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Authors
Ryne, R.
Abell, D.
Adelmann, A.
et al.

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SciDAC Advances and Applications in Computational Beam Dynamics

R. Ryne[4*], D. Abell[7], A. Adelmann[6], J. Amundson[2], C. Bohn[2,5], J. Cary[7], P. Colella[4], D. Dechow[7], V. Decyk[9], A. Dragt[10], R. Gerber[4], S. Habib[3], D. Higdon[3], T. Katsouleas[11], K.-L. Ma[8], P. McCorquodale[4], D. Mihalcea[5], C. Mitchell[10], W. Mori[9], C. T. Mottershead, F. Neri[3], I. Pogorelov[4], J. Qiang[4], R. Samulyak[1], D. Serafini[4], J. Shalf[4], C. Siegerist[4], P. Spentzouris[2], P. Stoltz[7], B. Terzic[5], M. Venturini[4], P. Walstrom[3]

[1]Brookhaven National Laboratory, [2]Fermi National Accelerator Laboratory, [3]Los Alamos National Laboratory, [4]Lawrence Berkeley National Laboratory, [5]Northern Illinois University, [6]Paul Scherrer Institute, [7]Tech-X Corporation, [8]University of California at Davis, [9]University of California at Los Angeles, [10]University of Maryland, [11]University of Southern California

[*]RDRyne@lbl.gov

Abstract. SciDAC has had a major impact on computational beam dynamics and the design of particle accelerators. Particle accelerators -- which account for half of the facilities in the DOE Office of Science Facilities for the Future of Science 20 Year Outlook -- are crucial for US scientific, industrial, and economic competitiveness. Thanks to SciDAC, accelerator design calculations that were once thought impossible are now carried routinely, and new challenging and important calculations are within reach. SciDAC accelerator modeling codes are being used to get the most science out of existing facilities, to produce optimal designs for future facilities, and to explore advanced accelerator concepts that may hold the key to qualitatively new ways of accelerating charged particle beams. In this poster we present highlights from the SciDAC Accelerator Science and Technology (AST) project Beam Dynamics focus area in regard to algorithm development, software development, and applications.

1. Introduction

Particle accelerators have enabled remarkable scientific discoveries and important technological advances that span several programs within the DOE Office of Science (DOE/SC). In the High Energy Physics (HEP) and Nuclear Physics (NP) programs, experiments associated with high-energy accelerators have led to important discoveries about elementary particles and the fundamental forces of nature, quark dynamics, and nuclear structure. In the Basic Energy Sciences (BES) program and the Biological and Environmental Research (BER) program, experiments with synchrotron light sources and spallation neutron sources have been crucial to advances in the materials, chemical, and biological sciences. In the Fusion Energy Sciences (FES) program, great strides have been made in developing heavy-ion particle accelerators as drivers for High Energy Density Physics (HEDP) research and ultimately inertial fusion energy. The importance of accelerators to the DOE/SC mission is evident from an examination of the DOE "Facilities for the Future of Science: A Twenty-Year Outlook." Of the 28 facilities listed, 14 involve new or upgraded accelerator facilities [1].

The successful development of large accelerator facilities involves enormous investments in the three paradigms of scientific research: theory, experiment, and simulation. Neglecting any of these can lead to a failure to meet performance requirements, cost overruns, and ultimately, project failure. As a result, simulation has played, and will continue to play, an essential and critical role in the development of virtually all the major accelerators in the USA and worldwide.

Recognizing the importance of particle accelerators to science and society, the present SciDAC initiative includes in its portfolio the project, "Advanced Computing for 21st Century Accelerator Science & Technology," also knows as the SciDAC Accelerator Science & Technology (AST) project. The goal of this project is to establish a comprehensive terascale simulation environment for the U.S. particle accelerator community in order to meet the needs of DOE/SC accelerator projects – especially its High Energy Physics and Nuclear Physics projects. The newly developed tools are now being used by accelerator physicists and engineers across the country to solve the most challenging problems in accelerator design, analysis, and optimization.

The AST project involves three main focus areas: computational beam dynamics, computational electromagnetics, and modeling advanced accelerator concepts. This paper highlights accomplishments in the beam dynamics area. A second paper in these proceedings, " Simulation of the Fermilab Booster using Synergia" by P. Spentzouris, presents a case study in the beam dynamics area. Electromagnetic modeling is described in the paper of K. Ko, "Impact of SciDAC on Office of Science Accelerators through Electromagnetic Modeling," and in the paper by R. Lee, "Progress/Achievements in ISIC/SAPP Collaborations for Electromagnetic Modeling of Accelerators," in these proceedings. Modeling advanced accelerators is described in the paper by W. Mori, "Recent Advances in Modeling Lasers/Plasma Accelerators: A Path towards Miniaturizing Accelerators from Kilometers to Meters," and the paper by D. Bruhwiler, "Massively Parallel Particle-in-cell Simulation of Advanced Particle Accelerator Concepts," in these proceedings.

2. Code Development

Particle simulation methods have been among the most successful and widely used methods in computational beam physics, plasma physics, and astrophysics. Under the SciDAC AST project a comprehensive, state-of-the-art set of parallel Particle-In-Cell (PIC) capabilities has been developed including:

- <u>IMPACT</u>: An integrated suite of codes consisting of 2 PIC codes, a linac design code, and an envelope code [2]. This package was originally developed to model high intensity ion linacs. Its functionality has been greatly enhanced so that it is now able to model high brightness electron beam dynamics (e.g. photocathodes), ion beam dynamics, and multi-species transport through a wide variety of transport systems.
- <u>BeamBeam3D</u>: A code for modeling beam-beam effects in colliders [3,4]. This code contains multiple models (weak-strong, strong-strong) and multiple collision geometries (head-on, long-range, crossing angle). It has been used to model the Tevatron, PEP-II, RHIC, and LHC
- <u>MaryLie/IMPACT</u>: A code that combines the high-order optics modeling capabilities of the MaryLie Lie algebraic beam transport code with the parallel PIC capabilities of IMPACT [5]. It is used to model space-charge effects in large circular machines such as the ILC damping rings.
- <u>Synergia</u>: A parallel beam dynamics simulation framework based on modern programming design [6]. Synergia combines multiple functionality, such as the space-charge capabilities of IMPACT and the high-order optics capabilities of MXYZPLT, along with a "humane" user interface and standard problem description.

The development of parallel terascale beam dynamics codes under the SciDAC AST project has involved the combined efforts of many personnel from multiple disciplines. An example is provided by the MaryLie/IMPACT (ML/I) code as shown in Figure 1. The development effort is shown diagrammatically in the figure below. The contributors come from 5 national laboratories (LBNL, LANL, FNAL, BNL, PSI), 3 universities (U. Maryland, UCLA, NIU), and a small business (Tech-X Corporation). The multi-physics nature of the code is provided for by having various teams provide specific capabilities (e.g. transfer maps for magnets and rf cavities, space-charge effects, wake field effects). Collaboration with SAPP-supported researchers and the ISICs contribute to the incorporation of optimized parallel PIC frameworks and Poisson solvers. The development team adopts, develops, and incorporates standards for items such as problem specification (i.e. the "MAD" front-end) and particle I/O. The code package includes a suite of test problems that serves the dual purpose of aiding in code verification and providing users with a starting point for learning to use the code.

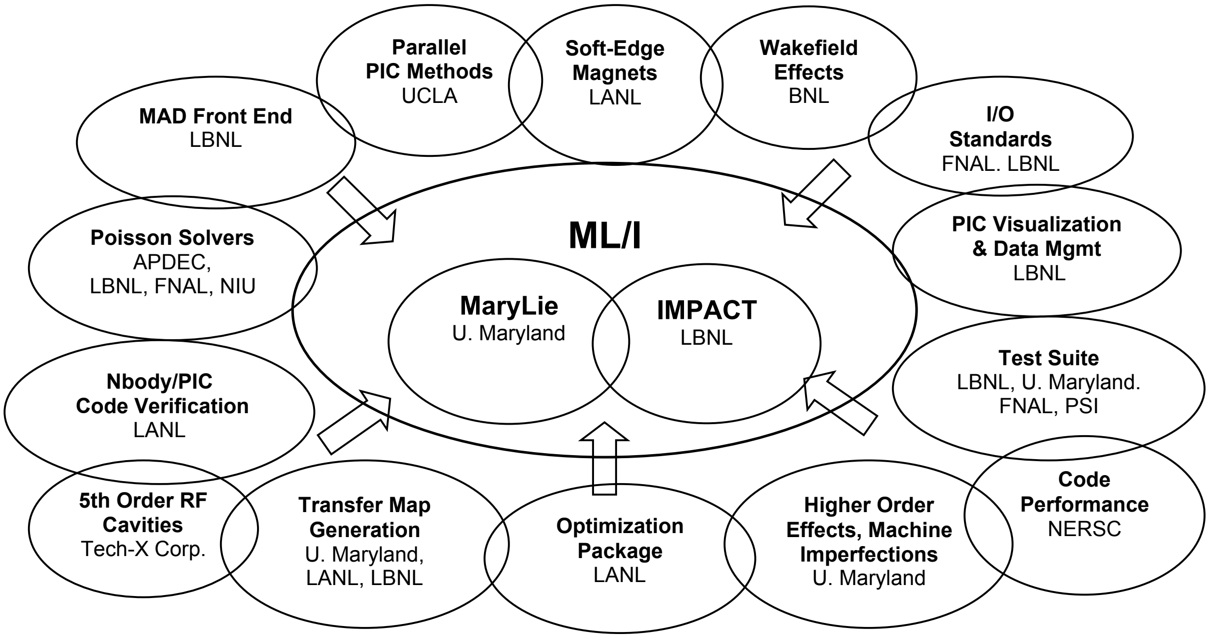

Figure 1. MaryLie/IMPACT (ML/I) code development is performed by a large, multi-disciplinary team whose members provide specific capabilities needed to produce a coherent, comprehensive, parallel, terascale beam dynamics code.

3. Algorithm Development; ISIC and SAPP Collaborations

Crucial to the development of the AST project's codes is the fact that many of them have been built using capabilities provided through collaborations with the SciDAC Integrated Software Infrastructure Centers (ISICs) and with other DOE/ASCR-supported activities such as the Scientific Applications Partnership Program (SAPP). The capabilities include parallel linear system solvers, eigensolvers, Poisson solvers, meshing technologies, adaptive grid technologies, statistical methods, and advanced visualization techniques. In some cases, the use of advanced algorithms has led to a performance increase of more than a factor of 100. The need to perform simulations accurately over a wide range of spatial and temporal scales, using high-end computing platforms of thousands of processors (100's of thousands in the future) makes the development of new, scalable, parallel algorithms not only desirable but *essential.*

Recent accomplishments related to algorithm development for beam dynamics codes, several of which involve ISIC and SAPP collaborations, include the following:

- Developed integrated Green function for high aspect ratio beams (J. Qiang, R. Ryne, LBNL)
- Statistical methods for phase space reconstruction from data [7] (D. Higdon, LANL)
- PARTVIEW/H5PART tools for large-scale data management and visualization in parallel PIC codes (J. Shalf, C. Siegerist, LBNL; A. Adelmann, PSI)
- Wavelet solver developed and incorporated in IMPACT (I. Pogorelov, LBNL, B. Terzic, NIU)
- APDEC solvers incorporated into ML/I code; progress on AMR/PIC (P. Colella, D. Serafini, P. McCorquodale)
- Developed shifted Green function for long-range beam-beam modeling (J. Qiang, LBNL)
- Multigrid solver developed, used to model RIA beam formation & transport (J. Qiang, LBNL)
- Wakefield module developed and incorporated into ML/I (R. Samulyak, BNL)
- Hybrid high performance visualization of particle data w/ large range of density scale (K.-L. Ma, UC Davis)

Further details on the development of solvers by the APDEC ISIC are described in the paper by D. Serafini, "Adaptive Mesh Refinement for Particle-in-cell Methods," in these proceedings. Further details on the application of visualization techniques for accelerator modeling are described in the paper by K.-L. Ma, "Scientific Discovery through Advanced Visualization," in these proceedings.

4. Applications

SciDAC AST beam dynamics codes have been applied to several important projects within the DOE Office of Science. Examples include existing colliders (Tevatron, RHIC, PEP-II), future colliders (LHC, under construction), proposed linear colliders (ILC), high intensity machines (the Fermilab booster, and the SNS ring under construction), linacs for radioactive ion beams (RIA, proposed), and electron linacs for 4th generation light sources (LCLS, under construction).

4.1. Application to the High Energy Physics (HEP) Program

SciDAC beam dynamics codes have been used to model several HEP machines including the Tevatron, the Fermilab booster, PEP-II, and ILC damping rings. Simulation results for the proposed ILC damping ring performed using MaryLie/IMPACT are shown in Figure 2. SciDAC Advanced Accelerator codes have also had an impact on HEP beam dynamics modeling. For example, the code QuickPIC has been used to model electron-cloud formation in the LHC and to study plasma afterburner concepts.

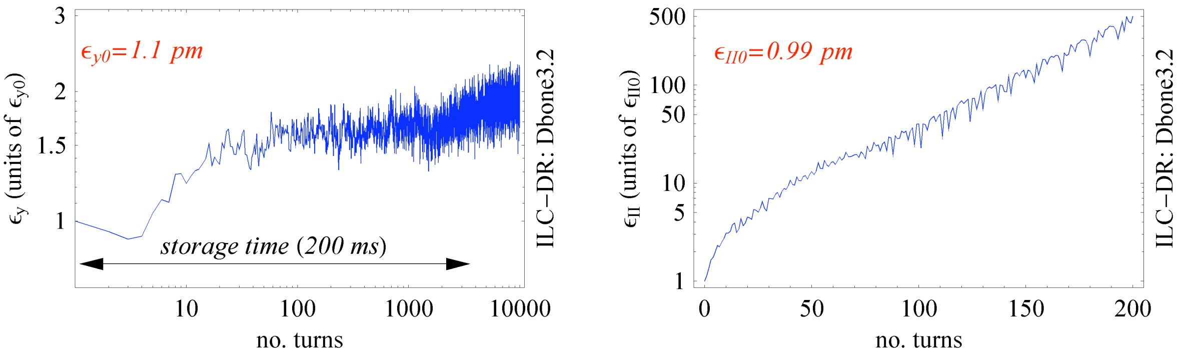

Figure 2. Results of ML/I simulations of an ILC "dog-bone" damping ring (DR) design showing space-charge induced emittance growth using different space-charge models. Left (nonlinear space charge model): the beam exhibits small emittance growth. Right (linear space charge model): the beam exhibits exponential growth due to a synchro-betatron resonance. The instability is a numerical artifact caused by the simplified (linear) space-charge model (M. Venturini, LBNL).

4.2. Application to the Nuclear Physics (NP) Program

SciDAC beam dynamics codes have been used to model the RHIC collider and the proposed RIA accelerator. An example of RIA modeling is shown in Figure 3.

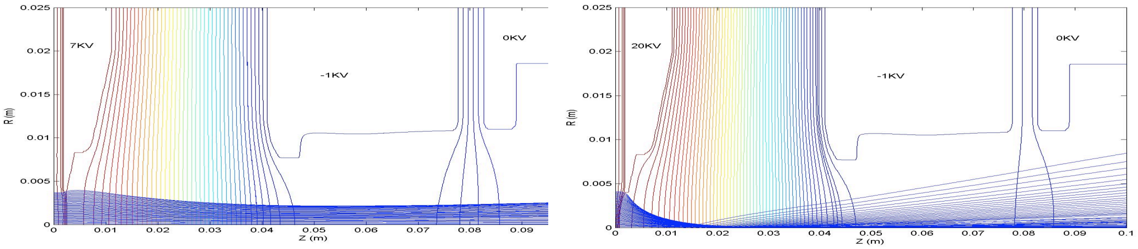

Figure 3. IMPACT-T simulation of the beam emerging from the RIA ECR ion source showing the effect of electrode voltage on the beam quality emerging from the source. Left: correct voltage. Right: incorrect voltage (J. Qiang, LBNL).

4.3. Application to the Basic Energy Sciences (BES) Program

SciDAC beam dynamics codes have been used to model the SNS, LCLS, and ALS. Examples related to the LCLS injector and to the design of an ultrafast streak camera for LCLS are shown in Figure 4.

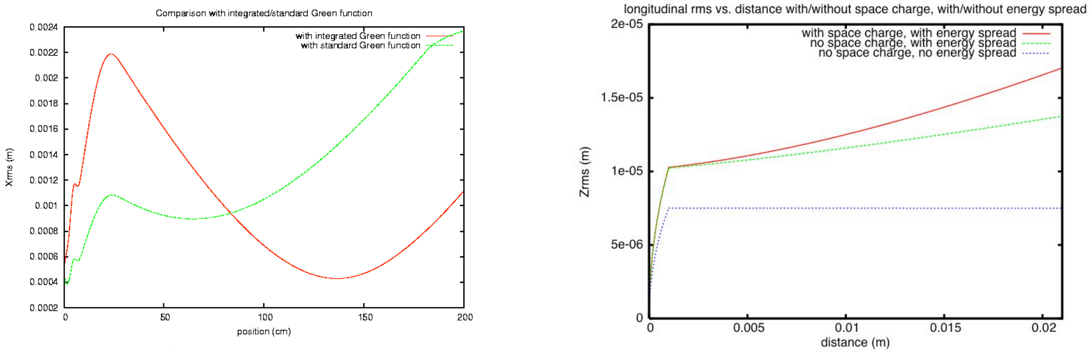

Figure 4. Left: LCLS simulation using IMPACT-T: Large effect observed when using integrated Green function compared with standard Green function (J. Qiang, LBNL and C. Limborg, SLAC). Right: Plot of rms bunch length vs distance in the proposed LCLS streak camera showing the effect of space charge on the bunch length (J. Qiang, LBNL).

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