Accelerator Modeling under SciDAC: Meeting the Challenges of Next-Generation Accelerator Design, Analysis, and Optimization

P. Spentzouris*, FNAL, PO Box 500, IL 60510, U.S.A.

Abstract

Under the US DOE Scientific Discovery through Advanced Computing (SciDAC) [1] initiative, a new generation of parallel simulation codes has been developed to meet the most demanding accelerator modelling problems for the DOE Office of Science (DOE/SC). Originally sponsored by DOE/SC's Office of High Energy Physics in collaboration with the Office of Advanced Scientific Computing Research, the new simulation capabilities have also been applied to other DOE projects, and to international projects as well. The new software has been applied to many projects, including the Tevatron, PEP-II, LHC, ILC, the Fermilab Booster, SNS, the JPARC project, the CERN SPL, many photoinjectors, and the FERMI@Elettra project. Codes have also been developed to model laser wakefield accelerators and plasma wakefield accelerators; these codes are being used both in support of advanced accelerator experiments, as well as to provide insight into the physics of ultra-high gradient accelerators. In this talk I will provide an overview of the computational capabilities that have been developed under our SciDAC project, and describe our plans for code development under the next phase of SciDAC.

THE SCIDAC PROGRAM

The U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program was created to bring together researchers from different scientific areas with math and computer scientists, to develop new computational methods for tackling some of the most challenging scientific problems which require large scale computing. The first five year phase of the program started in 2001, with main objective to develop scientific applications to *effectively* take advantage of terascale computing, by

- Creating a new generation of scientific simulation codes
- Creating the mathematical and computing systems software to enable these scientific simulation codes to use terascale computers
- Creating a distributed science software infrastructure to enable scientists to effectively utilize these codes.

Accelerator modeling is one of the SciDAC program areas. The emphasis of this project is on building teams of computer scientists, and computational and machine physicists to develop and apply the tools required by the field.

SciDAC Accelerator Science & Technology (AST) Project

The SciDAC Accelerator Science and Technology (AST) project was initiated in 2001. Its goals are to develop and apply an advanced, comprehensive, high-performance accelerator simulation environment, able to take full advantage of terascale computing resources and utilize them to solve challenging problems, which enable new discoveries in accelerator science and technology.

The SciDAC AST project is a large multi-institutional, multi-disciplinary collaboration. 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 US DOE/SC Office of High Energy Physics (HEP) in collaboration with the Office of Advanced Scientific Computing Research (ASCR). Under the AST project, accelerator scientists are working closely with computer scientists and applied mathematicians, associated with the SciDAC Integrated Software Infrastructure Centers (ISICs) and researchers in ASCR's Scientific Application Partnership program. This work covers many topics necessary in the development of efficient large scale computing accelerator modeling tools, such as 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. In this presentation I will focus mostly 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 [2]

*spentz@fnal.gov

- IMPACT: A 3D parallel PIC code used primarily for modeling beam dynamics in electron and ion linacs [3]
- MaryLie/IMPACT: A 3D parallel PIC code combining high order magnetic optics with spacecharge [14]
- OSIRIS: A fully electromagnetic 3D parallel PIC code, mainly for plasma accelerator simulation [5]
- QuickPIC: A 3D parallel PIC code for modeling plasma accelerators in the quasi-static limit and electron clouds [6]
- Synergia: A 3D parallel beam dynamics simulation PIC framework, which includes arbitrary order magnetic optics, space charge, and impedance models [7]
- UPIC: A framework for parallel PIC simulation [8]
- VORPAL: A parallel framework for modeling electromagnetic fields, fluids, particles, and their interactions. [9]

The impact of these codes to the accelerator community is evident both from the list of projects and accelerator facilities that are making use of AST codes. This list includes nearly every major present and proposed accelerator project in the USA, several international projects, as well as several small experiments and design efforts, such as the

- 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

The success of the AST project is also evident from the large number of presentations of members of the project or collaborators at this conference: there are twelve presentations [10]-[21] discussing AST or AST related codes, while AST applications were discussed in a number of other talks. These presentations are an excellent demonstration of the collaborative nature of the SciDAC program. For example, development of the CHEF libraries [11] is not SciDAC funded, but CHEF is used in one of the AST frameworks; also, VORPAL applications in electron cooling [18] are not SciDAC funded, but VORPAL development partially is.

SciDAC AST development accomplishments

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) [22]
- First multi-bunch, multi-turn injection simulation from linac-to-booster w/ self-consistent 3D space charge (Synergia; J. Amundson and P. Spentzouris) [7]
- 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) [23].
- First 3D simulation of a 1TeV Afterburner stage (QuickPIC; C.K.Huang et al.) [24].
- First 3D simulation of a GeV LWFA stage (OSIRIS; F.S.Tsung, W.Lu, M. Tzoufras et al. [25]

Details of the AST codes and their applications can be found in the talks and posters presented at this meeting [10]-[21]. Selected examples, covering development and applications not included in the above talks are discussed in the section below.

SCIDAC AST CODES AND APPLICATIONS

BeamBeam3d

BeamBeam3d is a multi-model parallel PIC code for simulating colliding beams, including models for weak-strong, strong-strong, head-on, crossing angle, and long range effects. It has been applied to Tevatron, LHC, PEP-II, and RHIC problems. BeamBeam3d features integrated and non-uniform grid Green function, and has multi-slice, multi-bunch, and multi-IP capabilities. An impedance model and map generation from lattice function measurements capability were recently added for Tevatron modelling. The scaling of the code performance at the NERSC SP3 is shown in Figure 1.

The validity of the 3D model has been verified by comparing to data from the VEP-II accelerator (see Figure 2). Coherent synchrobetatron beam-beam oscillations are a specific and unambiguous manifestation of beam-beam interactions. In a colliding beam accelerator bunches are subject to a beam-beam force from the electromagnetic fields generated by particles in the opposing beam. In a beam bunch with extended longitudinal length, particles in the head of the bunch couple indirectly with particles at the tail of the bunch through their mutual beam-beam interactions with an opposing beam bunch. The coupled system has oscillation modes at frequencies specific to the mode which can be observed experimentally.

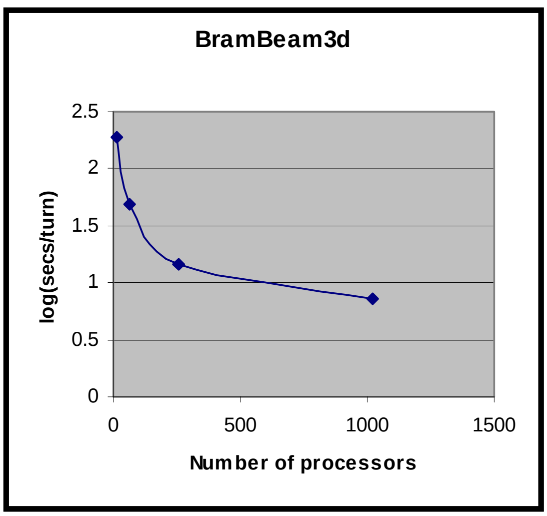

Figure 1: Scaling at the NERSC SP3: weak-strong model (100M particles, 512x512x32 grid, 4 slices).

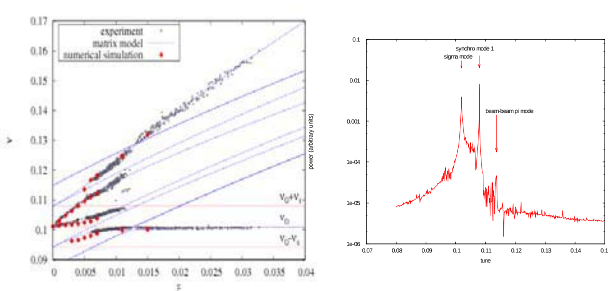

Figure 2: Left, beam-beam code validation comparing BeamBeam3d prediction with VEP-II data. Right, 2-bunch coherent spectrum for x=0.008. Shown are the beam-beam σ and π modes and one synchrobetatron mode.

QuickPIC

The code QuickPIC was originally developed to enable fast simulations of plasma-based accelerators. However, under SciDAC AST an enhanced version of the code was developed and adapted to the circular accelerator problem, by adding magnetic fields, non-neutral plasma, and lattice effects. QuickPIC was applied to modeling electron-cloud generation in the LHC (Figure 3), and it is used to model electron-cloud effects in the FNAL Main Injector. In this example, very basic research in advanced accelerator technologies turned out to have direct impact on near- and mid-term projects.

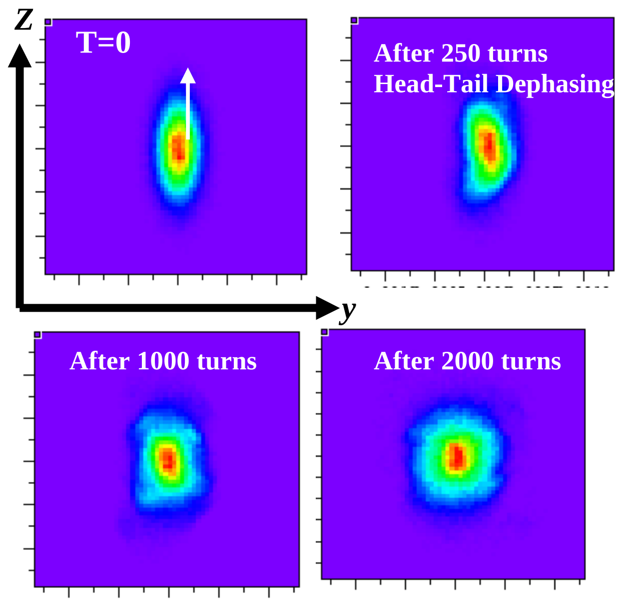

Figure 3: QuickPIC LHC modelling. Snap shots of Beam Evolution as a function of turn number.

Synergia

Synergia is a multi-language, extensible, parallel PIC framework which incorporates multi-physics capabilities and utilizes state-of-the-art numerical libraries, solvers, and physics models (Figure 4).

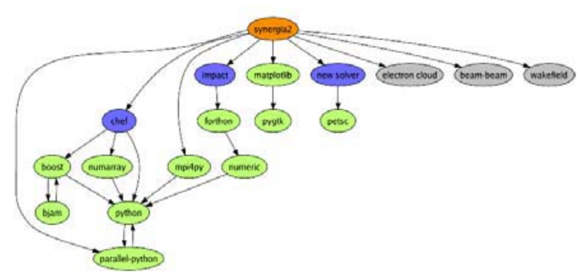

Figure 4: Synergia framework diagram.

Synergia features 3D space-charge and impedance modules, and arbitrary order Lie maps for magnetic optics (from CHEF, see [11]). It has unique capabilities for synchrotrons, boosters, and storage rings: multi-bunch, ramping and rf and magnet, multi-turn injection, and active feedback modelling. It utilizes multiple Poisson solvers, and FFT based from IMPACT [3], and a multigrid solver.

Synergia has been used extensively to model the FNAL Booster. Using Synergia, we performed the first-ever simulation of the process of linac microbunch capture, debunching, and acceleration, all using a 3D space-charge model, (Figure 5). We compared the results of our simulations to beam measurements, both under normal machine operations and during machine studies, (Figure 6). The simulations have helped provide guidance to accelerator operators to reduce losses and maximize the intensity of the Booster.

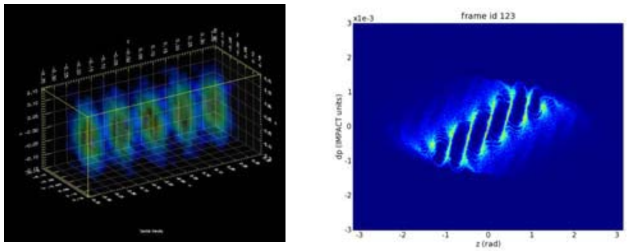

Figure 5: Left, Merging of 5 linac microbunches in the FNAL booster. Left, longitudinal phase space shows halo and space-charge "drag" during bunch merge.

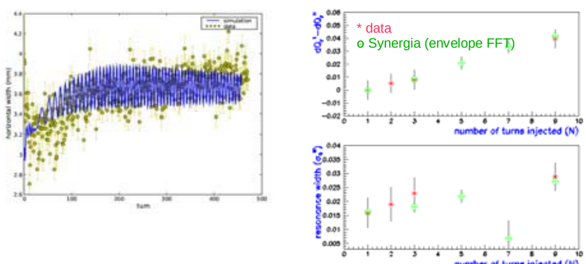

Figure 6: Left, 3D Booster simulation of beam profile evolution including injection, rf ramping compared with experimental data from the Ionization Profile Monitor. Right, measurement and simulation of the Booster space charge tune shift using a coasting beam and scanning the half integer resonance.

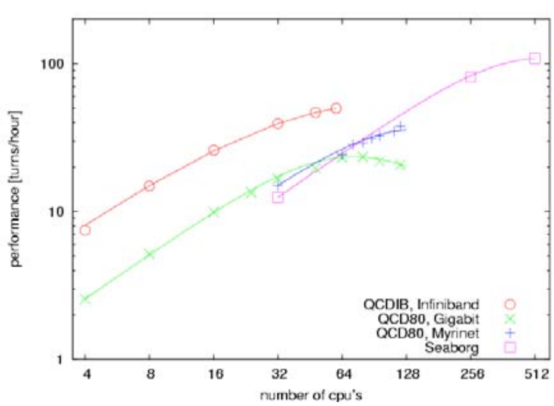

Figure 7: Synergia performance scaling on different platforms.

The Synegia code has been ported both to supercomputers and commodity PC clusters with fast networking, and has shown very good performance, (Figure 7).

Plasma Acceleration

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).

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. The first breakthrough was the observation of low energy spread bunches in a LWFA by three different groups [26]. Prior to this, LWFAs produced beams with such large energy spread that they were not suitable as useful accelerators. The experimental parameters for these experiments were guided by theory and simulation. All three groups achieved electron beams of slightly over 100 MeV with energy spread of a few percent, and simulations using SciDAC and codes have helped to explain the physics involved in the production of such beams and pointed the way to higher energies (Figure 8).

Figure 8: SciDAC codes used to successfully model LWFA experiments. 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 [26] using the VORPAL code.

The physics for the successful experiments was predicted prior to the measurements. A LWFA OSIRIS simulation is shown in Figure 9, depicting a sequence of 2D cuts through the 3D data of the electron density. The laser is propagating from left to right. After 0.24 cm (left column) there are no selfinjected electrons. After 0.43 cm (middle column) the self-injected electrons are seen. The electron beam shape is different in the two planes (xz and yz), an effect which has been seen experimentally. After

0.64 cm the first bunch has completely outrun the plasma wave and a second bunch has been injected. This simulation predicted that the initial bunch of trapped electrons induces a secondary wake which interferes with the primary wake, reducing its amplitude. If the drive laser pulse energy is just above the threshold for trapping, this beam loading effect suppresses further injection, creating an electron bunch isolated in phase space.

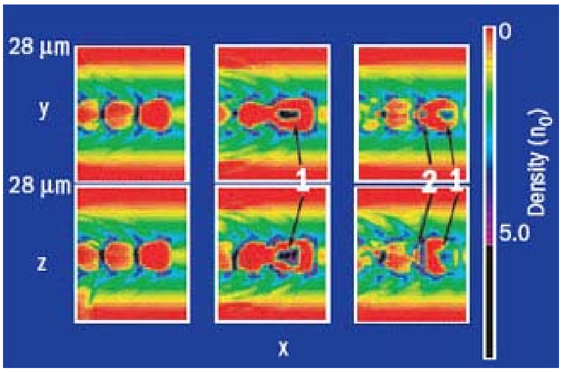

Figure 9: OSIRIS simulation predicting short electron bunch if acceleration path matched to de-phasing length.

THE FUTURE: IMPACT OF PETASCALE COMPUTING

The SciDAC program is about to begin its second five year funding cycle. Under SciDAC2 we will take advantage of the extraordinary opportunities presented by the petascale computing capabilities that will be available in the next five years. Our SciDAC2 project will aim to develop a comprehensive accelerator modelling framework capable of multi-physics simulation necessary for the end-to-end modelling required for the design of future accelerators such as the ILC. We will also continue along the path of our first SciDAC project, by developing common interfaces for code interoperation both for the existing and the new codes we will develop. Furthermore, the interfaces will be designed such that computational algorithms may be substituted where warranted.

We will build upon our existing work on the Synergia and ML/I frameworks to provide a framework capable of utilizing the existing and future physics modules. In addition, using the applied math and computer science tools that will be developed under SciDAC2, we will integrate algorithm optimization into the simulation environment, at the *user level*. This will allow the non-expert user to utilize the most appropriate algorithms available through our codes for his/her applications. Figure 10 shows the two main facets of this feature: (1) analysis infrastructure, which combines performance information and models from historical and runtime databases along with interactive analysis, including machine learning technology; and (2) control infrastructure, which encompasses decision-making components that evaluate progress based on domain-specific heuristics and metrics, along with services for dynamic component replacement.

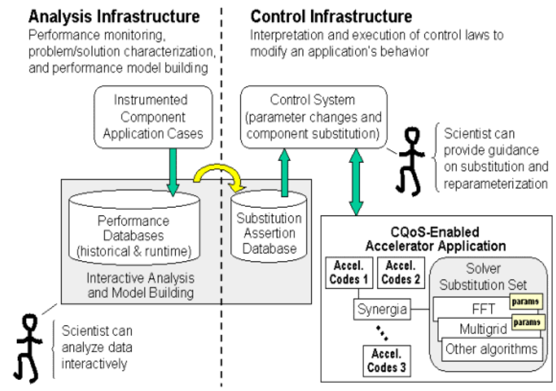

Figure 10: Accelerator modelling application using the infrastructure for computational quality of service.

We will also explore new synergies, for example by utilizing fully self consistent electromagnetics (EM) plus particle PIC codes (VORPAL) for EM design [10], in addition to the already existing AST EM codes [13], [20]. We will use these capabilities for applications such as self-consistent particle propagation in loaded cavities, secondary emission from cavities, feedback systems, beam diagnostics, and mode and wakefield calculations. Also, we are expanding the SciDAC accelerator modeling code suite to include codes such as the self-consistent electron cloud code WARP/POSINST [19], to augment our existing electron cloud modeling capabilities.

Our applications will focus on accelerator design and optimization for HEP projects: ILC, LHC, Tevatron, PEP-II, and proton drivers design, and our codes will be available for Nuclear Physics (RHIC, RIA, CEBAF) and Basic Energy Science (SNS, 4th generation light sources) projects. We will also continue to support efforts to push the energy frontier in advanced accelerators: exploring TeV scale afterburners with high fidelity and 10 GeV plus LWFA systems.

As with the first phase of our project, the emphasis will be on problems which require large scale (parallel) computing and we will work closely with machine designers and operators to apply our tools.

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