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### **Author**

Schachinger, L

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### Summary of the Working Group on Modelling and Simulation

L. Schachinger

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Summary of the Working Group on Modelling and Simulation\*

Lindsay Schachinger

Lawrence Berkeley Laboratory  
University of California  
Berkeley, CA 94720

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# Summary of the Working Group on Modelling and Simulation

Lindsay Schachinger  
Lawrence Berkeley Laboratory,\* Berkeley, CA 94720

## Abstract

The discussions and presentations in the Simulations and Modelling subgroup of the Fifth ICFA Beam Dynamics Workshop "The Effects of Errors in Accelerators" are summarized. The workshop was held on October 3-8, 1991 in Corpus Christi, Texas.

## 1.0 Introduction

The discussions and presentations in the Simulation and Modelling group were divided into roughly four areas. The first was the models themselves—maps and tracking codes—which are used to represent an accelerator. Our most heated discussions were in this area, and centered around the use of maps for tracking particles for many turns. The second area discussed was two recent measurements of slow particle loss, one at the Tevatron and the other at the SPS. We looked at how these measurements can be compared with tracking to give us a rough relationship between tracking dynamic aperture and real dynamic aperture. Thirdly, we discussed recently developed software and hardware tools. Many of the software tools use current computer science techniques such as object-oriented programming to simplify the use of elegant physics, or to make simulation systems easier to create, modify, and reuse. The fourth area of discussion was several examples of simulations, including those done for SSC, LHC, the proposed KEK B factory, and the Main Injector planned at Fermilab.

Most of the presentations mentioned in this paper are described in more detail in accompanying papers in these proceedings. This paper only explicitly references papers which are not included in the proceedings.

## 2.0 Models

Two sorts of models were discussed: element-by-element tracking codes and one-turn maps. The presentation and discussion on tracking codes centered on small machines and the validity of various approximations often made when writing a symplectic integrator for tracking. The map discussion focussed on maps produced by differential algebra (DA), and their use in analysis and tracking of lattices.

### 2.1 Tracking Small Machines

Étienne Forest gave a presentation about tracking in small rings, where many effects which are ignored for large rings (and often, unfortunately, for small rings, too) become important. Fringe fields, for example, become more important as ring size shrinks. In one extreme case the fringe fields contributed 50% of the chromaticity. Parallel face bends must be treated with

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care in small rings. For instance, the approximation that a rectangular bend is a sector bend with thin quads tacked on each end to change vertical focussing to horizontal is only correct near the design orbit. Once entrance and exit angles become large, this approximation breaks down. The Hamiltonian for a rectangular bend is

$$H = -\left(1 - \frac{x}{\rho}\right)\left((1 + \delta^2) - p_x^2 - p_y^2\right)^{1/2} + \frac{x}{\rho} + \frac{x^2}{2\rho^2} + V(x, y)$$

Many codes expand this Hamiltonian to first order in  $p_x$  and  $p_y$ , which is a good approximation for large rings, but should be done with care for small rings. One should take care that this approximation is not discarding terms which are comparable to the non-linear terms in  $V(x, y)$ , which contains multipole terms of quadrupole and higher order.

## 2.2 Analysis Using Maps

There are now several software packages available which allow one to generate a Taylor series map, exact to machine precision, using differential algebra (or automatic differentiation). It is also possible to create a map which is an explicit function of parameters of the machine elements—*e.g.*, quadrupole or sextupole strengths. Using normal form techniques, one can compute, for example, tune shift with amplitude, smear as a function of amplitude, and resonance strengths. In his tutorial about normal form analysis, Leo Michelotti pointed out that one must be careful to remember that this analysis is based on perturbation theory, and thus can fail if the expansion parameter gets too large. These techniques are extremely powerful, and are in the process of being adopted at many laboratories.

We discussed two ways of using such maps for correction of errors. The first is to calculate corrector strengths directly from a map which is an explicit function of those strengths. An example is the calculation of the tune shift with amplitude from a map which is a function of the strength of two families of octupoles. The octupole strengths can then be calculated which will set the tune shift with amplitude to zero.

The second way of using maps discussed was to use a property of the lattice calculated from a map as input to a correction algorithm. An example of this was a correction scheme presented by Étienne Forest which attempts to minimize tune shift with amplitude and non-linear chromaticities. Analytical expressions for these quantities, calculated using MACSYMA, contain properties of the bare lattice (such as  $d\beta/d\delta$ ) which are calculated using DA techniques. The result is expressions for the quantities to be minimized which are functions of the sextupole strengths in the ring. A non-linear optimization algorithm is then used to compute the sextupole strengths which will minimize these effects. In this case the goal is to improve the Touschek lifetime in the ALS. This is a particularly elegant example of the use of DA in a correction algorithm.

Since the Taylor series is approximate (only correct to the specified order), it is important to check any results derived from the map with a trusted element-by-element tracking program to see that the desired effect has been achieved. One should also beware that correcting one effect can cause another to worsen, which gives further reason to check the performance of a lattice after a correction scheme has been applied.

## 2.3 Tracking With Maps

It is tempting to use Taylor series maps for long-term particle tracking, since they can be 15 to 100 times faster than element-by-element tracking. Thus one can track machines such as SSC and LHC for  $10^7$  turns, which is about 1 hour of storage time, or approximately the SSC filling time. Another potential advantage is that the map is exact to a given order and symplectic, and errors due to round-off are lessened. Two members of the group, Yiton Yan at SSC and Frank Schmidt at LHC, had studied the use of maps from long-term tracking in some detail, and presented their results.

Yan showed turn-by-turn agreement between a 12th order map and tracking for 400 turns near the dynamic aperture for the SSC. He also presented data which show agreement in the  $10^6$  turn dynamic aperture between a 10th order map and element-by-element tracking. However, the two methods only agreed at  $10^6$  turns if the map was symplectified. Comparisons at  $10^5$  turns agreed without symplectification. The 12th order map was accurate to 8 digits for one turn compared to element-by-element tracking.

Schmidt found turn-by-turn disagreement between an 11th order non-symplectified map and element-by-element tracking for the LHC well inside the dynamic aperture. He looked at the amplitude of a single particle for  $10^4$  turns, and found amplitude growth of approximately 10% at 2000 turns. This amplitude growth was due predominately to phase errors. Schmidt and Yan agreed on the single turn accuracy of maps.

Aside from these disagreements about the accuracy of one-turn maps in specific cases, there was a great deal of uneasiness about the use of maps for long-term tracking in the group. It was felt that there was no guarantee that a given order map was accurate enough unless checked with element-by-element tracking, and if the goal is to go beyond the number of turns accessible by element-by-element tracking, then such checking is not possible. Therefore, long-term tracking with maps is to be done with caution, and the results should not to be taken as definitive.

### 3.0 Comparison of Experimental Measurements with Simulations

Two experiments to measure particle loss due to diffusion were discussed. These were of interest to our group because they test the predictions of tracking codes. We do not consider either experiment a stringent test of tracking, but they are useful as a rough measure of the difference between fairly naive tracking (but not so different from what is usually done in the design phase of a proton storage ring) and measurements of beam lifetime on real accelerators. The experiments were of interest purely as measurements of physical phenomena, but we will focus on the comparison with tracking, since that was our charge.

#### 3.1 E778 Diffusion Measurements

This part of the E778 experiment at the Fermilab Tevatron, presented by R. Talman, set out to measure diffusion by measuring the profile of a horizontally kicked beam with a flying wire at regular intervals, for a total of 20-30 minutes.<sup>1</sup> Sixteen special sextupoles were powered to provide known, dominant nonlinearities in the machine, and the horizontal tune was near  $2/5$ . The data fit a diffusion model very well, over a range of conditions. The interesting result was that the radius inside which particles were not lost experimentally was about half the radius of the largest regular contour in phase space from tracking (which would be naively associated with the dynamic aperture). Thus, there is measurable slow particle loss even inside closed, regular contours in horizontal phase space.

An earlier E778 experiment, using a different measurement technique, found that the 400 turn tracking dynamic aperture was approximately 30% larger than the measured aperture.<sup>2</sup> In this previous experiment the dynamic aperture was defined as the width of the base of the beam distribution as measured by flying wires. Particle loss was sped up with noise, and beam profiles were only measured for 100 seconds.

So while fast particle loss agrees with tracking to approximately 30%, slow particle loss is not predicted at all well by short-term tracking in the presence of time-independent fields and nonlinearities alone. Perhaps this is not surprising, but this tracking was not atypical of the sort of tracking often done in an attempt to determine dynamic aperture. This experiment shows that such approximations can be in error by factors of two.

#### 3.2 SPS Diffusion Measurements

The SPS experiment, described by Frank Schmidt, was similar in that eight special sex-

tupoles were used to provide non-linearities, but different in that the usual diffusion in the machine was enhanced approximately 10 times via ripple in the quadrupole power supplies. The measurement technique for determining the dynamic aperture was also different: a scraper was used to measure the radius inside which particles were not lost. Loss measurements were made for approximately 20 minutes after the tune modulation was turned on. Qualitatively, there was a correlation of loss rate (dynamic aperture) with ripple amplitude. The effect of the addition of ripple at two frequencies was much worse than a simple linear superposition would predict, which is to be expected if the two ripple frequencies cause resonance overlap.

Particles were tracked with ripple for  $10^6$ ,  $5 \cdot 10^6$ , and  $10^7$  turns ( $10^7$  turns is approximately 10 minutes in the SPS). There was a significant difference (a decrease of  $\sim 25\%$ ) in the dynamic aperture between  $10^6$  and  $10^7$  turns. The tracking dynamic aperture for  $10^7$  turns and the measured dynamic aperture were in fairly good agreement (the tracking dynamic aperture was  $\sim 10\text{-}20\%$  larger). Here we see again that to predict long-term stability it is necessary to track for many turns. The "onset of chaos" as indicated by the Lyapunov exponent was in some cases  $\sim 20\%$  smaller than the measured dynamic aperture, indicating that it can be a pessimistic predictor of dynamic aperture.

## 4.0 Computing Tools

There are several new software tools available for accelerator physics simulations. Some take advantage of modern computer science techniques, and some are elegant implementations of DA packages. Advances in computing speed are being exploited for multi-particle long-term tracking, with the hope that for the SSC it will be possible to do element-by-element tracking for the full injection time in the year or two.

We also heard a presentation about a system developed at CEBAF which allows the substitution of a simulated machine for the real machine for testing correction algorithms for controls.

### 4.1 DA Libraries

Differential algebra libraries are now available in many forms. The original FORTRAN library is available from M. Berz<sup>3</sup>. At SSCL, Yiton Yan has developed a FORTRAN library which is optimized for the CRAY, and which uses dynamic memory allocation. At Fermilab, Leo Michelotti has developed an elegant C++ DA library, which allows the user to manipulate DA vectors using standard arithmetic symbols such as + and \*. Johan Bengtsson at LBL has developed a Pascal-based input language for the original Berz FORTRAN package<sup>4</sup>. All these packages have advantages over the simple FORTRAN library, and their development is evidence that DA techniques are being more widely used.

### 4.2 Beamline Class

At Fermilab, Leo Michelotti has developed a C++ beamline class which is quite powerful. It allows the description of beamlines, calculation of twiss parameters, and also tracking. Since C++ is used, the tracking function (called "propagate") will accept either particle coordinates or a DA vector, either of which will be propagated through the lattice in the appropriate manner. Several analysis methods are also provided—for example, there is one to compute the driving terms for transverse resonances. The underlying physical description of the beamline is modular, and can be either one of the standard modules provided (such as matrix, or kick-code) or user-specified. This is an elegant tool which combines standard tracking and analysis techniques with DA.

### 4.3 The Integrated Scientific ToolKit

Vern Paxson presented work being done at SSCL and LBL on the Integrated Scientific Tool



Kit<sup>5</sup>. ISTK has three major components—Glish, a language for writing control sequences, Glistk, a toolkit for writing user-interfaces, and SDS, a standard data format. These tools all work together very well—for example, it is easy to make buttons created with Glistk send events understood by Glish, and the events can include SDS datasets as values. ISTK provides a powerful environment for creating interactive, graphical simulations which can easily move to controls, since it encourages the use of independent modules by making interprocess connections simple to create.

#### *4.4 Tracking with the Hypercube*

Tracking with maps would not be necessary if we had more computer power at our disposal. George Bourianoff described the efforts at SSCL to use parallel computers for multi-particle tracking. Multi-particle tracking is well-suited to coarse-grained parallelism, since each particle is independent of the others. Therefore requirements for communication between nodes is minimal, and one gets full advantage of each node. Since supercomputer speeds are saturating, but single chip speeds are still climbing rapidly each year, parallel machine speeds will surpass CRAY's for many problems in the near future. Already, the 64 node Hypercube can perform element-by-element tracking for 64 particles for  $10^5$  turns in 20% less time than the CRAY Y/MP.

#### *4.5 Simulation of Correction Algorithms at CEBAF*

Jörg Kewisch of CEBAF described their scheme for simulating correction algorithms in the context of controls. This system allows one to replace the accelerator with a simulation which writes data to the shared memory which serves as the machine database. The controls algorithms then read the simulated data from shared memory, just as though it were data from the real machine, and compute corrector strengths. In this way, a correction algorithm can be tested on simulated data in the context of the controls system. This addresses the issue of testing controls correction algorithms when the machine is not yet built, but requires a working controls system.

### **5.0 Simulations of Correction Schemes**

A full day of presentations and discussions at the workshop were devoted to examples of simulations of correction schemes. A wide variety of machines were represented. Only decoupling in SSC and LHC will be described here. Others presentations are described in the accompanying papers in these proceedings.

#### *5.1 Decoupling SSC and LHC*

In a presentation by George Bourianoff, we heard about plans for decoupling the SSC. a discussion followed which compared SSC with LHC. There was agreement that coupling adversely affects the dynamic aperture and must be corrected. SSC and LHC are expected to have random and systematic skew quad errors of comparable magnitude, but the effects in the two machines will be different, and, currently, different correction schemes are envisioned.

The SSC has two very long arcs, which makes local correction in the arcs necessary, since otherwise the systematic skew quadrupole errors can build up to unacceptable levels. The horizontal and vertical integer tunes must be split for performance to be acceptable. The current correction scheme calls for skew quads in half-cell centers specifically chosen not to enhance vertical dispersion. There are approximately 100 correctors. The correction scheme will use measurements of the beam transfer function at many ( $\sim 100$ ) local monitors to minimize the coupling. For details, see R. Talman's paper on a universal correction algorithm for accelerators in these proceedings.

The LHC has 8 arcs, and uses skew quads in the interaction regions for correction. There

are four families, for a total of 92 skew quad correctors, in the current scheme. Correction is done by minimizing the distance of closest approach of the tunes, zeroing off-diagonal matrix elements, and zeroing the first order difference and sum resonance driving terms.

There was some disagreement between the two groups as to whether systematic or random skew quad errors were more damaging. However, it is important to note that both agreed that coupling is not simply a linear phenomenon that can be ignored in machine simulations which are meant to predict dynamic aperture. There are two ways in which coupling can decrease dynamic aperture: one is by the excitation of skew resonances, and the other—due to random skew quadrupole errors—is through the random distortion of lattice functions.<sup>6</sup>

## 6.0 Conclusions

Many advances in simulation for accelerator design have been made in recent years—both in the application of mathematical techniques new to accelerator physics and in the adoption of current computing techniques—which give us a powerful set of tools for analyzing lattices. However, as always, these tools must be used with care. In estimating dynamic aperture it is important to be aware of the approximations being made by the chosen tracking program. If one-turn maps are used, an entire set of investigations is necessary to check (as much as is possible) that the order of the map is sufficient. Once tracking has been done, one must understand the reasons for particle loss (*e.g.*, are the lost particles crossing an avoidable resonance?). In fact, given the unavoidable approximations in any tracking code, the real utility of long-term tracking is in the insight it gives into potential mechanisms for particle loss.

Recent measurements of dynamic aperture on proton storage rings have shown that long-term tracking is necessary to accurately predict long-term dynamic aperture. This is an interesting and important area of study, and more quantitative comparisons of measurements and simulations are needed.

We have a rich collection of tools for simulation and modelling at our disposal. However, as was demonstrated again and again in the course of this workshop, there is a real danger of obtaining inaccurate results unless the physics in the tools is appropriate to the problem at hand.

## 7.0 Acknowledgments

Many thanks to George Bourianoff for serving as scientific secretary for this working group. His notes and comments were very helpful.

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LAWRENCE BERKELEY LABORATORY  
UNIVERSITY OF CALIFORNIA  
INFORMATION RESOURCES DEPARTMENT  
BERKELEY, CALIFORNIA 94720