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ADVANCED METHODS FOR THE COMPUTATION OF PARTICLE
BEAM TRANSPORT AND THE COMPUTATION OF
ELECTROMAGNETIC FIELDS AND BEAM-CAVITY INTERACTIONS

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1 ABSTRACT

The University of Maryland Dynamical Systems and Accelerator Theory Group carries out research in two broad areas: the computation of charged particle beam transport using Lie algebraic methods and advanced methods for the computation of electromagnetic fields and beam-cavity interactions. Important improvements in the state of the art are believed to be possible in both of these areas. In addition, applications of these methods are made to problems of current interest in accelerator physics including the theoretical performance of present and proposed high energy machines.

The Lie algebraic method of computing and analyzing beam transport handles both linear and nonlinear beam elements. Tests show this method to be superior to the earlier matrix or numerical integration methods. It has wide application to many areas including accelerator physics, intense particle beams, ion microprobes, high resolution electron microscopy, and light optics.

With regard to the area of electromagnetic fields and beam cavity interactions, work is carried out on the theory of beam breakup in single pulses. Work is also done on the analysis of the high frequency behavior of longitudinal and transverse coupling impedances, including the examination of methods which may be used to measure these impedances. Finally, work is performed on the electromagnetic analysis of coupled cavities and on the coupling of cavities to waveguides.

In addition to its research effort, the Dynamical Systems and Accelerator Theory Group is actively engaged in the education of students and post-doctoral research associates. To this end, it presents a regular graduate seminar course in accelerator physics, directs graduate students in M.S. and Ph.D. thesis research, and guides and fosters the research of post-doctoral research associates.

Substantial progress in research has been made during the past contract/grant period. There have also been important educational accomplishments. These achievements are summarized in the following report.

2 Educational Accomplishments

One of the major goals of the Dynamical Systems and Accelerator Theory Group is the education of students, postdoctoral research associates, and visiting scientists. Listed below are present and past students associated with the program, postdoctoral research associates, and visiting scientists.

2.1 Present Graduate Students

Dan Abell

Thesis work in progress on the computation and analytic properties of transfer maps.

Wen Hao Cheng

Now in his second year as a Graduate Research Assistant studying the current carrying capacity of an alternating phase focussing linac. He is also starting to work on the calculation of the transverse impedance of an obstacle in a beam pipe.

Shicheng Jiang

Now in his first year as a Graduate Research Assistant working on the impedance of a thick iris.

2.2 Past Graduate Students

David Douglas, Ph.D. 1982.

Thesis: Lie Algebraic Methods for Particle Accelerator Theory.

Employment: Previously employed by the Lawrence Berkeley Laboratory.

Presently employed by the Continuous Electron Beam Accelerator Facility.

Etienne Forest, Ph.D. 1984.

Thesis: Lie Algebraic Methods for Charged Particle Beams and Light Optics.

Employment: Currently employed by the Lawrence Berkeley Laboratory.

Janko Milutinovic, Ph.D. 1984.

Thesis work done in Elementary Particle Theory while simultaneously receiving training in Accelerator Theory.

Employment: Accelerator Theory at Brookhaven National Laboratory.

Liam Healy, Ph.D. 1986.

Thesis: Lie Algebraic Methods for Treating Lattice Parameter Errors in Particle Accelerators.

Employment: Previously at CERN. Presently with celestial mechanics group at the Naval Research Laboratory.

Robert Ryne, Ph.D. 1987.

Thesis: Lie Algebraic Treatment of Space Charge.

Employment: Previously employed by Lawrence Livermore National Laboratory. Presently employed by the Los Alamos National Laboratory.

Petra Schuett (1987-88).

Worked one year at Maryland on Lie algebraic methods and Poisson solvers while simultaneously completing her Ph.D. thesis work on Wake-Field Acceleration under Thomas Weiland at DESY.

Employment: Presently with the Theoretische Elektrotechnik Group at the Darmstadt Technische Hochschule.

Govindan Rangarajan, Ph.D. 1990.

Thesis: Invariants for Symplectic Maps and Symplectic Completion of Symplectic Jets.

Employment: Lawrence Berkeley Laboratory.

Rui Li, Ph.D. 1990.

Thesis: Analytic and Numerical Investigation of the Longitudinal Coupling Impedance

Employment: Continuous Electron Beam Accelerator Facility.

John Diamond, M.S. 1990

Spent two years as a Graduate Research Assistant working on the penetration of electromagnetic fields through circular holes in a thick metallic wall. Also carried out symbolic manipulation program calculations for various complicated beamline elements such as combined function quadrupoles and combined function bends. In addition, responsible for general computational support. Now working at Adroit Systems, Alexandria, VA.

William Detlefs, M.S. (in Applied Math with Thesis) 1991

Thesis: Longitudinal Coupling Impedance of a Thin Iris Collimator.

Employment: Now a graduate student with support in Physics at Cal Tech.

2.3 Other Students

Dimitris Vassiliadis (1987-88)

Spent 1 1/2 years working as a Graduate Research Assistant on Alternating Phase Focussing. Now affiliated with a group working on chaos.

Jeffrey Skibo (1988-89)

Spent one year exploring possible further work on the use of Lie algebraic methods in the treatment of space charge. Also responsible for general computational support. Now working in space physics.

Eric Salter (1990-91)

Spent one year working on the calculation of the impedance of a thick iris. Also did programming for MARYLIE and provided general computational support. Now serving as a Teaching Assistant.

Glenn VanderWoude (1988-)

Undergraduate student and National Merit Scholar. Responsible for general computational support.

2.4 Present Ph.D. Professional Staff

Fernando Casas (1992-)

Visiting postdoctoral fellow, supported by Spanish Government.

Ivan Gjaja (1991-)

Postdoctoral research associate and SSC fellow.

Branislav Radak (1992-)

Postdoctoral research associate.

Johannes van Zeijts (1987-)

Postdoctoral research associate.

2.5 Past Ph.D. Professional Staff

Herbert O. Moser (1985)

Visiting Scientist. Presently at IMM Institut fur Mikrotechnik, Mainz Germany.

Hiromi Okamoto (1989-90)

Visiting postdoctoral research associate. Presently at Nuclear Science Laboratory, Institute for Chemical Research, Kyoto Japan.

Filippo Neri (1983-90)

Postdoctoral Research Associate. Presently at Los Alamos National Laboratory.

3 Research Accomplishments

Most of the major objectives set forth in the 1989 proposal have been met, and additional objectives have been achieved as well. A brief summary of work accomplished over the last contract/grant period is given below.

3.1 Task A: Charged Particle Beam Transport

1. The program MARYLIE 3.0, comprising approximately 32,000 lines of code, is nearly ready for wide distribution and general use. A detailed instruction manual, consisting of some 470 pages and set in TEX, is substantially complete.¹ Preliminary versions of the code have been tested on VAX, CRAY, IBM, SUN, and UNIX computers, and are in use in various laboratories in the United States, Canada, and Europe.
2. Several major improvements and additions have been made to various MARYLIE components. Some of these improvements and additions are listed below:
 - (a) The MARYLIE fitting routines have received dramatic improvements. Suppose the device or machine under study has a set of properties A (focal lengths, aberrations, tunes, chromaticities, etc.), and we wish to adjust various parameters to achieve a set of properties B that may be quite far from A . A new MARYLIE procedure determines a set of target values that moves continuously from A to B . The MARYLIE fitting routines then continuously adjust parameter values to follow the moving target values until the final target B values are achieved. This new algorithm has remarkable convergence properties, and allows the solution of fitting problems that were previously intractable or impossible by earlier techniques.
 - (b) Optimizing routines have been added. These routines adjust parameters to optimize arbitrary merit functions, and are of use when fits are not possible.
 - (c) Scanning routines have been added that facilitate parameter studies. These routines automatically scan parameter space, and prepare convenient graphical output.
 - (d) The logic of the fitting, optimizing, and scanning procedures has been extended so that it is possible to fit in an "inner loop" while scanning or optimizing in an "outer loop".
 - (e) A routine has been added to MARYLIE for the numerical computation of the transfer map for a combined function bend.² A

combined function bend is a sector dipole with superimposed normal and skew quadrupole, sextupole, and octupole fields. This MARYLIE feature has been used extensively at Brookhaven National Laboratory for the design of compact synchrotron light sources with superconducting bends.

- (f) A routine has been added to MARYLIE for the analytical computation of the transfer map for a combined function quadrupole.³ A combined function quadrupole is a quadrupole with superimposed normal and skew sextupole and octupole fields. The FORTRAN for this routine was produced by symbolic manipulation, and comprises some 3000 lines of dense code. This new MARYLIE feature, because of its high execution speed, has been essential to the design and ultimate success of the final expansion telescope for the Los Alamos Neutral Particle Beam program.
 - (g) A routine has been added to MARYLIE for the numerical computation of the transfer map for a solenoid including fringe-field effects.⁴ The addition of this routine makes it possible to model beam transport systems with solenoids. The effect of solenoidal fields in detectors and the skew quadrupole correction of solenoidal effects can also be studied. Finally, the performance of electron microscopes can be studied.
 - (h) Routines have been added to MARYLIE for the generation of various particle distributions. The generation and subsequent tracking of these distributions is useful for the study of the performance of transport lines, telescopes, and final focus systems. These routines also calculate all moments, through order 6, of the various distributions. These moments are of interest for studying emittance growth.
- 3. A version of MARYLIE 3.1, a third-order code including error effects, has been assembled and used to study the importance of misalignment effects in the Final Focus Test Beam facility under construction at Stanford.⁵
 - 4. Versions of MARYLIE 5.0, a fifth-order code, are in use at Los Alamos. These versions contain extensive GENMAP routines that compute trans-

fer maps for octupole and decupole corrected rare-earth-cobalt quadrupoles including all fringe field effects.^{6,7,8}

5. Work has begun on MARYLIE 5.1, a fifth-order code including error effects.
6. Lie algebraic map multiplication rules have recently been worked out through seventh order using symbolic manipulation. These rules are a key step in the construction of a seventh-order Lie algebraic program.
7. A new hybrid code that uses both Taylor series and Lie algebraic methods has been developed. This code, called Tlie, works numerically to arbitrary order.⁹ That is, given any Hamiltonian expanded to some order, it can compute by numerical means the associated transfer map to the same order. It can also multiply maps of any specified order. Tlie has been used to cross check other existing codes, and for fifth and higher order aberration studies at Los Alamos. In addition, it has been used to study the importance of misalignment and higher-order aberration effects for the Stanford Final Focus Test Beam Facility.⁵
8. The computation of error effects in nonlinear Hamiltonian systems using Lie algebraic methods has been worked out in detail, and applied to the problem of steering magnets and mispowered dipoles.¹⁰ These computations will be implemented in MARYLIE 3.1 and 5.1, and cross checked with Tlie.
9. Self consistent Lie algebraic calculations have been carried out for cylindrically symmetric beams with linear and nonlinear space-charge effects.¹¹ These calculations agree well with particle in cell simulations. However, they are orders of magnitude faster since they compute the transfer map directly rather than follow the trajectories of a large number of particles. Moreover, they provide aberration data that is inaccessible to particle in cell codes due to their large statistical noise.
10. A theory and procedure has been developed for the construction of complete third-order achromats.¹² A complete third-order achromat bends a charged particle beam, but otherwise has an identity transfer map through third order for the full six-dimensional phase space including

time of flight terms. The theory of such achromats makes use of normal form procedures. It is expected that such achromats may be of use in the design of time of flight mass spectrometers and certain high performance storage rings.

11. General moment invariants have been found for linear Hamiltonian systems.^{13,14,15} This work generalizes the concept of emittance to the full six-dimensional phase space, and shows that there are three conserved *eigen emittances* (constructed from second-order moments) for general linear Hamiltonian systems. It also shows that there are an infinite number of invariants for such systems that can be constructed from third and higher-order moments. These higher-order invariants may be of use for studying nonlinear effects.
12. Based on the work just described, a general new theory has been developed for the description of beams in a full six-dimensional phase space.¹⁶ This theory generalizes the usual Twiss beam envelope description (used for the earlier two-dimensional phase space description) by the introduction of *envelope matrices* and *eigen phase advances* in addition to the *eigen emittances* described above. The computation of eigen emittances, envelope matrices, and eigen phase advances has been made a standard MARYLIE command. It is expected that these new tools will facilitate the calculation and description of projected emittance growth due to linear cross couplings.¹⁷
13. Work has begun on the computation of the dynamic aperture for a ring using the one-turn map for tracking studies.¹⁸ This method appears promising provided suitable procedures can be found for symplectifying high-order Taylor expansions. If successful, tracking using the one-turn map (or at least a small number of lumps) should be orders of magnitude faster than the usual element to element tracking, and should also permit a much more accurate treatment of real magnets with distributed multipoles and fringe-field effects.
14. The use of Taylor series maps raises at least two questions. First, what is the domain of convergence of the series? Second, how can a truncated expansion be made symplectic? Work has begun on the first

question as part of the thesis research of Dan Abell, and preliminary results have been found for the anharmonic oscillator and the pendulum problem. Work on the second question constituted part of the thesis of Dr. Govindan Rangarajan, and more work on this question is in progress.^{15,19,20}

15. Some of the work undertaken, both on symplectification methods and the description of charged particle beam transport using moments, raises various questions concerning the symplectic group $Sp(6)$ and the full group of symplectic maps. Some of these questions have been answered including certain questions about $Sp(6)$ representations and questions about the existence of *invariant metrics*.^{15,21} It is expected that these tools will be of use for further study. For example, representation theory is useful in the construction and understanding of invariants such as emittance invariants. Invariant metrics may be useful in characterizing the nonlinear component of a transfer map, and the convergence of various symplectification procedures.
16. Work has begun on writing an extensive set of Lecture Notes on Non-linear Dynamics and Lie Methods with Applications to Accelerator Physics.²²

3.2 Task B: Computation of Electromagnetic Fields and Beam-Cavity Interactions

1. Beam Cavity Interactions/Beam Breakup

Work was completed on the theory of beam breakup with coupling between cavities [a]. Results were obtained as a function of the ratio of Q^{-1} to the dispersion curve band width and to the separation of modes. For zero band width the results reduce to those for cumulative beam breakup. For Q^{-1} less than the separation between the modes, the results reduce to regenerative beam breakup. Thus our formalism contains the more general case, but reduces to the usual results in these limits.

The theory of single bunch beam breakup has been extended to include BNS damping as well as Autophasing [b,c,d]. Universal curves have

been obtained for the suppression of beam breakup as a function of the energy gradient introduced into the bunch and these have been compared with the formalism of Balakin [e].

2. Coupling Impedance

The coupling impedance of an obstacle in a beam pipe was formulated in terms of an integral equation for the axial electric field at the wall at the location of the obstacle [f]. This formulation permitted the study of the impedance in the high frequency limit [f], as well as for a periodic array of obstacles [g]. In addition results were obtained for a small obstacle [h] as well as for a large number of obstacles [i] in order to study the transition to the periodic result. In this work confirmation was obtained of the prediction by Palmer [j] that the impedance would increase only as the square root of the number of obstacles due to a "shadowing" effect. The integral equation method was also applied to the calculation of the transmission coefficient for a thin wire in the same cavity geometry [k], and the results showed that the wire measurement of impedance is more reliable than had been anticipated. All of these calculations are described in detail in Rui Li's thesis [ℓ]. In addition, the method was also applied to the calculation of the impedance of a multi-cell, multi-block structure [m].

3. Impedance of an Iris Collimator

A method has been developed to calculate the impedance of an iris within a beam pipe [n]. Numerical calculations have been carried out for zero iris thickness [o] and asymptotic results obtained for a small iris in both the low and high frequency limits.

4. Penetration of Fields through Holes in a Conducting Wall

Work has been completed on the calculation of the penetration of electromagnetic fields through small holes of general shape in a wall of zero thickness [p]. In this analysis, variational forms are constructed for the polarizability and susceptibilities of the hole. With judiciously chosen trial functions, one can obtain accurate values of these parameters for a variety of shapes. The procedure was then extended to a circular hole in a thick wall [q] and numerical values accurate to at least 4 significant figures were obtained over the complete range of the ratio wall

thickness/hole radius from 0 to ∞ .

5. Free Electron Lasers

A universal scaling function has been obtained for FEL gain for a laser including optical guiding [r]. This is obtained from a variational formulation in the exponential region before saturation, incorporating the energy spread, emittance, and focussing of the electron beam and the diffraction and guiding of the radiation.

The fields in a variety of compact wiggler designs have been calculated. These included a bifilar helix [s] and a slotted cylindrical shell [t].

The effect of wiggler errors on FEL gain has also been calculated [u] with results that are somewhat less serious than earlier estimated.

6. Miscellaneous

During the contract period, a number of other reports have been written primarily at LANL and CERN on a variety of subjects.

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5.1 Task A

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