32. COSY INFINITY and Its Applications in Nonlinear Dynamics*

(Chapter of "Computational Differentiation: Techniques, Applications, and Tools", Martin Berz, Christian Bischof, George Corliss, and Andreas Griewank, eds., SIAM, 1996.)

Martin Berz† Kyoko Makino† Khodr Shamseddine† Georg H. Hoffstätter‡
Weishi Wan§

Abstract

The Fortran-based environment COSY INFINTIY, as well as the related codes DAFOR and DAPRE, is presented. The codes contain modules for the computation of derivatives to very high orders in many variables, with a particular emphasis on sparsity. The main use of the code lies in the field of nonlinear dynamics, where it is used for the computation of perturbation expansions of Poincare maps to high orders as well as their analysis based on normal forms and other methods. Using Remainder Differential Algebraic Methods, quantitative and mathematically rigorous statements about long-term stability can be made for general systems. The code is currently used by more than 150 registered users, mostly in the field of beam physics for the study and design of particle accelerators.

Keywords: COSY INFINITY, high-order derivatives, sparsity, nonlinear dynamics, differential algebra.

1 DAFOR and DAPRE

The programs DAFOR and DAPRE [Berz1987a], [Berz1990f], [Berz1990a] represent a package consisting of a precompiler to automatically transform Fortran 77 code lines to new code in which elementary operations are executed step by step via calls to elementary routines. The package DAPRE contains runtime library routines to execute these elementary operations for various data types, including vectors, intervals, and, foremost, truncated Taylor series [Berz1987b]. In this case, the main emphasis lies on the ability to handle high orders in many variables as efficiently as possible. This is achieved with a sophisticated indexing scheme based on a family of address arrays that are calculated upon first call [Berz1989a]. With this approach, the logistic overhead for bookkeeping of addresses is kept to a minimum. Depending on the machine type, the overhead is often as little as 30% of the raw execution time needed for floating-point operations. Typical applications of the package in the field of beam physics require the computation of Taylor series in six variables of order ten, resulting in about 10^4 coefficients.

*This research was financially supported by the Department of Energy, Grant No. DE-FG02-95ER40931, and the Alfred P. Sloan Foundation.

†Department of Physics and Astronomy, Michigan State University, East Lansing, MI. 48824, USA.
‡Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22603 Hamburg, Germany.
§APAS Department, University of Colorado, Boulder, CO 80309-0391, USA.

2 COSY INFINITY

Besides being called from Fortran obtained through precompilation, the run-time libraries of DAPRE can also be invoked from the dedicated language environment of COSY INFINITY. This environment has object-oriented features and a syntax similar to that of PASCAL [Berz1990b], [Berz1995a] and also allows one to link easily with Fortran source code. In this sense, it represents an efficient environment for using new data types. At the same time, it allows the direct use of existing Fortran-based code, a requirement that is of importance for many applications in physics, where large, dedicated simulation libraries exist.

Besides these features, many of which can also be found in Fortran 90, the code allows incremental and interactive compilation. This unique feature makes it suitable as a control language in which to set up the problem to be studied. It also allows interactive changes of the control structure.

The code COSY INFINITY originated in the field of beam physics, where it is used as a major design and analysis tool by more than 150 registered users. In this field, high-order nonlinearities correspond directly to relevant quantities called image aberrations, which traditionally have been very hard to compute and describe.

Many codes compute aberrations to second and third order [Wollnik1988a], [Brown1979a], [Dragt1985a]. A comprehensive description of the theory behind the perturbative approach to compute aberrations can be found in [Brown1982a]. With advanced and dedicated formula manipulators, it was possible to extend the work to fifth order [Berz1987c], [Berz1988a], but it seems hard to imagine that the traditional methods can be extended substantially. In contrast, the forward differentiation techniques and the differential algebraic extensions used in the code COSY routinely allow the computation of aberrations of orders around ten.

COSY also allows the computation of aberrations of systems that are otherwise particularly hard to treat, especially those occurring due to the fringe fields of particle optical elements [Hoffstätter1993a], [Hoffstätter1994b].

3 Applications in Nonlinear Dynamics

Several of the features in COSY are connected to the study of the nonlinear dynamics around a fixed point. The differential algebraic picture connected to the description of nonlinear effects lends itself particularly well to an introduction of perturbative normal form methods [Berz1991d], [Forest1989a], [Berz1992c] and to their application for general problems of nonlinear dynamics. The general idea behind repetitive normal forms is to perform a nonlinear change of variables such that the motion in the new variables becomes highly regular. Indeed, in the simplest nonresonant case, it just follows an approximately circular motion. Since a mere change of coordinates does not affect the general topological properties, this approach usually allows for a much more detailed analysis of the motion. The method is based on an iterative removal of terms, where in the mth step, only the mth order of the map is affected. Specifically, a change of coordinates of the form

$$\vec{A}_m = \vec{E} + \vec{T}_m$$

is performed, where $\vec{E}$ is the unity map and $\vec{T}_m$ possesses only monomials of order m. It turns out that $\vec{A}_m$ is invertible, and to mth order, we have $\vec{A}_m^{-1} =_m \vec{E} - \vec{T}_m$.

Of course, the full inversion of $\vec{A}_m$ contains higher-order terms, which is one of the reasons iteration is needed. We note that, in principle, the parts of $\vec{T}_m$ higher than order m can be chosen freely, but if symplectic symmetry is to be preserved, there is an essentially unique transformation that is canonical. To study the effect of the transformation, we now infer up to order m:

$$\begin{aligned}
\vec{A}_m \circ \vec{M}_m \circ \vec{A}_m^{-1} &=_m \left(\vec{E}+\vec{T}_m\right) \circ \left(\vec{R}+\vec{S}_m\right) \circ \left(\vec{E}-\vec{T}_m\right) \\
&=_m \left(\vec{E}+\vec{T}_m\right) \circ \left(\vec{R}+\vec{S}_m-\vec{R}\circ\vec{T}_m\right) \\
&=_m \vec{R}+\vec{S}_m+\left(\vec{T}_m\circ\vec{R}-\vec{R}\circ\vec{T}_m\right).
\end{aligned}$$

For the first step, we have used $\vec{S}_m \circ (\vec{E}-\vec{T}_m) =_m \vec{S}_m$, which holds because $\vec{S}_m$ is nonlinear and $\vec{T}_m$ is of order m. In the second step, we used $\vec{T}_m\circ(\vec{R}+\vec{S}_m-\vec{R}\circ\vec{T}_m) =_m \vec{T}_m\circ\vec{R}$, which holds because $\vec{T}_m$ is of exact order m and everything in the second term is nonlinear except $\vec{R}$. This result can be used to simplify $\vec{S}_m$ by choosing the commutator $\vec{C}_m = \{\vec{T}_m, \vec{R}\} = \left(\vec{T}_m\circ\vec{R}-\vec{R}\circ\vec{T}_m\right)$ appropriately. A careful analysis reveals that the commutator is able to remove all terms of up to order m except those that describe a nonlinear rotation.

By virtue of providing approximate invariants of the motion, the normal form methods can be used to perform a rigorous analysis of problems of nonlinear stability, leaning on ideas similar to those occurring in the stability theories of Lyapunov and Nekhoroshev [Turchettia1990a]. By Remainder Differential Algebraic methods [Makino1996a], these approaches can even be made fully mathematically rigorous [Berz1994c]. To this end, let us assume that the whole region of normal form coordinates up to the maximum radius $r_{\max}$ corresponds to Cartesian coordinates within the area to which motion should be restricted. Let us assume further that nowhere in the $r-\phi$ diagram is the invariant defect larger than Δr. If we launch particles within the normal form region below $r_{\min}$, then all these particles require at least

$$N = \frac{r_{\max}-r_{\min}}{\Delta r}$$

turns before they reach $r_{\max}$. Considering the small size of Δr in practical cases, this can often assure stability for a rather large number of turns.

The appeal of the method outlined here hinges critically on the ability to determine rigorous bounds for Δr, and its practical usefulness is directly connected to how sharp these bounds are. However, in practice these functions have a tremendously large number of local maxima, and a computation of their bounds requires great care. For every one of the $l-1$ regions in phase space, we are faced with the task of finding n bounds for the maxima $\Delta r^{(j)}$ of deviation functions

$$\Delta r^{(j)} \geq \max[r^{(j)}(\vec{M}(\vec{x})) - r^{(j)}(\vec{x})],$$

where $r^{(j)}(\vec{x})$ is the normal form radius in the jth normal form subspace of a particle at position $\vec{x}$. The regions in which the bounds for the maxima have to be found are the regions where $r^{(j)}(\vec{x}) \in [r_i^{(j)}, r_{i+1}^{(j)}]$. Unfortunately, despite the many local maxima, it is necessary to find rigorous bounds with an accuracy of about 10^{-6}, and for some applications to 10^{-12}.

Many rigorous interval optimization methods were used to try to find bounds for the motion, but because of the complexity, all of them surrendered to blow up. On the other hand, using the Remainder Differential Algebra methods outlined in [Makino1996a], we were able with only moderate effort to obtain bounds with sufficient sharpness [Berz1994c] and to guarantee stability of orbits for in the range of 10^6 to 10^9 turns in a mathematically rigorous sense.

References

[Berz1987a] M. BERZ, *The differential algebra Fortran precompiler DAFOR*, Tech. Report AT–3: TN–87–32, Los Alamos National Laboratory, Los Alamos, N.M., 1987.

[Berz1987b] ——, *The method of power series tracking for the mathematical description of beam dynamics*, Nuclear Instruments and Methods, A258 (1987), pp. 431 +.

[Berz1987c] M. BERZ AND H. WOLLNIK, *The program HAMILTON for the analytic solution of the equations of motion in particle optical systems through fifth order*, Nuclear Instruments and Methods, A258 (1987), p. 364.

[Berz1988a] ——, *Analytical solution of the equations of motion to high orders: The formula manipulator HAMILTON and the fifth order code COSY*, AIP Conference Proceedings, 177 (1988), p. 301.

[Berz1989a] ——, *Differential algebraic description of beam dynamics to very high orders*, Particle Accelerators, 24 (1989), p. 109.

[Berz1990a] ——, *Differential algebra precompiler version 3 — Reference manual*, Tech. Report MSUCL – 755, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Mich., 1990.

[Berz1990b] ——, *COSY INFINITY version 3 reference manual*, Tech. Report MSUCL – 751, National Superconducting Cyclotron Lab., Michigan State University, East Lansing, Mich., 1990.

[Berz1990f] ——, *The DA precompiler DAFOR*, Tech. Report, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1990.

[Berz1991d] ——, *High-order computation and normal form analysis of repetitive systems*, in Physics of Particle Accelerators, M. Month, ed., vol. AIP 249, American Institute of Physics, 1991, p. 456.

[Berz1992c] ——, *Differential algebraic formulation of normal form theory*, in Proc. Nonlinear Effects in Accelerators, M. Berz, S. Martin, and K. Ziegler, eds., IOP Publishing, 1992, p. 77.

[Berz1994c] M. BERZ AND G. H. HOFFSTÄTTER, *Exact estimates of the long term stability of weakly nonlinear systems applied to the design of large storage rings*, Interval Computations, 2 (1994), pp. 68–89.

[Berz1995a] ——, *COSY INFINITY Version 7 reference manual*, Tech. Report MSUCL–977, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Mich., 1995.

[Brown1979a] K. L. BROWN, *The ion optical program TRANSPORT*, Tech. Report 91, SLAC, 1979.

[Brown1982a] ——, *A first- and second-order matrix theory for the design of beam transport systems and charged particle spectrometers*, Tech. Report 75, SLAC, 1982.

[Dragt1985a] A. J. DRAGT, L. M. HEALY, F. NERI, AND R. RYNE, *MARYLIE 3.0 - a program for nonlinear analysis of accelerators and beamlines*, IEEE Transactions on Nuclear Science, NS-3,5 (1985), p. 2311.

[Forest1989a] E. FOREST, M. BERZ, AND J. IRWIN, *Normal form methods for complicated periodic systems: A complete solution using differential algebra and Lie operators*, Particle Accelerators, 24 (1989), p. 91.

[Hoffstätter1993a] G. H. HOFFSTÄTTER AND M. BERZ, *Efficient computation of fringe fields using symplectic scaling*, in Third Computational Accelerator Physics Conference, AIP Conference Proceedings 297, 1993, p. 467.

[Hoffstätter1994b] ——, *Accurate and fast computaton of high–order fringe field maps via symplectic scaling*, Nuclear Instruments and Methods, 352 (1994).

[Makino1996a] K. MAKINO AND M. BERZ, *Remainder differential algebras and their applications*, in Computational Differentiation: Techniques, Applications, and Tools, M. Berz, C. Bischof, G. Corliss, and A. Griewank, eds., SIAM, Philadelphia, Penn., 1996, pp. 63–74.

[Turchettia1990a] G. TURCHETTI, *Nekhoroshev stability estimates for symplectic maps and physical applications*, Springer Proceedings in Physics, 47 (1990).

[Wollnik1988a] H. WOLLNIK, B. HARTMANN, AND M. BERZ, *Principles behind GIOS and COSY*, AIP Conference Proceedings, 177 (1988).