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ADVANCED METHODS FOR THE COMPUTATION OF PARTICLE  
BEAM TRANSPORT  
AND  
THE COMPUTATION OF ELECTROMAGNETIC FIELDS AND  
MULTIPARTICLE PHENOMENA

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## **ABSTRACT**

Since 1980, under the grant DEFG02-96ER40949, the Department of Energy has supported the educational and research work of the University of Maryland Dynamical Systems and Accelerator Theory (DSAT) Group. The primary focus of this educational/research group has been on the computation and analysis of charged-particle beam transport using Lie algebraic methods, and on advanced methods for the computation of electromagnetic fields and multiparticle phenomena. This Final Report summarizes the accomplishments of the DSAT Group from its inception in 1980 through its end in 2011.

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# 1 Introduction

The University of Maryland Dynamical Systems and Accelerator Theory (DSAT) Group has been carrying out long-term research work in the general area of Dynamical Systems with a particular emphasis on applications to Accelerator Physics. Work has been devoted to both the development of new methods and the application of these methods to problems of current interest in accelerator physics, including the theoretical performance of present and proposed high-energy machines and light sources.

In particular, Lie algebraic methods have been developed for computing beam transport in both linear and nonlinear beam elements. These methods have several advantages over the earlier matrix or numerical integration methods. They have wide application to many areas including accelerator physics, intense particle beams, ion microprobes, high resolution electron microscopy, and light optics.

Much of this work is documented in the draft manuscript *Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics*, which is available on the DSAT Web site

<http://www.physics.umd.edu/dsat/>

Currently some 2026 pages are posted, with additions being made monthly. In future discussion this material will be referred to simply as the Lie Methods book.

A considerable amount of this material is new to the fields of Nonlinear Dynamics and Accelerator Science, and cannot be found easily, or even at all, elsewhere. Although primarily aimed at the field of Accelerator Science, it is also meant to be of interest to the broader community. Indeed, since its appearance on the Web, several people in the broader Nonlinear Dynamics community have greeted its availability with enthusiasm.

In addition to carrying out research, the DSAT Group was actively engaged in the education of students and post-doctoral research associates. To this end, it held weekly group meetings/seminars, directed graduate students in M.S. and Ph.D. thesis research, and guided and fostered the research of Post-doctoral Research Associates and Visiting Scientists. A list of past Ph.D. students, including their thesis topics, is provided in Section 6. Additional information, including links to their theses, and information about

undergraduate and M.S. students as well as Post-doctoral Research Associates and Visiting Scientists, can be found at the DSAT web site.

## 2 Past Work

Over the past several years a new method, employing Lie algebraic tools, has been developed for the computation of charged particle beam transport and accelerator design. It represents the action of each separate element of a beamline or accelerator, including nonlinear effects, by a transfer map expressed as a product of Lie transformations. These maps can then be combined, manipulated, analyzed, and applied, following well-defined Lie-algebraic rules, to compute, analyze, and simulate a wide variety of beam transport phenomena. The goal is to treat all nonlinear phenomena with the same ease as matrix methods treat linear phenomena [1-5].

These map methods have been implemented through third order in the code *MaryLie 3.0*. It consists of a Main Program and approximately 500 sub-routines that together comprise approximately 40,000 lines of Fortran code. The program is fully documented by a 930-page Users' Manual. Copies of this Manual, and instructions how to obtain the MaryLie code, are available at the DSAT Web site.

A Hybrid Lie-PIC Beam Transport Code (MaryLie/IMPACT) has been constructed in collaboration with R. Ryne (LBNL) and other members of the DOE Accelerator Physics SciDAC consortium. MaryLie/IMPACT incorporates both the full linear and nonlinear beam-line element library of MaryLie and standard PIC routines for space-charge effects [6]. The library includes all standard beam-line elements as well as REC quads and solenoids with fringe fields through fifth order. (That is, the code of *MaryLie 5.0* has been incorporated.) The MaryLie code has also been modified to handle true acceleration (it had previously only treated synchrotron oscillations about a fixed design energy) so that it is fully applicable to linear accelerators and ramping synchrotrons or storage rings, as well as quiescent storage rings and static devices such as beamlines and spectrometers. PIC routines have been incorporated and tracking with space charge has been implemented by splitting all beam-line elements into sequences of MaryLie tracking steps interspersed with space-charge kicks based on the PIC routines. Finally, the lattice translator part of the code has been enlarged so as to accept both

MAD and MaryLie input formats.

Both MaryLie 3.0 and MaryLie/IMPACT are available at no cost to all U.S. Government supported projects and laboratories. A Multi-Platform Graphic User Interface version of MaryLie 3.0, prepared jointly with G.H. Gillespie Associates, Inc., is available for non-government sponsored use [7]. The Gillespie Associates version has, in addition to ease of use, the virtue of enabling ready comparison of results from various codes. See the web site

<http://www.ghga.com/accelsoft/>

Many of these map methods, all originally discovered and developed by our Maryland group, have also become standard components of many other codes including MAD, BMAD, Six Track, and Cosy Infinity. Some of them are summarized in the *Handbook of Accelerator Physics and Engineering* edited by Alex Chao and Maury Tigner [8,9]. Correspondingly, their use is now routinely covered in U.S. Particle Accelerator Schools. Finally, map and Lie methods have been used and developed extensively at SLAC for the design and operation of the SLC, the FFTB Facility, and the PEP II B-factory, and for the design of the ILC [10-13]. They also played a key role in dynamic aperture and long-term tracking studies for the LHC [14,15].

Some of the fundamental Lie algebraic advances pioneered by the DSAT group are listed below:

- Emphasis on the modern map approach to the description of dynamical systems and, in the case of accelerator physics, emphasis on the symplectic or near symplectic nature of these maps. Thus, if synchrotron radiation effects and multi-particle including wake-field effects are neglected, the transfer map for any beam-line element, including all nonlinear effects, is a symplectic map.
- Treatment of full 6-dimensional phase space including all synchro-betatron effects and acceleration.
- Development and compilation of extensive information about the symplectic group and symplectic maps.
- Lie algebraic representation of symplectic maps, as factored products, in terms of Lie transformations whose generators (Lie operators) are

characterized by homogeneous polynomials. Thus, the Lie algebraic approach provides a unique way of describing (parameterizing) symplectic maps: for every set of homogeneous polynomials there is a unique symplectic map, and for every symplectic map there is a unique set of homogeneous polynomials that generate this map. By contrast, if a symplectic map is described by a Taylor series, many more coefficients are required and these coefficients are not independent, but instead are constrained by a large number of nonlinear relations arising from the symplectic condition. In addition to its applications in charged-particle beam optics and light optics, this factored-product Lie algebraic representation has now been widely used in quantum chemistry [16].

- Introduction and development of Truncated Power Series Algebra (TPSA) to manipulate these polynomials [17].
- Introduction of an invariant scalar product within the space of these polynomials to measure their magnitudes, and to decompose quadratic Lie operators into Hermitian and non-Hermitian parts.
- Formulas and algorithms for computing symplectic maps for arbitrary Hamiltonians including those for ‘s-dependent’ beam-line elements.
- Development of Surface Methods for the computation of realistic transfer maps for actual beam-line elements based on the use of accurate 3-dimensional field data [18-23].
- Formulas for multiplying and inverting symplectic maps in Lie form. Thus, maps for successive beam-line elements can be combined to obtain grand maps for complete beam lines, or one-turn maps for rings.
- Normal form analysis of one-turn symplectic maps. This analysis is a nonlinear generalization of matrix diagonalization. Suppose  $\mathcal{M}$  is a one-turn symplectic map. Then there is a symplectic map  $\mathcal{A}$  such the map  $\mathcal{N}$  given by

$$\mathcal{N} = \mathcal{A}^{-1}\mathcal{M}\mathcal{A}$$

is in normal form. The map  $\mathcal{N}$  provides complete information about tunes, anharmonicities, chromaticities, and momentum compaction to

the order to which  $\mathcal{M}$  is specified. The map  $\mathcal{A}$  provides complete information about linear and nonlinear dispersion, linear and nonlinear lattice functions, and Courant-Snyder invariants including their nonlinear generalizations. It can also be used to construct matched particle distributions, including all nonlinear effects. All this analysis includes arbitrary coupling between the transverse and temporal degrees of freedom. Also, unlike the older approach to calculating nonlinear phenomena, which employed either various integrals over lattice functions or elaborate Hamiltonian perturbation theory, and which could not be pursued to high order due to algebraic complexity, normal form analysis uses Lie algebraic tools to compute (to any desired order) all quantities directly from the one-turn map. And (as described above) this map is in turn also computed using Lie algebraic tools.

- Introduction of resonance bases that permit the calculation of normal forms. They can also be used to characterize nonlinear-resonance driving terms in the one-turn map. The magnitude of these terms is correlated with the size of the dynamic aperture.
- Canonical treatment of errors by extending phase space to 8 dimensions. This development makes it possible to treat by map methods all misplacement, misalignment, and mispowering errors. When used in conjunction with extended normal form routines, these methods enable the determination of closed orbits in machines with errors and the effects of these errors on tunes, anharmonicities, chromaticities, momentum compaction, dispersion, lattice functions, and Courant-Snyder invariants. All tools are now in place for the construction of *MaryLie 7.1*, a seventh-order code that will treat all error and nonlinear effects through seventh (16-pole) order.
- Symplectic tracking using individual maps, lumps (a lump is a collection of elements combined together and treated by a single transfer map), and full one-turn maps. Both generating-function and Cremona-map methods were invented for this purpose, and their use can yield speed improvements over conventional element-by-element-tracking methods by at least an order of magnitude. They can also be employed for realistic maps, including all fringe-field and high-order multipole effects, without any loss in speed.



- Construction of aberration-corrected systems including microscopes, telescopes, spot-forming systems, and high-order achromats.
- Moment analysis, computation of eigen-emittances for general phase-space distributions, and map-based moment transport. These methods are now being used to analyze mechanisms for producing electron beams with very high transverse brightness [24].
- Symplectic classification of all analytic vector fields. This classification makes it possible to uniquely factor an arbitrary map into symplectic and nonsymplectic parts. In the field of accelerator physics, this factorization is expected to have application to the treatment of synchrotron radiation damping.
- Lie formulation of symplectic integration. This formulation was fundamental for many subsequent developments in the field. Similar Lie formulations are now also employed in the field of quantum computing [25,26].
- Lie formulation of and Lie methods for light optics. These methods are now appearing in optics text books [27-29].

### 3 Recent Work

Recent work has been devoted to four areas. The work in each of these areas is summarized briefly below:

#### 3.1 Calculation of transfer maps for realistic beam-line elements

Although high-order methods have been developed for the representation, manipulation, analysis, and application of transfer maps, the maps currently used for most beamline-elements themselves are, for the most part, still highly idealized. (The only exceptions are iron-free elements, such as air-core solenoids and REC quadrupoles, for which fields can be computed analytically, and for which MaryLie was the first code to provide high-order

and realistic maps for such elements.) Fringe-field and  $s$ -dependent (including high-order multipole) effects are generally neglected or only treated approximately.

Fringe-field effects are known to be potentially important. (For example, the third-order aberrations of an air-core solenoid are infinite in the hard-edge limit. Some third-order aberrations of dipoles are also infinite in the hard-edge limit.) Therefore, for high-order calculations to be credible, it is essential to include in a realistic way fringe-field and  $s$ -dependent multipole effects. For this purpose it is necessary to have some analytical representation of body and end fields that exactly satisfies the Maxwell equations and has reliably computable high derivatives. Typically numerical data is available on some 3-dimensional grid, and the problem is to produce the desired representation using this data.

Past work of others in this area has advocated fits based on on-axis data or midplane data, and employing various assumed profile functions (*e.g.* Enge profiles) or trigonometric series. These fits were then used to generate 3-dimensional off-axis or off-midplane field representations by repeated (to high order) differentiation. However, these methods are inherently unstable because high derivatives cannot be computed reliably from numerical data. Also, errors typically grow rapidly (as some high power of distance) as one extrapolates *outward* from interior to exterior points. Finally, the trigonometric series have poor convergence properties (particularly when repeatedly differentiated) because they presume a nonexistent periodicity. These results are well known to numerical analysts, and can be demonstrated to those who doubt.

These problems can be overcome by the use of *surface* data. This data is fit and then used to compute interior fields by integrating the Maxwell equations *inward*. The advantage of using surface field data followed by inward integration are numerous:

- Only functions with known (orthonormal) completeness properties and known (optimal) convergence properties are employed.
- The Maxwell equations are exactly satisfied.
- The results are manifestly analytic in all variables.

- The error is globally controlled. It is (or should be) well known that solutions to vacuum Maxwell equations take their extrema on boundaries. But this is exactly where a controlled fit has been made.
- Due to the smoothing properties of the Maxwell Green function (inward integration), the interior fit is relatively insensitive to errors in the surface data. The sensitivity to noise in the data decreases rapidly (as some high inverse power of distance) with increasing distance from the surface, and this property improves the accuracy of the high-order interior derivatives needed to compute high-order transfer maps.

Thus, for the first time, there is now a reliable method for the computation of transfer maps describing particle motion through realistic fields. It is expected that this method will become the method of choice when accurate results are required for the the design of future machines with demanding performance. (For example, it has ben found experimentally that in some cases insertion of a wiggler in a storage or damping ring lattice seriously diminishes the dynamic aperture. The use of surface methods makes it possible to predict such degradation in advance, and to formulate alternate designs with improved performance.)

The use of surface data has been implemented for the case of elements with small sagitta. In this case the surface is that of a straight cylinder that fits within the element aperture and extends beyond the fringe-field regions at both ends. The surface of a circular cylinder can be used in the case where the aperture is roughly circular. The surface of cylinders with elliptic or rectangular cross sections can be used to good advantage when the gap width is larger than its height.

This use of straight cylinders has been extensively documented and benchmarked, including calculation of the transfer map for the prototype Cornell wiggler for ILC damping rings. Some 330 pages are devoted to this purpose in the Lie Methods book. A distillation of this material, prepared jointly with Chad Mitchell from LBNL, has been published in *PRSTAB*. See publication 1 in Section 4.

Extensive work has also been done, and is being done, on the treatment of curved beam-line elements such as dipoles with substantial sagitta. In this case the Maxwell equations are not separable in coordinates that satisfactorily surround the design orbit, and the straight-cylinder methods applicable

to elements with small sagitta cannot be used. However, it is the case that if both normal fields and the scalar potential are known on an arbitrary surface, then there are kernels that allow the computation of the interior vector potential and all its derivatives. And all the virtues of surface methods listed above continue to hold. (For the case of a dipole with large sagitta, it is convenient to use the surface of a bent box with straight ends. The bent box contains the body fields of the dipole, and the straight ends contain the fringe fields.) Some 65 pages are currently devoted to this purpose in the Lie Methods book, with more in preparation. In addition to benchmarking to verify numerical accuracy, this method will be applied to a proposed Brookhaven light source bending dipole. It is expected that a distillation of these results will be published as a Part II sequel to publication 1 in Section 4.

### **3.2 Preparation of a detailed publication on Poincaré Analyticity and the Complete variational Equations**

According to a theorem of Poincaré, the solutions to differential equations (including the equations for charged-particle motion) are analytic functions of (and therefore have Taylor expansions in) the initial conditions and various parameters provided that the right sides of the differential equations are analytic in the variables, the time, and the parameters. Some 140 pages of the Lie Methods book now describe how these Taylor expansions may be obtained, to any desired order, by integration of what we call the *complete* variational equations. There it is also illustrated that remarkably, in a Duffing equation stroboscopic map example, these Taylor expansions, truncated at an appropriate order thereby providing polynomial approximations, can well reproduce the behavior (including infinite period doubling cascades and strange attractors) of the solutions of the underlying differential equations. A distillation of some of this material (produced jointly with Dobrin Kaltchev from TRIUMF) has been submitted to and accepted for publication in *Physica D: Nonlinear Phenomena*. See publication 2 of Section 4.

### **3.3 Applications of Moment Invariants and Eigen Emittances**

Some book sections have been drafted for the chapter on Beam Description and Moment Transport. In particular, eigen emittances are defined (based on quadratic moments of a beam distribution) and a Classical Uncertainty Principle and a Minimum Emittance Theorem are proved for arbitrary (but linear) symplectic transport in a fully 6-dimensional phase space. In collaboration with coauthors in Los Alamos, the eigen emittance concept has now been key to the design of ultra-bright electron sources (applicable, for example, to X-ray light sources) using novel new ways of producing initial electron distributions. See publications 3 through 5 of Section 4.

In addition, communication is occurring with the Muon Accelerator Program (MAP) at BNL. The use of eigen emittances should also be useful in analyzing the results of beam cooling experiments. In this case one can measure all quadratic moments before and after a cooling channel. Next, compute the eigen emittances of the beam before and after. Ideally, one would like to find that all the eigen emittances have decreased, or at least the minimum of the eigen emittances has decreased.

### **3.4 Continued development and documentation of Lie algebraic methods**

Work continues on the development and documentation of Lie methods. Over the past 3 years some 570 pages have been added to the Lie Methods book. In addition to the material described in Subsections 3.1 through 3.3 above, extensive material (some 65 pages) has been added on Geometric Integration including Integration on Manifolds and Symplectic Integration. In particular, a new Lie method (far faster and far more accurate than methods in current use) has been discovered for integrating the BMT equations for spin transport.

In addition, summary descriptions of Lie and Map methods have been written for the upcoming second edition of the *Handbook of Accelerator Physics and Engineering*. See publications 7 through 9 of Section 4.

## 4 Recent Publications and Reports

1. C. Mitchell and A. Dragt, “Accurate Transfer Maps for Realistic Beam-line Elements: Part I, Straight Elements”, 19 pages, *Phys. Rev. ST Accel. Beams* **13**, 064001 (2010).
2. D. Kaltchev and A. Dragt, “Poincare Analyticity and the Complete Variational Equations”, 50 pages; “Supplementary Material for Poincare Analyticity and the Complete Variational Equations”, 26 pages, to appear in *Physica D: Nonlinear Phenomena* (2012).
3. B. Carlsten, K. Bishofberger, L. Duffy, S. Russell, R. Ryne, N. Yampolsky, and A. Dragt, “Arbitrary emittance partitioning between any two dimensions for electron beams”, 16 pages, *Phys. Rev. ST Accel. Beams* **14**, 050706 (2011).
4. L. Duffy, K. Bishofberger, B. Carlsten, A. Dragt, Q. Marksteiner, S. Russell, R. Ryne, and N. Yampolsky, “Exploring Minimal Scenarios to Produce Transversely Bright Electron Beams Using the Eigen-Emittance Concept”, 7 pages, arXiv:1107.2070 (2011). To appear in *Nuclear Instruments and Methods A*.
5. N. Yampolsky, B. Carlsten, R. Ryne, K. Bishofberger, S. Russell, and A. Dragt, “Controlling Electron-Beam Emittance Partitioning for Future X-Ray Light Sources”, 4 pages, arXiv:1010.1558 (2011).
6. A. Dragt, *Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics*, 2026 pages (2012). Some 570 pages have been added in the past 3 years. Available on the Web at <http://www.physics.umd.edu/dsat/>
7. M. Venturini and A. Dragt, “3-D Multipole Expansion, Calculation of transfer Maps from field Data, Fringe Fields”, 3 pages, to appear in *Handbook of Accelerator Physics and Engineering*, second edition, A. Chao, K. Mess, M. Tigner, and F. Zimmermann, edit., World Scientific (2012).

8. A. Dragt, “Taylor Map, Henon Map, Standard Map”, 2 pages, to appear in *Handbook of Accelerator Physics and Engineering*, second edition, A. Chao, K. Mess, M. Tigner, and F. Zimmermann, edit., World Scientific (2012).
9. A. Dragt, “Lie Algebraic Methods”, 7 pages, to appear in *Handbook of Accelerator Physics and Engineering*, second edition, A. Chao, K. Mess, M. Tigner, and F. Zimmermann, edit., World Scientific (2012).

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5. Forest, E., *Beam Dynamics: A New Attitude and Framework*, Harwood (1998).
6. Ryne, R., Adelman, A., Colella, P., Qiang, J., Serafini, D., Samulyak, R., Habib, S., Mottershead, T., Neri, F., Walstrom, P., Decyk, V., and Dragt, A., “MaryLie/IMPACT: A Parallel 5th Order Beam Optics Code with Space Charge”, *Proceedings of the 2003 International Particle Accelerator Conference* (2003).
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19. Dragt, A.J. and M. Venturini, “Accurate Computation of Transfer Maps from Magnetic Field Data”, *Nuclear Instruments and Methods*, A427, p. 387 (1999).



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## 6 DSAT Ph.D. Students

Chad Mitchell, Ph.D. 2007

Thesis: Calculation of Realistic Charged-Particle Transfer Maps.

Employment: Postdoctoral Research Associate, Physics Department, University of Maryland. Subsequently an NRC Fellow at the Naval Research Laboratory. Now employed by Lawrence Berkeley Laboratory.

Marco Venturini, Ph.D. 1998.

Thesis: Lie Methods, Exact Map Computation, and the Problem of Dispersion in Space Charge Dominated Beams.

Employment: Previously Postdoctoral Research Associate, Physics Department, University of Maryland. Subsequently employed by Stanford Linear Accelerator Center. Now employed by Lawrence Berkeley Laboratory.

Alexei Fedotov, Ph.D. 1997.

Thesis: Longitudinal Coupling Impedance of a Hole in the Accelerator Beam Pipe at Finite Frequencies.

Employment: Previously Postdoctoral Research Associate, Physics Department, University of Maryland. Now employed by Brookhaven National Laboratory.

Shicheng Jiang, Ph.D. 1996.

Thesis: An Analytical and Numerical Investigation of the Coupling Impedance of Irises in a Beam Pipe.

Employment: Cable and Wireless, Inc.

Dan Abell, Ph.D. 1995.

Thesis: Analytic Properties and Cremona Approximation of Transfer Maps for Hamiltonian Systems.

Employment: Previously a Postdoctoral Research Associate, Physics Department, University of Maryland. Subsequently employed by Brookhaven National Laboratory. Now employed by Tech-X Corporation.

Wen Hao Cheng, Ph.D. 1995.

Thesis: Beam Dynamics of the Alternating Phase Focusing Linac and Dependence of the Penetration of Electromagnetic Fields Through a Small Coupling Hole in a Thick Wall on Frequency.

Employment: Previously employed by Lawrence Berkeley Laboratory. Now employed by Intel.

Rui Li, Ph.D. 1990.

Thesis: Analytic and Numerical Investigation of the Longitudinal Coupling Impedance.

Employment: Thomas Jefferson National Accelerator Facility.

Govindan Rangarajan, Ph.D. 1990.

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

Employment: Previously at Lawrence Berkeley Laboratory. Now Professor of Mathematics, Indian Institute of Science, Bangalore, India.

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: Now with the Theoretische Elektrotechnik Group at the Darmstadt Technische Hochschule.

Robert Ryne, Ph.D. 1987.

Thesis: Lie Algebraic Treatment of Space Charge.

Employment: Previously employed by Lawrence Livermore National Laboratory and the Los Alamos National Laboratory. Now employed by the Lawrence Berkeley National Laboratory.

Liam Healy, Ph.D. 1986.

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

Employment: Previously at CERN. Now with Celestial Mechanics Group at the Naval Research Laboratory.

Etienne Forest, Ph.D. 1984.

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

Employment: Previously employed by the Lawrence Berkeley Laboratory. Now employed by the KEK High Energy Physics Laboratory, Tsukuba, Japan and also a Professor at the Graduate University for Advanced Studies, Kanagawa, Japan.

David Douglas, Ph.D. 1982.

Thesis: Lie Algebraic Methods for Particle Accelerator Theory.

Employment: Previously employed by the Lawrence Berkeley Laboratory. Now employed by the Thomas Jefferson National Accelerator Laboratory.