Beam dynamics

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Abstract. We describe some of the accomplishments of the Beam Dynamics portion of the SciDAC Accelerator Science and Technology project. During the course of the project, our beam dynamics software has evolved from the era of different codes for each physical effect to the era of hybrid codes combining start-of-the-art implementations for multiple physical effects to the beginning of the era of true multi-physics frameworks. We describe some of the infrastructure that has been developed over the course of the project and advanced features of the most recent developments, the interplay between beam studies and simulations and applications to current machines at Fermilab. Finally we discuss current and future plans for simulations of the International Linear Collider.

1. Introduction
The SciDAC Accelerator Science and Technology Beam Dynamics project has advanced the simulation of particle accelerators through a progression from an era where entirely new codes were needed for each physical effect to a new paradigm where state-of-the-art implementations of individual models are integrated into powerful hybrid codes. This progression is continuing with the development of multi-physics frameworks for the simultaneous integration of many physical effects. We describe this progression and its culmination in the frameworks MaryLie/IMPACT and Synergia2 below. We have also developed new infrastructure modules as part of these frameworks; two such modules are described here, H5Part and a new Poisson solver. We also consider the sorts of new simulations made possible by Synergia2, considering a case in the Fermilab Booster.

Applications to existing and planned accelerators are the raison d’etre of accelerator simulation development. We list the areas in which we have modeled collective effects in existing machines at Fermilab. Finally, we discuss current and future applications of our code to the International Linear Collider (ILC).

2. Evolution of beam dynamics software
The software packages developed and used by the Beam Dynamics project has evolved from a time in which each category of physical effect was represented by a separate code to an era where hybrid codes combine the best of existing physical models into a single package. Now, at
the end of SciDAC1, we are moving on to true multi-physics frameworks where new effects can be easily incorporated into the existing infrastructure.

Two very capable single-particle optics packages were available at the beginning of the project. MaryLie\textsuperscript{[6]} is a sophisticated implementation of Lie mapping techniques producing mappings up to fifth order in the phase-space variables. MaryLie includes a wide range of tools for dealing with single-particle optics. The CHEF libraries\textsuperscript{[1, 2, 3, 4]} are a comprehensive set of libraries for beam physics. CHEF uses automatic differentiation to generate mappings at arbitrary orders. The program IMPACT\textsuperscript{[5]} was also available for the calculation of collective space-charge effects. While IMPACT featured a state-of-the-art parallel implementation of space-charge calculations, its linear optic model was very simple; it was limited to linear maps of a restricted set of elements.

During the SciDAC project, we developed two new programs to combine the best features of IMPACT with MaryLie and CHEF. The first is MaryLie/IMPACT\textsuperscript{[7]}, which, as the name implies, incorporates the IMPACT space charge model into the MaryLie code. The second is Synergia\textsuperscript{[8]}, which extends IMPACT's main loop to call CHEF for single-particle mappings. Synergia also includes a Python wrapping mechanism that allows the user to write simulations using human-friendly Python scripts which then send commands in the more technical IMPACT input format. Both MaryLie and Synergia have been successfully used to model various accelerators over the course of the project. The following sections contain examples of some of the Synergia applications.

Having demonstrated the ability to combine sophisticated single-particle optics codes with parallel collective-effects codes, we are now moving into an era where the codes transform into frameworks for the combination of multiple models of physical effects. MaryLie/IMPACT is growing to accommodate effects from many contributors including software modules for physical effects such as wakefields and more sophisticated magnet models to computational topics such as parallel I/O and visualization. At the same time, Synergia has evolved into Synergia2, a Python-steered accelerator physics framework. Whereas Synergia used Python only for the user interface, Synergia2 creates actual Python programs, calling modules written in Fortran and C++ for the computationally intensive calculations. The use of Python greatly simplifies the process of adding new physical models to Synergia2. At the same time, the main loop has become almost arbitrarily flexible, allowing the user to create simulation logic with little effort.

Synergia2 also takes advantage of the wide variety of existing physical and numerical software. In Fig. 1, we show the variety of modules incorporated in Synergia2, including modules planned for inclusion during further development.
3. Infrastructure development

While much of the Beam Dynamics effort in SciDAC1 involved integration and physical modeling, effort was also spent on the development of software infrastructure. Two examples of the efforts are H5Part and a new Poisson solver.

H5Part[10] is a portable, high-performance, parallel data interface for particle simulation. It utilizes the HDF5[11] library to provide an interface for efficient, cross-platform particle storage with bindings for the most popular scientific computing languages. It has been used to enable advanced visualization of beam simulations using existing visualization packages.

Another infrastructure development was motivated by the needs of the ILC; we developed a new, more flexible Poisson solver for space charge applications. The existing solvers in IMPACT all use a fixed grid spacing. Such a fixed spacing is inefficient in the case of a small beam in a large pipe as well case case of a beam with a large aspect ratio. Both cases apply to the ILC damping ring. The new solver utilizes state-of-the-art multigrid methods from PETSc[9], taking advantage of another the work done in another SciDAC project. The PETSc-based solver uses a finer grid where the particle density (and, hence, curvature) is greatest, and a rougher grid for mostly empty spaces, where the curvature is the least, as shown in Fig. 2. The result is a solver that produces similar accuracy to a uniform grid, while utilizing only half as many grid points, with a corresponding speed increase. The new solver is also flexible in that it may be modified to be used with a variety of boundary conditions.

4. Interplay between beam studies and simulations

Although the focus of the Beam Dynamics project is software, the software would be meaningless if it did not produce meaningful physical results that can be compared with experiments in existing machines. Throughout the project we have compared the results of our simulation tools with beam studies, including performing the studies themselves.

In a recent example, we studies the interaction between space charge, the sum resonance and skewed quads in the Fermilab Booster. Fig. 3 shows the results of a study where the Booster was tuned to be close to the sum resonance, then the settings of the skew quads and the total injected current were varied. The experimental data show that the vertical width grew sharply after roughly 1000 turns, accompanied by a dramatic loss of beam. The simulated results using Synergia2 show similar behavior, including the variation with current.

Figure 2. Transverse view of beam particles (red) in a circular pipe with a uniform cylindrical grid (left), and a non-uniform cylindrical grid (right). Similar accuracy is obtained with either grid, even though the grid on the right only contains half as many grid points as the grid on the left.
Figure 3. Experimental data from study of space charge interaction with skewed quads in the Fermilab Booster compared with simulation results from Synergia. The top row shows the drop in total beam current correlated with the growth of vertical beam width in the bottom row. In the experimental plots, the red line is the signal and the green is the derivative of the signal. In the simulation plots, the red line is half current, the green is full current and the blue is zero current.

5. Applications to Fermilab machines
Applying our simulations to existing machines has been an important part of the project. At Fermilab, our efforts have focused mostly on the Booster because it is the Fermilab machine which is most affected by space charge. However, we also participated in simulations of beam-beam effects in the Tevatron and electron cloud generation in the Main Injector. At the current time, beam-beam and electron cloud effects are modeled by individual codes. We plan to incorporate beam-beam and electron cloud modeling into Synergia2 and MaryLie/IMPACT during the next phase of development.

6. Advanced features in Synergia2
The Python-based steering in Synergia2 enables simulations of machines at a much greater level of sophistication than was previously possible. Not only can we use sophisticated models of single-particle optics and collective effects such as space charge, we can also incorporate the machine logic into the simulations. An example is our model of the RPOS mechanism in the Fermilab Booster. The RPOS system controls the acceleration of the beam by using feedback from the beam position monitors to adjust the phase of the RF system in order to maintain the beam in the center of the ring while the strength of the bending magnets is ramped. In space-charge simulations using Synergia2, we model this process by periodically measuring the mean position of the beam particles, then updating the parameters of the RF model in a manner similar to the RPOS circuit. In this manner we can investigate possible couplings that would have been out of the reach of earlier, less sophisticated simulations.

7. Applications to the International Linear Collider
The most important machine for future accelerator modeling efforts is the ILC. The collective effects in the ILC requiring high-performance computing include space charge, electron cloud and impedance in the damping ring and wakefields in the main linac. In addition, beam-beam
effects need to be investigated at the interaction point. The plans for the next phase of the
Beam Dynamics project are focused on providing high-fidelity modeling of these effects.

Work on the damping ring has begun with investigations of the single-particle optics, as in
Fig. 4. The Poisson solver work described in Sec. 3 is necessary for space charge calculations
due to the large aspect ratio of the electron and positron beams. Electron cloud and impedance
effects need to be incorporated into the MaryLie/IMPACT and Synergia2 frameworks in order to
enable truly multi-physics simulations. Modeling of the main linac will also require integration
of sophisticated electromagnetic field calculations into the frameworks. This work will be crucial
for an accurate understanding of the physics of the ILC.

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References
[1] L. Michelotti, FERMILAB-CONF-91-159 Presented at 14th IEEE Particle Accelerator Conf., San Francisco,
CA, May 6-9, 1991.
[2] L. Michelotti, FERMILAB-FN-535-REV.
[3] L. Michelotti. Published in Conference Proceedings: Automatic Differentiation of Algorithms: Theory,
Implementation, and Application. Society for Industrial and Applied Mathematics. First International
Workshop on Computational Differentiation. 1991.
[4] L. Michelotti. Published in Conference Proceedings: Advanced Beam Dynamics Workshop on Effects of
Errors in Accelerators, their Diagnosis and Correction. Corpus Christi, Texas. October 3-8, 1991. American
Institute of Physics: Proceedings No.255. 1992.
[5] J. Qiang, R. D. Ryne, S. Habib and V. Decyk, J. Comp. Phys. 163, 434 (2000).
[6] Dragt, A. J., D. R. Douglas, E. Forest, F. Neri, L. M. Healy, P. Schtt, and J. van Zeijts, 1999, MARYLie 3.0
User’s Manual (University of Maryland, Physics Department Report).
[7] http://scidac.nersc.gov/accelerator/tml/manual.pdf
[8] J. Amundson, P. Spentzouris, R. Ryne and J. Qiang, Journal of Computational Physics, Volume 211, Issue 1,
1 January 2006, Pages 229-248.
[9] S. Balay, K. Buschelman, V. Eijkhout, W. Gropp, D. Kaushik, M. Knepley and L. McInnes and B. Smith,
H. Zhang, ANL-95/11, 2004.
[10] A. Adelmann, R. Ryne, J. Shalf, C. Siegerist, Particle Accelerator Conference, Knoxville 2005.
[11] http://www.ncsa.uiuc.edu/HDF5