Advanced Computing for 21st Century Accelerator Science and Technology

Progress Report on University of Maryland Activities 15 July 2001 – 14 July 2005

Alex J. Dragt
Department of Physics
University of Maryland
College Park, Maryland 20742

September 2004

Prepared for the U.S. Department of Energy under Grant DEFC0201ER41191

Report ER41191-1

Overview

Dr. Dragt of the University of Maryland is one of the Institutional Principal Investigators for the SciDAC Accelerator Modeling Project *Advanced Computing for 21*st *Century Accelerator Science and Technology* whose principal investigators are Dr. Kwok Ko (Stanford Linear Accelerator Center) and Dr. Robert Ryne (Lawrence Berkeley National Laboratory). This report covers the activities of Dr. Dragt while at Berkeley during spring 2002 and at Maryland during fall 2003.

Work on Code Development

Completion of MaryLie 3.0 and Construction of MaryLie-IMPACT: MaryLie 3.0, a Program for Charged Particle Beam Transport Based on Lie Algebraic Methods, was completed. It consists of approximately 40,000 lines of code organized into approximately 500 routines, and is accompanied by a 900-page Users' Manual. The purpose of MaryLie is to aid in the design and evaluation of both linear charged particle beam transport systems and circulating storage rings. The capabilities of MaryLie are further described below. As an additional part of the SciDAC effort, MaryLie has had added to it the space-charge and RF gap modeling capabilities of the code IMPACT to produce the code ML/I (MaryLie-IMPACT).

The MaryLie (and hence also the ML/I) program employs algorithms based on a Lie algebraic formulation of charged particle trajectory calculations, and is able to compute transfer maps for and trace rays through single or multiple beam-line elements. This is done for the full 6-dimensional phase space *without* the use of numerical integration or traditional matrix methods. All nonlinearities, including chromatic effects, through third (octupole) order are included. (Significant portions of ML/I also contain 5th-order MaryLie code.) In addition, MaryLie is exactly symplectic (canonical) through all orders.

MaryLie may be used both for particle tracking around or through a lattice and for analysis of linear and nonlinear lattice properties. It may also be used to transport moments without the need for particle tracking. When used for tracking, it is both versatile and extremely fast. Tracking can be performed element by element, lump by lump, or any mixture of the two. (A lump is a collection of elements combined together and treated by a single transfer map.) The speed for element by element tracking is

comparable to that of other tracking codes. When collections of elements can be lumped together to form single transfer maps, tracking speeds can be orders of magnitude faster.

MaryLie also has extremely powerful analytic tools. They include the calculation of tunes and first and second-order chromaticities (dependence of tunes on energy) and anharmonicities (dependence of tunes on betatron amplitudes) and first, second, and third-order temporal dispersion (dependence of closed-orbit transit time on energy, sometimes called the phase-slip factor, and related to momentum compaction, the dependence of the closed-orbit length on energy); first, second, and third-order ordinary dispersion, and all other linear lattice functions and their energy dependence through second order; nonlinear lattice functions; nonlinear phase-space distortion; transfer map normal forms; nonlinear resonance driving terms; nonlinear invariants; expected Fourier coefficients for tracking data; and moment data including eigenemittances and high-order moments.

To facilitate actual machine design, MaryLie has extensive fitting, scanning, and optimization routines. These routines make it possible to fit, scan, or optimize essentially all quantities that can be computed by MaryLie including those computed in user written subroutines. MaryLie also provides full geometrical information including the orientation and location of beamline elements in 3-dimensional space.

Finally, MaryLie can be used to give an explicit representation for the linear and nonlinear properties of the total transfer map of a system. This information can be used to evaluate or improve the optical quality of a single pass system such as a beam transport line or linear collider. For a circulating system such as a storage ring, the one-turn transfer map can be used to compute the linear aperture, and it is hoped that the explicit knowledge of this map can eventually be used to predict the dynamic aperture without the need for extensive long-term tracking.

Work on Algorithm Development

Map Generation for Realistic Beamline Elements: The ability to generate transfer maps represents a key component needed in a beam optics code. Previously most codes have modeled only idealized elements. We have developed methods for using numerical field data (e.g. measured or computed) on some enclosing surface S to generate realistic and robustly accurate transfer maps. This is a major modeling advance. The known surface data is used to generate data in the interior volume V that are both exactly Maxwellian and analytic so that the required associated Taylor expansions can be computed to any desired order. These methods enjoy the smoothing property associated with Laplace's equation: any solution of Laplace's equation must take its extrema on the boundary. Since these methods make controlled fits on S, the error is guaranteed to be controlled (and less) everywhere in the interior V. Preliminary application has made to the case of next generation wigglers installed in CESR and anticipated for the ILC damping rings. Excellent agreement has been demonstrated between fields calculated from the surface data and the field available at interior grid points. (By contrast, the traditional method of

using midplane data at discrete points to extrapolate out gives poor results.) Use of these new methods allows realistic treatment of all fringe-field and multipole-error effects. These map generation algorithms (through 5^{th} or perhaps 7^{th} order) will eventually become standard parts of MaryLie and ML/I.