APPLICATIONS OF DIFFERENTIAL ALGEBRAIC METHODS IN BEAM PHYSICS

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Abstract

Differential Algebraic (DA) methods, at the most fundamental level, have been developed to solve analytic problems by algebraic means. Over the last 20 years or so, they gained widespread application in many areas of beam physics. In this paper, an overview is given, starting with some history, its mathematics, and some specific applications. So far, the method has not been extensively utilized in the case of linear accelerators. Hopefully, this compendium of examples will illustrate its power and potential usefullness even for high power superconducting linac design and simulation.

OVERVIEW OF DA

Historically, Differential Algebra has roots in automatic and computational differentiation, and the truncated power series algebras (TPSA). Any textbook on numerical analysis contains many examples of potential inaccuracies of numerical differentiation of functions, and the buildup of errors with increasing order of the derivatives. To overcome this, it was noticed that by propagating the value and derivatives of the identity function, one can compute arbitrary high order derivatives of very complicated functions fast on a computer, with accuracy limited only by the underlying floating point representation of numbers on a computer. The ordered set of partial derivatives of these functions can be related very easily to its Taylor series, and hence the TPSAs. Augmenting this mathematical structure with the analytic operations of differentiation and integration yields the Differential Algebra [1].

From the point of view of beam physics, this is important since the object that contains explicitly the functional dependence of the system's behavior as a function of whatever parameter or quantity is needed, is contained in such a DA vector. This DA vector is called the Poincaré section or return map for periodic systems, or the transfer map (or simply the map) of a single pass system. The task that beam physicist often face is the computation and analysis of the map of the system.

CODES THAT UTILIZE DA

Over the last twenty years or so, the theory matured so that an efficient implementation on a computer became possible. The first codes to tackle the problem were precursors of the code COSY INFINITY. Today, there are many codes that have DA-based libraries. DA itself is just the framework on which the beam physics codes can be built, in themselves do not contain any physics. While the theory of the DA methods is well established, its implementation on a computer environment varies greatly. In the tradition of the accelerator physics community, each lab, university, or even group develops and uses its own computer codes. Besides COSY INFINITY [2], some of other codes based on DA are: MXYZPTLK (Fermilab), ZLIB (SLAC), DACYC (TRIUMF), TLIE (MARYLAND), PTC (KEK), SIXTRACK (CERN), UAL (BNL), and others.

All codes, except COSY focus on high energy periodic accelerators. COSY has some unique features that make it ideal even for other types of charged particle machines, as we will show in the examples section. These include dependence on system parameters such as mass and charge, not restricted to relativistic energies, own object oriented language, optimization at the language level, flexibility in manipulation of DA vectors, relative easy of extension its already extensive library of optical elements, etc.

SOME ADVANCED DA METHODS

As explained in the preceding sections, DA allows computation of maps. More generally, DA allows complex operations to be performed on a computer very elegantly. Here we outline some of these.

Ordinary differential equations (ODE) and partial differential equations (PDE) can be formulated as a fixed point problem. In many cases it can be shown that the corresponding operators in DA are contractive, and converge to the exact solution in finitely many steps, starting with an arbitrary initial condition. Therefore, differential equations can be solved elegantly in DA.

Once maps are computed, one needs to manipulate them. For example, a beam line's map consisting of many elements may be obtained by concatenating maps of individual pieces. Practical examples are the maps of fringe fields. In general, maps of fringe fields (or any fields that depend explicitly on the independent parameter) are time consuming to compute, since they require numerical integration in DA. Because they are so expensive to compute, one can do it once and for all. The saved map can be recalled when necessary, and composed with the actual map. Composition of maps in DA is readily available.

Perhaps even more interestingly, sometimes one needs the inverse of the map. Inversion also can be cast into a fixed point problem, and solved in DA. This is useful in a variety of situations, but in general allows us to solve nonlinear systems of polynomial equations explicitly. Instances where this is useful are use of mirror symmetric systems, reconstructive correction of aberrations, making implicit relations explicit, and so on.

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These and some other elementary operations can be combined to deliver design and analysis tools for the accelerator physicists that are fast and highly accurate.

APPLICATION OF DA METHODS IN BEAM PHYSICS

In addition to pushing perturbation theory to very high orders, DA allows many applications in beam physics. Without claiming that the following list is exhaustive, we enumerate some important applications:

- Calculation of high order Taylor expansions of transfer maps
- Mass and charge dependence of trajectories
- Inclusion of system parameters in the expansion (quadrupole strength, length of a drift, dipole placement error, an RF phase, etc.)
- Sensitivity studies (for example pitch/yaw of a magnet, or general misplacements, misalignments)
- Normal form methods (tunes, amplitude dependent tune shifts, chromaticities, resonance strengths, etc.)
- Tracking with the map, including symplectic tracking (faster than ray tracing)
- Reconstructive correction of aberrations
- Spin-orbital coupling, including normal form
- Correction of beam-beam effects
- Validated integration of differential equations
- Global optimization
- Simplifies system optimization (local optimization)

In the next section the power of the approach is illustrated with some specific examples.

EXAMPLES

The examples in this section were chosen in such a way as to illustrate capabilities of the code in different systems:

- Computation of wire model magnet fringe fields for LHC
- Aberration correction in single pass systems
- Beam-material interaction simulation in single pass (possibly repetitive) systems
- Efficient and accurate long-term symplectic tracking with the map for periodic systems

Magnet fringe fields

Modern superconducting magnets are current dominated, and their design is done by sophisticated codes such as ROXIE. The code creates a wire current model of the magnet, such as shown in Figure 1.

The model consists of several hundred thousand wire pieces, approximating the real strands of superconducting coils, and measurements of actual magnets built according to the model showed that this is an approach that allows achieving a high degree of accuracy.

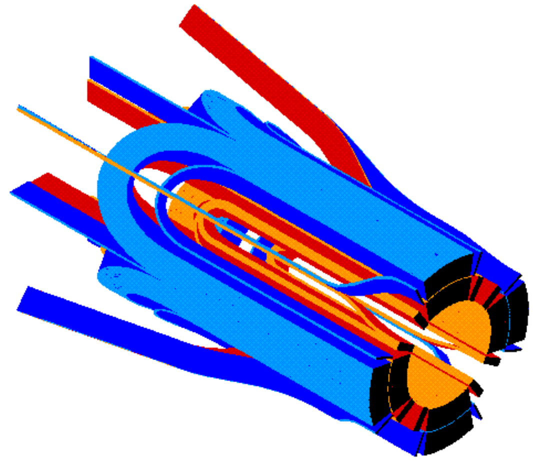

Figure 1. Wire current model of the lead end of the LHC's High Gradient Quadrupoles, as created by the code ROXIE..

The computation of the magnetic fields at an arbitrary point is equivalent to summing up the contributions of the various straight wire pieces according to the Biot-Savart law. By evaluating the Biot-Savart law in DA, we got not only the value of the magnetic field at that point, but also its Taylor expansion. This allows the direct computation of the multipole content of the fields, without resorting to numerical Fourier transforms, which can get inaccurate for small amplitude high order multipoles.

Moreover, the Taylor expansion of the fields makes possible the straightforward computation of the curl of the field, that is a check of the Maxwell equations. This test can be used to ascertain the accuracy of the computation and the correctness of the model. It is well-known that the model should consist of closed loops of current to obey the Maxwell equations. This method has been used to detect flaws in the model and correct them.

Once we know the fields, a DA integration produces the transfer map through this filed. The method of producing maps through these complicated fields can be extended and made more sophisticated. For example, work is in progress to obtain the necessary field data by the so-called surface field method.

Aberration correction

A system that is perfect for the need of high order aberration correction is the Rare Isotope Accelerator Fragment Separator. In the proposed RIA, the primary beam's collision with a target will produce a variety of isotopes that need to be collected, selected, and delivered in identifiable form to the experimental stations. Due to the kinematics of the nuclear reactions, the fragment separator should be of high resolution and large acceptance. This requires the consideration and correction of aberrations of up to 5^{th} order.

DA allows the computation of the Taylor expansion of the final position with respect to initial conditions, which is directly related to the various aberrations. If the system is implemented in the code COSY Infinity, the map and the aberrations can be easily obtained, and the object oriented language that allows optimization at the language level permits system performance optimization.

A layout of the first half of a fragment separator, for which most 3rd order aberrations have been corrected, is shown in Figures 2 and 3.

Figure 2. Horizontal envelope in a proposed layout of the RIA Fragment Separators.

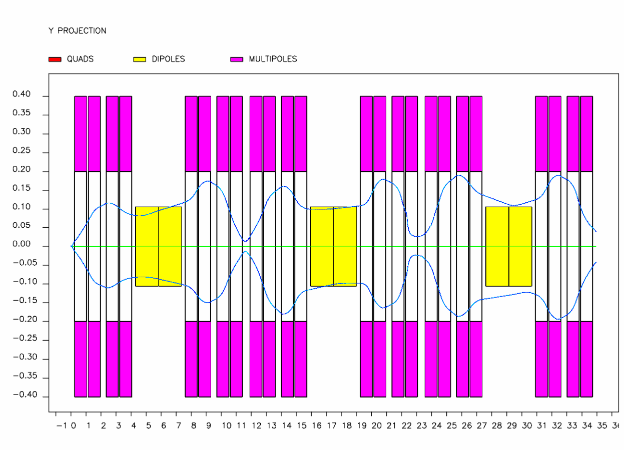

Figure 3. Vertical envelope in a proposed layout of the RIA Fragment Separators.

Among others, the following aspects can be studied elegantly by the DA-enabled code COSY INFINITY:

- Basic layout designs, taking into account footprint constrains
- 5th order designs, including correction of most harmful high order aberrations
- Effects of the fringe fields and beam-material interactions on the performance of the system, including identification of limiting factors
- Sensitivity and error analysis of the systems
- Magnet aperture requirements
- Optimized resolving power, including optimization of the resolving power of the two "sub-separator" parts
- Wedge and absorber locations and shapes
- Optimized ion optics for the gas catcher
- Ideal beam dump location.

The details of the design are still work in progress, to be addressed in future publications.

Beam-material interactions

Beam-material interactions are difficult to treat in the traditional language of accelerator physics, including the map approach. This is due to the stochastic processes that take place in absorbers and wedges. It is possible to employ a split operator approach, in which the average deterministic effects are incorporated in the map, while the stochastic effects are treated as random kicks. Examples when such an approach is useful are the muon cooling simulations, and the fragmentation of heavy ions and separation of isotopes.

Such an integrated approach to nuclear processes and beam optics is being pursued in an extensive code development program, based on COSY. The resulting code will be utilized for RIA Fragment Separator design. The nuclear physics, present in a variety of codes have been incorporated as function callable directly from COSY. The fragmentation cross-sections are based on the EPAX parameterization, the charge state distributions on GLOBAL, while the energy loss and the straggling (energy loss and angle) on ATIMA. So, a suite of codes work seamlessly together to aid in separator design.

As an example of the power of DA we show how the map inversion technique can be used to obtain the final energy as a function of initial coordinates, which is a component of the transfer map of an absorber, or a wedge. Denoting the initial and final energies of a particle with initial coordinates $\vec{z}_i$ by E_i and E_f, the equation that needs to be solved for E_f is:

$$Range(E_i) - Thickness(\vec{z}_i) - Range(E_f) = 0$$

The thickness dependence on initial conditions takes into account the shape of the wedge. In general the equation is a complicated multivariable nonlinear equation for E_f. In practice, the range is given by a spline (obtained in ATIMA from first principles), and the shape is determined by two polynomials specifying the entrance and exit shape of the wedge. By evaluating the range splines in DA, one obtains the Taylor expansion of the range around the energies of the reference particle. Now, the above equation takes the general form $f(\vec{z}_i, \delta_f) = 0$, where δ_f is the final relative energy of the particle with the given initial conditions. Let's say that the vector of initial conditions is *n* dimensional. Then, introducing the *n* dimensional identity function, the above equation can be written as a system of equations in the form

$$\mathbf{M}(\vec{z}_i, \delta_f) = (\vec{z}_i, 0),$$

where **M** can be regarded as a map, with components

$$\mathbf{M} = \begin{pmatrix} id(1) \\ id(2) \\ \vdots \\ id(n) \\ f \end{pmatrix}$$

As explained in the previous sections, in DA the map can be inverted, and since **M** is origin preserving, we obtain

$$\left(\overrightarrow{z_i}, \delta_f\right) = \mathbf{M}^{-1}\left(\overrightarrow{z_i}, 0\right)$$

From which we can read off δ_f as being

$$\delta_f = \left(\mathbf{M}^{-1}\left(\overrightarrow{z_i}, 0\right)\right)_{n+1}.$$

Finally, this value of δ_f can be incorporated in the transfer map of the wedge.

We note that the derivation of the final energy spread according to the above algorithm would be only formal if we would not have a procedure to invert nonlinear multivariable polynomial functions. Herein lies the power of DA. Generally speaking, DA provides a local mechanism to solve systems of polynomial equations explicitly.

Symplectic tracking with the map

Traditionally, numerical integration methods have been viewed as numerical approximations to a single trajectory. The methods have been developed and selected based on local accuracy, efficiency, robustness, and ease of implementation. A shift of point of view happened when the integration methods began to be regarded as a discrete dynamical system that approximates the flow of the corresponding differential equation. This gave rise to the field of Geometric Numerical Integration, in which accelerator physics played a very important catalytic role.

Today, there are many kinds of geometric integration methods; here we are concerned with symplectic methods. Broadly, these can be categorized into splitting and composition and generating function methods. Generating functions are well-known from any advanced classical mechanics course. These can be utilized for symplectic tracking with the map. However, the four Goldstein type of generating functions that are well-known from graduate physics are not sufficient for practical purposes, as has been shown in many examples over the years. Fundamentally, it does matter how one represents the map describing the system by a generating function. The studies in this direction are called symplectification methods. It was shown that besides the Goldstein generating functions there are infinitely many more that in principle could be used for tracking. Moreover, out of this huge set, there is one, named EXPO, that in general gives the best results. Technically, it provides the optimal symplectification with respect to Hofer's metric. For details see [3].

For the purpose of this paper suffice to mention that the implementation of the whole theory is possible due to the power of DA. The computation of the generating function itself involves function composition and inversion. The iteration of the resulting map is also done very elegantly in DA in vectorized or parallel fashion.

The theory of extended generating functions, symplectification, and optimal symplectic tracking by the EXPO method have been implemented in the code COSY INFINITY. The method gave very good results in all cases studied over the last few years, including the LHC, Tevatron, Proton Driver, Neutrino Factory, etc. Now it is the default tracking method in COSY.

This concludes the examples section. We tried to illustrate the power of DA in a variety of systems: single pass, single pass repetitive, and periodic systems. We also showed the variety of problems that can be tackled by employing the power of DA. Our hope is that some of these applications, and perhaps some new ones, will find their way into the linac community, and DA will prove useful for linear accelerator design and simulation too.

SUMMARY

As a summary we would like to emphasize a few main points. We hope that the theory and examples illustrated that if the dynamics has a good polynomial approximation Differential Algebraic methods have many advantages over conventional numerical methods. We showed how DA can be used to:

- Accurately compute complicated fields and easily characterize field quality
- Compute high order Taylor transfer maps
- Perform system analysis, parameter dependencies, and error sensitivities
- Enable straightforward powerful optimization
- Correct aberrations
- Track particles of periodic systems long-term, quickly, and accurately
- Incorporate in the map the deterministic portions of the beam-material interactions
- In some cases allow optimization even for non-polynomial dynamics (for example beam-beam compensation)

Some applications that come to mind for linac design and simulation are the accurate simulation of nonlinear effects in cavities, optimization of cavity failure modes, error sensitivities, and acceptance studies. Hopefully these and others will be pursued in the future.

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