAL booster
- FNAL Main Injector
- L'OASIS LWFA experiments
- SLAC PWFA experiments
- Plasma afterburner design
- RHIC
- RIA
- SNS
- LCLS
- Photoinjector design
- Advanced streak camera design
- CERN SPS
- JPARC commissioning
- FERMI design
- International code benchmarking via CERN PS experiments

It is worth pointing out that, while the accelerators of the DOE/SC program offices have their unique needs, there is also significant overlap, and this has contributed to the wide impact of the AST project as evidenced by the above list of projects. For example, the BeamBeam3D code, originally developed for modeling HEP colliders, is being used to model NP accelerators like RHIC. The IMPACT code, originally developed for modeling beam dynamics in ion linacs, has been enhanced and is being applied to model HEP and BES photoinjectors [16]. Another example of this cross-cutting nature is the simulation of electron effects: The codes WARP and POSINST, developed separately for applications in the HEP and FES programs, respectively, have been merged into a state-of-the-art capability for modeling electron-cloud effects [17] that is included in a SciDAC2 proposal. The impact of AST has also been enhanced in unexpected ways; for example, the QuickPIC code, originally developed for modeling plasma accelerators, has been enhanced and used for electron-cloud studies [18].

The widespread usage of AST codes in the accelerator community is a testament to the fact that SciDAC and the AST project have succeeded in developing and distributing a new generation of accelerator modeling tools that have been adopted by the accelerator community. This has led to a number of important “firsts” in computational accelerator simulation. In thte subject matter covered in this presentation (beam dynamics and advanced accelerator concepts) these include:

- First Million particle, million turn, strong-strong colliding beam simulation for LHC (BeamBeam3D; J. Qiang) [19]
- First multi-bunch, multi-turn injection simulation from linac-to-booster w/ self-consistent 3D space charge (Synergia; J. Amundson and P. Spentzouris) [13]
- First 100M simulation of a linac for an x-ray light source w/ self-consistent 3D space charge (IMPACT-Z; I. Pogorelov, J. Qiang)
- First self-consistent electromagnetic simulation of an intense beam in an ILC 'crab' cavity (VORPAL; J.R. Cary, C. Nieter & VORPAL team) [20].
- First 3D simulation of a 1TeV Afterburner stage (QuickPIC; C.K.Huang et al.) [21].
- First 3D simulation of a GeV LWFA stage (OSIRIS; F.S.Tsung, W.Lu, M. Tzoufras et al. [22]

Details of the AST codes and their applications can be found in the accelerator-related talks and posters presented at this meeting. Selected examples, covering several applications to the HEP, NP, and BES programs of DOE, are shown below.

2.1. Damping Ring Design for the International Linear Collider

SciDAC beam dynamics codes have been used to support several important projects of the DOE Office of High Energy Physics (HEP) including the Tevatron, the PEP-II B-factory, the Fermilab Booster, the Large Hadron Collider, and the International Linear Collider (ILC). The ILC, in particular, is currently the highest priority future accelerator project of the DOE/HEP and the international high energy physics community. As presently envisioned, the accelerator complex would be comprised two opposing 20 km linacs, along with a number of other accelerator subsystems: an electron source, pre-linac, energy compressor, spin rotator, bunch compressor, main linac, positron production undulator, beam delivery system, interaction region, and extraction lines. The initial application of SciDAC AST codes to the ILC involved modeling the damping rings. These represent a significant technical challenge and have been the subject of a concerted design effort. Under the AST project, damping ring simulations were performing using the MaryLie/IMPACT code [23]. These simulations were performed to study the effect of space charge on the beam dynamics in the damping rings, to assure that, though small, the integrated effect of the space charge would not spoil the beam emittance. The simulations showed that the predicted emittance was strongly dependent on the space-charge model, and in particular that it was insufficient to use a linear space model. In the next two years, it is expected that large scale simulations using SciDAC codes will be performed of nearly every accelerator system in the accelerator complex to verify and optimize the designs and to support the design effort.

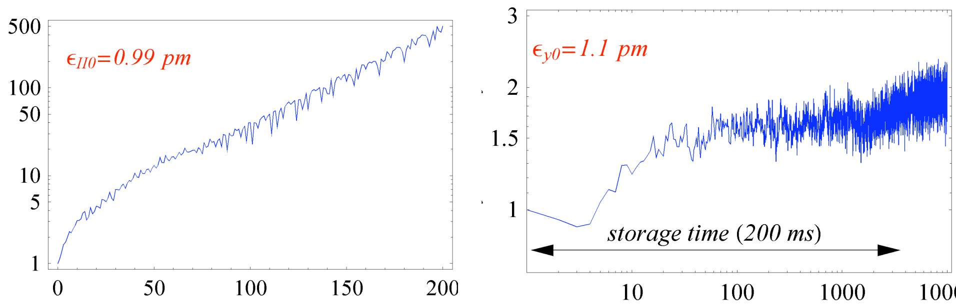

Figure 9. MaryLie/IMPACT simulation results of an early ILC damping ring (DR) design. Studies of space-charge induced emittance exhibited an exponential instability (left) that was found to be unphysical and due to the use of a simplified (linear) space charge model. Simulations using a realistic (nonlinear) space charge model showed that the emittance growth was not unstable and that it saturated at an acceptable level. (M. Venturini, LBNL)

2.2. Modeling space-charge effects in the Fermilab booster

The Tevatron complex at Fermilab is currently the highest energy collider operating in the world, and will be so until the turn-on of the LHC in 2008. SciDAC codes have been, and will continue to be used to maximize its performance until it is shut down later in the decade. SciDAC simulations of the Tevatron itself under AST included a comprehensive study of beam lifetime and luminosity as a function of machine operating parameters. Extensive studies have also been performed of the Fermilab booster, a key accelerator subsystem in the accelerator complex. Beam losses in the booster currently represent the main bottleneck to operation at high intensity that limits the number of protons that can be provided to the Tevatron and to the Fermilab neutrino program. Under SciDAC, we have studied the performance of the Fermilab booster using the Synergia framework. Developed under the AST project, Synergia is a parallel, multi-physics, beam dynamics simulation framework based on modern programming design [13]. Synergia combines multiple functionality including the space charge capabilities of IMPACT, the high order optics capabilities of MXYZPLT, a software module for inclusion of wakefield effects, and other physics modules, all with a powerful user interface and standard problem description.

Accurate simulation of the booster including 3D space charge effects was not possible prior to SciDAC. Under the AST project we developed and applied Synergia to help understand space charge effects and their impact on intensity limitations in the booster. The beam dynamics involves collective, nonlinear processes, and as a result the beam forms a low density halo that leads to particle loss and radioactivation. Using Synergia, we performed the first-ever simulation of the process of microbunch capture, debunching, and acceleration, all using a 3D space-charge model [13]. The simulations have helped provide guidance to accelerator operators to reduce losses and maximize the intensity of the beam in the booster.

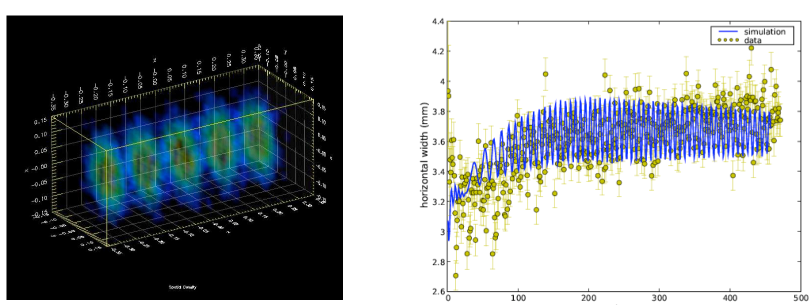

Figure 10. Left: Synergia simulation showing a train of 5 microbunches from the Fermilab linac debunching after being injected into the Fermilab Booster. Right: beam size as a function of turn number in the Fermilab booster, showing a comparison of experimental results and the results of large scale simulations using Synergia. (P. Spentzouris, J. Amundson, FNAL).

2.3. Simulation of beam-beam effects in colliders

Beam-beam modeling is crucial to understanding the beam behavior in high intensity colliders and to develop compensation mechanisms to control beam instabilities and emittance blowup. Beam-beam modeling will also be important for understanding and controlling the behavior of collisions in the ILC, where operation in the high-disruption regime means that there can be significant luminosity loss, even from small bunch distortions and other effects. The ability to perform large strong-strong beam-beam simulations is extremely challenging because of the huge amount of particle movement between beam-beam collisions. Under SciDAC, we developed the BeamBeam3D code, a comprehensive 3D parallel PIC code for studying beam-beam effects under a wide range of conditions [24]. It is interesting to note that early on the in the AST project we reached a milestone by performing the first ever million-particle, million-turn "strong-strong" (i.e. self-consistent) beam-beam simulation. As we near the end of SciDAC1, we have far exceeded our early accomplishments in beam-beam modeling. Working with the PERC ISIC, we have began performing 100M particle simulations on 1024 processors on the Seaborg cluster at NERSC [25]. Besides being able to perform large simulations, we have now added several important new physics capabilities to BeamBeam3D, including multi-bunch, multi-interaction point, and multi-slice modeling. The BeamBeam3D code has been applied to all the colliders of the HEP and NP programs, the Tevatron, PEP-II, and RHIC, as well as the soon-to-be-operating LHC. In the future, BeamBeam3D will be used to study beam-beam effects in the ILC. Figure 11 shows BeamBeam3D simulations results for RHIC and results of a comparison with experimental results at the VEPP-2M collider.

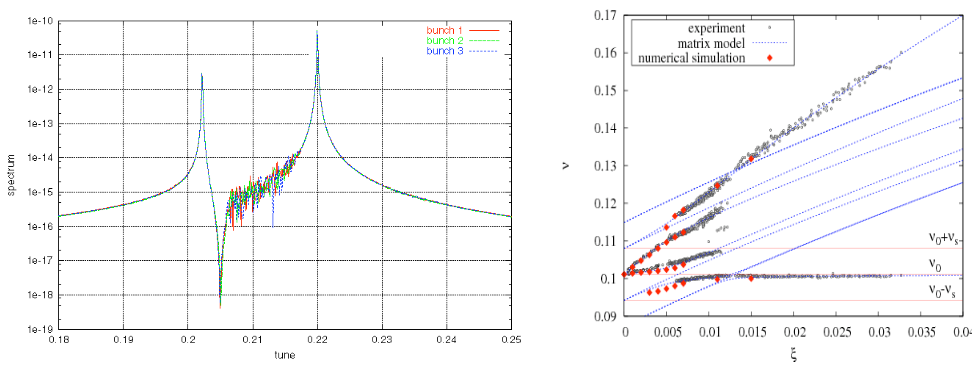

Figure 11. Left: Power spectrum from a strong-strong, multi-bunch BeamBeam3D simulation of colliding beams in RHIC (J. Qiang, LBNL, and W. Fischer, BNL). Right: Comparison of BeamBeam3D simulations with experiment at the VEPP-2M collider. There is poor agreement when using a matrix model, and good agreement when using the self-consistent BeamBeam3D code (J. Amundson and P. Spentzouris, FNAL).

2.4. Simulation of high brightness electron beams and light sources

High brightness electron beams are important to a number of projects across DOE/SC including HEP (ILC), NP (CEBAF and proposed electron-ion colliders), and the light sources of the BES program. The IMPACT suite of codes developed under the AST project has been applied to several photoinjector projects nationwide including photoinjectors at ANL, BNL, Cornell, FNAL/NIU, JLAB, LBNL, and SLAC/LCLS. Our predictive capability has benefited from our ability to run large, 3D simulations. As seen in Figure 12, left, accurate prediction of beam emittance, for example, requires "multi-slice" modelling. In another example, we have recently performed the first-ever 100M particle simulation of a linac for a light source to accurately study the microwave instability. But, beyond the ability to perform simulations with large numbers of particles and grid points, the development multi-physics modelling capabilities, and the development of new computational algorithms, has also been crucial. For example, Coulomb collisions are important in certain situations, such as emission from a nano-needle cathode (Figure 12, right). In some situations, it is essential to be able to model beams with large energy spread; a technique for doing this was developed and implemented in IMPACT under SciDAC. And, in certain situations, the beams have a very large geometrical aspect ratio. Under the AST project we developed include a new class of 3D parallel Poisson solvers specially designed to efficiently model beams that have high aspect ratios [16].

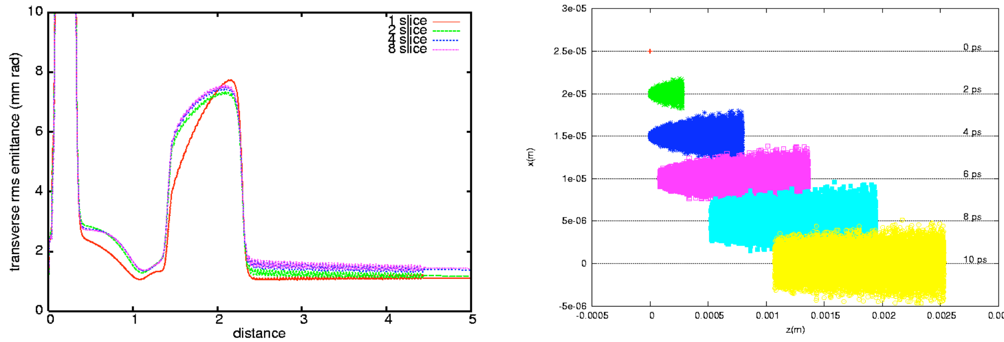

Figure 12. Left: Simulation of the LCLS photoinjector showing the need for “multi-slice” modelling to predict the beam emittance (J. Qiang, LBNL and C. Limborg-Deprey, SLAC) [16]. Right: Simulation of beam formation during emission from a nano-needle tip; the data are shifted downward at 2 ps intervals for clarity in the figure (J. Qiang, LBNL).

2.5. Application of advanced accelerator codes to beam and electromagnetic modeling

Major progress has been made under SciDAC in the area of parallel codes for modeling large, geometrically complex electromagnetic (EM) structures. The EM codes developed under AST have already been described in invited talks and posters at this meeting. I do want to mention, however, an example of how codes developed under the Advanced Accelerator (AA) portion of the AST project have had unexpected application outside their original area. VORPAL was originally developed in part under the AA effort to model plasma-based accelerators. But its general capabilities for modeling intense charged particle beams in EM structures have led the code to be applied to a number of other important projects including ILC (Figure 13). As already mentioned, VORPAL was used for the first self-consistent electromagnetic simulations of an intense beam in an ILC 'crab' cavity. Similarly, the code QuickPIC was originally developed to enable fast simulations of plasma-based accelerators. However, and enhanced version of the code was developed and applied to modeling electron-cloud generation in the LHC, and it will soon be used to model electron-cloud effects in the FNAL Main Injector. In these examples involving VORPAL and QuickPIC, very basic research in advanced accelerator technologies turned out to have direct impact on near- and mid-term projects.

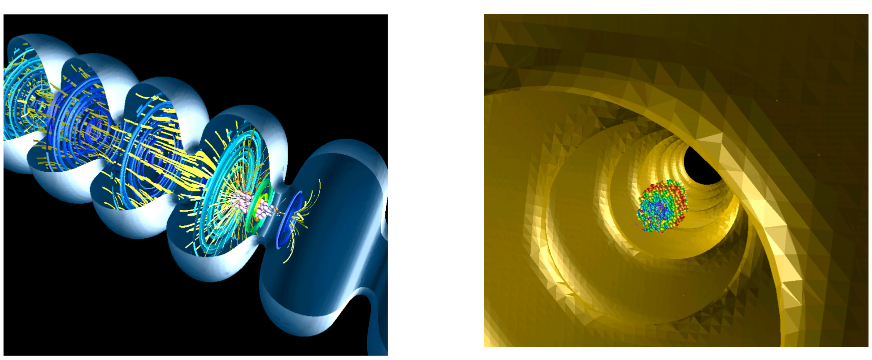

Figure 13. Left: Parallel 3D electromagnetic simulation of a Tesla SRF cavity using VORPAL. The magnetic field lines encircle the axis, while the electric field lines are along the direction of propagation. Right: Cut-cell representation of the Tesla cavities using VORPAL showing a beam propagating through the cavity (J. R. Cary et al., Tech-X).

3. Impact of SciDAC on discovery and developing new methods of particle acceleration

I began this presentation talking about the early development of accelerators in the 1920's and 1930's and commented on how much progress has been made since that time. It is appropriate, at this SciDAC meeting, to compare that progress with the progress made in computing technology.

One can look back to the mid-1940's and to the EDVAC and ENIAC computers to get a sense of how far we have come in 60 years. The ENIAC, for example, was capable of 5000 operations per second. Compared with the most powerful computer today, the IBM blue gene capable of 280 Teraflops on the Linpak benchmark, this corresponds to an increase by a factor of 56 billion. Analogously, Lawrence's first cyclotron accelerated hydrogen ions up to 80,000 eV. Considering that the highest energy accelerator of the present era – the Large Hadron Collider (LHC) at CERN set to come on line in 2007 – accelerates proton beams to an energy of 7 trillion eV, this corresponds to an increase by a factor of nearly 90 million.

This audience is familiar with the well-known Moore's law describing the exponential increase in computing power over a period of time. The analogy in the field of accelerator science is the Livingston plot [26]. Figure 14 shows the plot describing the increase in energy of colliders. Like Moore's law, the exponential increase in accelerator energy has been made possible due to the fact that, as one technology matures, a new technology has been developed that keeps the growth going. Drawing a comparison to developments in microprocessors where the roadmap shows that new technology will be needed by around 2020, in the case of accelerators radio frequency (rf) technology is also expected to reach its apex by around 2020 with the International Linear Collider (ILC), and a new technology (that of the Compact Linear Accelerator, CLIC), is likely soon thereafter. But it appears that, beyond around 2030, innovative new approaches will be needed to get back on the Livingston Curve.

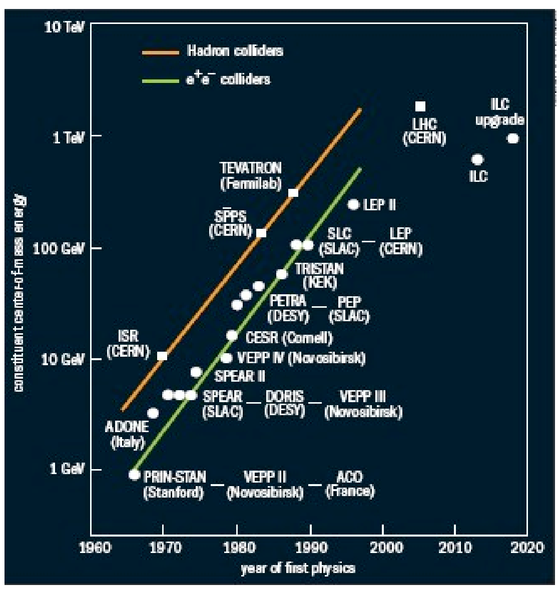

Figure 14. An adaptation of the "Livingston Curve," displaying the center-of-mass energies of the particle constituents in past, present, and proposed high energy accelerators [26,27]. In the case of the hadron machines, energies have been adjusted to account for quark and gluon constituents.

The Advanced Accelerator (AA) thrust area of the SciDAC AST project is devoted to developing and using advanced computational tools to help advance the frontiers of particle accelerator technology. It is hoped that eventually AA technologies will keep us on the Livingston curve and allow us to reach the highest energies possible. Also, AA technologies are expected to have near-term impacts in many areas of science, technology and medicine through the development of compact accelerators that will be smaller, cheaper, and more ubiquitous than present-day technology allows.

The AA thrust area of the AST project has focused on technologies that use plasmas and lasers to reach new regimes of accelerating gradient. The gradient, along with the geometrical layout of an accelerator, determines its size. Obviously, having a high gradient makes it possible to reach a given energy in a smaller space than if one employed a lower gradient. And just as obviously, if we reach a "brick wall" in gradient, i.e. if we cannot continue to develop technologies to reach higher gradients, then the only way to reach the highest energies is to make accelerators larger and larger, which consequently makes them more expensive (and eventually, prohibitively expensive). The gradients in rf accelerators are now typically on the order of a few million volts per meter (MV/m) to around 20 MV/m, and with improvements in rf technology, gradients of around 50 MV/m are expected to be used in future rf accelerators. But, a number of issues, such as rf cavity breakdown, set a limit on the maximum achievable gradient. Going to higher frequencies allows for higher gradients, but also brings in other problems in high energy accelerators (wakefield effects are more challenging, for example). As a result, few people believe that conventional accelerators will be built with gradients higher than 100 MV/m, and even that is optimistic.

Consider, then, that using advanced concepts, gradients in excess of 40000 MeV/m (40 GeV/m) have *already* been measured in laboratory experiments. This is possible because AA technologies replace the metal accelerating cavity with another medium (like the ionized gas that constitutes a plasma) that is not subject to rf breakdown. But, major challenges remain, in particular harnessing these extraordinarily high gradients into useful accelerators. Under the AST project, researchers have been working closely with experimentalists to understand two types of AA concepts, Laser Wakefield Accelerators (LWFAs) and Plasma Wakefield Accelerators (PWFAs).

In wakefield accelerators an intense electromagnetic field is made to exist in a plasma, either by an incident laser beam (in the LWFA concept) or with an incident particle beam (in the PWFA concept). If a beam bunch that is to be accelerated is then made to pass through the plasma at the correct phase with respect to the excitation, it can gain an enormous amount of energy over a very short distance. There are many technological challenges, but two of the most important are (1) to extend the interaction length and (2) to produce a high quality beam, and to preserve it, as it is accelerated in the plasma. Both of these challenges have now begun to yield thanks to advances in experiment, theory, and simulation. In fact, I think it is fair to say that the progress in AA concepts has occurred at a rate much greater than most people imagined was possible during the 1990's when AA research began to be carried out in earnest. In particular, I want to mention some notable breakthroughs in experiment and simulation that have occurred within the last few years.

The first breakthrough was the observation of low energy spread bunches in a LWFA. Prior to this, LWFAs produced beams with such large energy spread that they were not suitable as useful accelerators; some high energy particles were produced, but so were a huge number of low energy particles. Then, in 2004, three groups around the world succeeded in producing beams with low energy spread from a LWFA [28]. The experimental parameters for these experiments were guided by theory and simulation. The results were so impressive that they became the focus of an issue of Nature (Figure 16, left) [28]. All three groups achieved electron beams of slightly over 100 MeV with energy spread of a few percent. Simulations using SciDAC and other codes [22,28] have helped to explain the physics involved in the production of low energy spread beams from LWFAs and pointed the way to higher energies (Figure 16, right).

A second major experimental achievement – breaking the 1 GeV barrier in a LWFA – occurred within the last few months [29]. Given that a conventional rf electron linac, with a gradent of, say, 20 MeV/m, would require 50 m to reach 1 GeV, it is noteworthy that the LWFA-based system takes only 3 cm to do so, allowing it to be sited in the basement of what is essentially an office building with a small experimental area. This was accomplished using a capillary discharge plasma. Work is already underway to reach the next milestone – a 10 GeV electron beam using a LWFA - through increasing the interaction length and/or increasing the laser power.

Figure 16. SciDAC simulations indicated the physics behind production of monoenergetic beams in recent wakefield accelerator experiments, and this is guiding future development. Left: Plasma density, including the wake and trapped particle bunches (bright dots on black, on the center line), from a SciDAC simulation of a channel guided wakefield accelerator experiment [28] using the VORPAL code [15]. Right: Scaling upward in laser energy, 3D simulations using the OSIRIS code have shown formation of low energy spread bunches at energies exceeding a GeV [30].

A third breakthrough involved taking an already high energy electron beam and doubling its energy [31]. This occurred at SLAC, in a series of PWFA experiments that culminated in an experiment known as E167. In these experiments, a cell of order 1 m in length containing lithium gas was self-ionized by an incoming electron bunch. The head of the bunch excites the wake and loses energy, while the tail of the bunch surfs the wake and gains energy. The nominal incident energy of the electron beam was 28.5 GeV. In recent experiments the tail of the beam's energy was doubled. The SciDAC codes OSIRIS and QuickPIC have been used extensively to unravel the nonlinear physics in these experiments. (Figure 17, left, shows results from QuickPIC.) The success of PWFA experiments provides added impetus to the concept a "plasma afterburner" as a possible means to extend the reach of high energy accelerators further into the energy frontier. Recently the SciDAC code QuickPIC was used to design a virtual TeV afterburner, in which the energy of a 500 GeV electron beam was doubled in only 25 meters. The simulations (Figure 17, right) showed that, despite some hosing, the wake structure remained stable, and the resulting TeV beam had a 5% energy spread. It is interesting to note that, prior to SciDAC, such a simulation would have taken roughly 2.5 million processor hours; using the SciDAC code QuickPIC such a run now takes only 5000 processor hours.

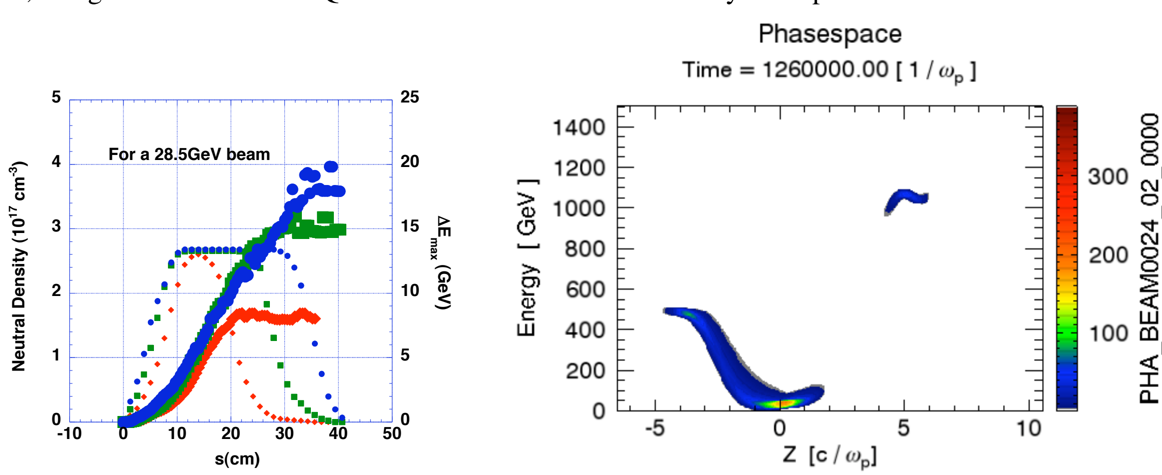

Figure 17. Left: Predicted energy gain in the SLAC E167 experiment using the code QuickPIC (M. Zhou et al.) Right: QuickPIC simulation of a TeV plasma afterburner (C. Huang et al., UCLA).

For all the above mentioned advances in LWFAs and PWFAs, large-scale computing played an important role providing understanding of the incredibly complex phenomena that occur in the plasmas. These physical systems involve simultaneous interactions of beams, plasmas, particle ionization, and radiation, all under extreme conditions. Simulations, including those performed with the SciDAC codes OSIRIS, VORPAL, and QuickPIC, have provided a window to explore how the electromagnetic wake develops, how particles are trapped and accelerated by the wake, how energy is drawn out of the wake (and out of the laser beam in LWFAs), and how it is possible for this to occur in such a way that the resulting beam has low energy spread.

To conclude this section of my talk, let me point out that the progress in advanced accelerator technologies in the past few years has proceeded at a much faster pace than many people had expected. Furthermore, while advanced accelerator R&D aims to address the long-range needs of accelerator-based high energy physics, the successes so far provide strong evidence that these technologies will also have significant near- and mid-term applications. The ability to place compact, inexpensive accelerators in university and high-tech research labs, and in hospitals, will have huge consequences for science, industry, and medicine.

4. Summary and Future Prospects

Particle accelerators are exemplary of the US DOE's "Extraordinary Tools for Extraordinary Science." Particle accelerators and the technologies associated with them have a profound impact on US science and technology, and on US economic competitiveness. They are also highly beneficial to people's lives, not only through the technological advances that they enable, but also through applications related health, the environment, and homeland security. The tremendous advances in accelerator science in the previous 75 years have been made through a combination of theory, experiment, simulation, and above all, innovative ideas. Under SciDAC, simulation has become increasingly important, as more realistic, three-dimensional, multi-physics simulations have become possible.

The SciDAC Accelerator Science and Technology project has led to the development of a new generation of accelerator modeling tools that have been adopted by the accelerator community and applied to a number of important projects of the DOE Office of Science. The development of these codes would not have been possible without the successful collaboration between the accelerator physics community and advanced scientific computing community. The establishment of such collaborations – a key element of the SciDAC paradigm – provides the foundation for seizing the opportunities and meeting the challenges of petascale computing for accelerator science and technology.

Looking to the future, a number of exciting and challenging accelerator projects are on the horizon. In the near term, the LHC is set to come on line in 2008; SciDAC codes will be used to help commission and optimize this machine, allowing it to reach its full potential as quickly as possible to explore the frontiers of high energy physics. SciDAC codes will continue to be used to enhance the operation of existing DOE/SC colliders (the Tevatron, PEP-II, RHIC) during their operational lifetimes. SciDAC codes will also be used to support the operation of the Fermilab complex, including its neutrino program.

In the mid-term, SciDAC codes will play a pivotal role in the design of the ILC. The ILC presents many challenges in beam dynamics modeling and electromagnetic modeling. In beam dynamics, in particular, the challenges are daunting – electron-cloud modeling, design of low emittance transport, simulation and prevention of instabilities, assessment of space charge and radiation effects, modeling collisions in the high disruption regime, and simulations that include beam diagnostics, controls, and feedback systems so as to sustain machine operation at the design luminosity. All these phenomena need to be included in an advanced computational model to reduce cost and risk, to optimize performance, and to help assure success.

While ILC is the top priority for HEP, SciDAC codes will also be ready to be applied to other projects if HEP needs require them, including possible upgraded facilities for neutrino physics, a super B-factory, and an LHC upgrade. In the area of nuclear physics, large-scale simulation is already playing a role in the design of a proposed Rare Isotope Accelerator, and activities have been proposed under SciDAC2 to address this as well as linac-ring colliders and other NP projects. A t the same time, SciDAC is enabling simulation of laser and plasma wakefield experiments to develop these new technologies for use in future accelerators.

In the DOE Basic Energy Sciences program, tremendous opportunities exist in the near- and mid-term. The SNS has just delivered its first neutrons and will soon be fully operational, opening the door to a new era in neutron science. A new era in light source science and *ultrafast* science is also beginning. The Linac Coherent Light Source (LCLS) at SLAC is set to come on line in 2009 and will be the world's first X-ray free electron laser; operating with x-ray pulses whose duration is measured in femtoseconds (a quadrillionth of a second), LCLS will make it possible to view and analyze chemical and biological processes in real time. This and other 4^{th} generation light sources present many challenges, including the production of ultra-high brightness beams in photoinjectors, the maintenance of beam quality, and control of prevention of the microbunching instability in the presence of space charge, wakefields, and coherent synchrotron radiation. To address these issues, researchers are forming collaborations to develop simulation capabilities for large-scale, start-to-end modeling of accelerator-based x-ray light sources.

In closing, I want to say a word about the things that I have not addressed in this talk. First, at this DOE meeting I have of course emphasized the US accelerator infrastructure and the impact of SciDAC to US accelerator science and technology. But accelerator R&D, and the development of large accelerator facilities, is an international activity. There are many important accelerator facilities and important accelerator modeling activities worldwide that I have not described here but deserve to be mentioned in the broader context. Members of the SciDAC AST project have benefited greatly from international collaborations with researchers at CERN, GSI, JPARC, KEK, PSI, RAL, and other laboratories worldwide.

Finally, in this presentation I have emphasized the role of the DOE Office of Science to accelerator science and technology, and I have described the impact of SciDAC to its programs, especially its high energy physics programs. But, as I hope is obvious from this presentation, accelerator science spans all the programs of the Office of Science. Computational accelerator physicists in the HEP, NP, BES, and FES programs are already collaborating; I have no doubt that this will continue in the future, and think it likely that such cross-program collaborations will grow. Also, there is a growing interest in accelerator science in other agencies including NSF and in DOE/NNSA. There is ample opportunity for collaboration among these and other agencies in accelerator science in general, and in computational accelerator science in particular. I think it is now clear that accelerators and the technologies associated with them are so important that a coherent, coordinated effort would be highly beneficial and would best serve science and the nation.

Acknowledgements

The SciDAC Accelerator Science and Technology (AST) project was originally sponsored by the DOE/SC Office of High Energy and Nuclear Physics. Since the reorganization of DOE/SC, AST has been sponsored by the Office of High Energy Physics. The project has been performed in close collaboration with researchers supported by the Office of Advanced Scientific Computing Research (ASCR), through the SciDAC Integrated Software Infrastructure Centers (ISICs) and through the Scientific Application Partnership Program (SAPP). Many people have contributed to the AST project. I want to acknowledge the contributions of my co-PI, Kwok Ko, who also headed the electromagnetic (EM) modeling area of the project. The contributions of Kwok and his EM team are well documented in these proceedings and those of previous SciDAC conferences. In the area of beam dynamics (which I headed under the AST project), I want to acknowledge the contributions of key personnel at several institutions: Ji Qiang, Miguel Furman, Ilya Pogorolov, and Marco Venturini

(LBNL); James Amundson, Panagiotis Spentzouris, and Eric Stern (FNAL); Salman Habib, Filippo Neri, and Peter Walstrom (LANL); Roman Samulyak (BNL); Dan Abell and Doug Dechow (Tech-X); Alex Dragt (U. Maryland). The advanced accelerator effort (AA) of AST was headed by Warren Mori (UCLA). Other key personnel in the AA effort are: F. Tsung (UCLA); Tom Katsouleas (USC); David Bruwhiler and John Cary (Tech-X); Eric Esarey and Cameron Geddes (LBNL). In the area of rf cavity modeling using VORPAL, I want to acknowledge the contributions of C. Nieter, P. Stoltz, and P. Messmer (Tech-X). ISIC and SAPP personnel who made significant contributions include P. Colella, P. McCorquodale, and D. Serafini (APDEC ISIC); Hongzhang Shan, Erich Strohmaier, and Kathy Yelik (PERC ISIC); Viktor Decyk (UCLA), Kwan-Liu Ma (UC Davis), Cristina Siegerist and John Shalf (LBNL). We have also benefited from valuable interactions with international collaborators, including Andreas Adelmann (PSI), Frank Gerigk (CERN), Ingo Hofmann (GSI), and Masanori Ikegami (KEK).

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