

# Recent Advances in Differential Algebraic Methods

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An overview of the background of Taylor series methods and the utilization of the differential algebraic structure is given, and various associated techniques are reviewed. The conventional Taylor methods are extended to allow for a rigorous treatment of bounds for the remainder of the expansion in a similarly universal way. Utilizing differential algebraic and functional analytic arguments on the set of Taylor models, arbitrary order integrators with rigorous remainder treatment are developed. The integrators can meet pre-specified accuracy requirements in a mathematically strict way, and are a stepping stone towards fully rigorous estimates of stability of repetitive systems.

## 1. Introduction

We begin with a recent enhancement that allows to not only obtain transfer maps to high order, but at the same time and with very limited additional computational effort also determine fully rigorous bounds for the remainders in the Taylor expansion of a given order. The approach is based on utilizing the three differential algebraic (DA [1]) operations of addition, multiplication, derivation and their inverses on so-called Taylor model [2, 3, 4] objects for the direct solution of the Picard fixed point form of the differential equation. Employing Schauder's theorem and compactness and convexity arguments for certain function spaces described by Taylor models, it is possible to construct verified integrators that perform a rigorous error analysis of their steps [5]. Compared to other verified integrators, the ones developed here avoid the so-called wrapping effect problem [6, 7, 8], which hampers conventional such approaches, and would otherwise prevent the treatment of typical beam physics problems.

One of the applications of the availability of maps with rigorous remainder bounds is the determination of optimal generators for symplectic tracking [9, 10, 11]. Besides the conventionally known four generators, there is an infinite family of others, all of which can be determined with DA methods. It is possible to identify those of the family that yield optimal symplectification in the sense of a metric that is invariant under symplectomorphisms. This assures that the generator is not only optimal for a given Poincare sections, but simultaneously for all others around the ring, and that it works as well for the millionth turn as it does for the first.

Using the rigorous remainder bounds of maps, it is possible to not only assure the existence of the generators locally, but to determine regions of phase space over which with certainty the map can be represented by a given generator. In practical examples it is found that as expected, the optimal generators maximize this region [11, 12].

The methods are particularly useful for the study of systems where conventional symplectic tracking via kick approximations is not possible because the Hamiltonian cannot be decomposed into two explicitly solvable parts, as in all split-operator approaches. This is for example the case when the so-called kinematic correction is relevant, as in the case of the various accelerators and rings for neutrino machines. Symplectification can in this case be achieved with the use of generating functions; but because of the inherent strong nonlinearity, the use of optimal symplectification is of prime importance. Various examples of the performance of the methods for such machines are given in [11].

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All the methods discussed here have been implemented within the DA environment of COSY INFINITY [13]. In order to facilitate interaction with other language environments, the COSY system has recently been ported to a language independent environment, which allows automatic code generation for use as F90 and C++ objects [4]. The advantage of the resulting tight and robust wrappers is that most of the inherent speed and efficiency of the original FORTRAN-based COSY tools is maintained, which has not been possible with native object oriented implementations.

## 2. Differential Algebras

The differential algebraic approach [14, 15, 16] took the computation of Taylor maps

$$\bar{z}_f = \mathcal{M}(\bar{z}_i) \quad (1)$$

of dynamical systems from the then customary third [17, 18, 19, 20] or fifth order [21] all the way to arbitrary order in a unified and straightforward way. The Taylor maps have many applications, as many of the physical quantities that are encountered in practice are more or less directly connected to Taylor coefficients. Since its introduction, the method has been widely utilized in a large number of new map codes. [13, 22, 23, 24, 25, 26, 27, 28]

The basic idea behind the method is to bring the treatment of functions to the computer in a similar way as the treatment of numbers. In a strict sense, neither functions (for example,  $C^\infty$ ) nor numbers (for example, the reals  $R$ ) can be treated on a computer, since neither of them can be represented with the finite amount of information that can be stored on computers (after all, a real number is an equivalence class of bounded Cauchy sequences of rational numbers).

However, from the early days of computers we are used to dealing with numbers by extracting information deemed relevant, which in practice usually means the approximation by floating point numbers with finitely many digits. In a formal sense this is possible since for every one of the operations on real numbers, like addition and multiplication, we can craft an adjoint operation on the floating point numbers such that the following diagram commutes:

$$\begin{array}{ccc} a, b \in R & \xrightarrow{T} & \bar{a}, \bar{b} \in FP \\ \downarrow * & & \downarrow \circledast \\ a * b & \xrightarrow{T} & \bar{a} \circledast \bar{b} \end{array} \quad (2)$$

Of course, much to the chagrin of those doing numerics, in reality the diagrams commute only “approximately,” which typically makes the errors grow over time.

The approximate character of these arguments can be removed by representing a real not by one floating point number, but rather by an interval of floating point numbers providing a rigorous upper and lower bound. By rounding operations down for lower bounds and up for upper bounds, rigorous bounds can be found for sums and products, and adjoint operations can be made such that the above diagram commutes exactly. In practice, while always maintaining rigor, the method sometimes becomes rather pessimistic, as over time the intervals often have a tendency to grow.

Historically, the treatment of functions in numerics has been done based on the treatment of numbers; and as a result, virtually all classical numerical algorithms are based on the mere evaluation of functions at specific points. As a consequence, numerical methods for differentiation, which are so relevant for the computation of Taylor representations of the map (1), are very cumbersome and prone to inaccuracies because of cancellation of digits, and not useful in practice for our purposes.

The success of the new methods is based on the observation that it is possible to extract more information about a function than its mere values. Indeed, considering the commuting diagram in Equation (2), one can demand the operation  $T$  to be the extraction of the Taylor coefficients of a pre-specified order  $n$  of the function. In mathematical terms,  $T$  is an equivalence relation,

and the application of  $T$  corresponds to the transition from the function to the equivalence class comprising all those functions with identical Taylor expansion to order  $n$ .

Since Taylor coefficients of order  $n$  for sums and products of functions as well as scalar products with reals can be computed from those of the summands and factors, it is clear that the diagram can be made to commute; indeed, except for the underlying inaccuracy of the floating point arithmetic, it will even commute exactly. In mathematical terms, this means that the set of equivalence classes of functions can be endowed with well-defined operations, leading to the so-called Truncated Power Series Algebra (TPSA) [14, 15].

This fact was realized in the first paper on the subject [15], which led to a method to extract maps to any desired order from a computer algorithm that integrates orbits numerically. Similar to the need for algorithms within floating point arithmetic, the development of algorithms for functions followed, including methods to perform composition of functions, to invert them, to solve nonlinear systems explicitly, and to introduce the treatment of common elementary functions [29, 30].

However, very soon afterwards it became apparent [16, 31] that this only represents a half-way point, and one should proceed beyond mere arithmetic operations on function spaces of addition and multiplication and consider their analytic operations of differentiation and integration. This resulted in the recognition of the underlying differential algebraic structure and its practical exploitation [1], based on the commuting diagrams for addition, multiplication, and differentiation and their inverses:

$$\begin{array}{ccccc}
 f, g & \xrightarrow{T} & F, G & f, g & \xrightarrow{T} & F, G & f & \xrightarrow{T} & F \\
 +, - \downarrow & & \downarrow \oplus, \ominus & \cdot, / \downarrow & & \downarrow \odot, \oslash & \partial, \partial^{-1} \downarrow & & \downarrow \partial_{\circ}, \partial_{\circ}^{-1} \\
 f \pm g & \xrightarrow{T} & F \oplus_{\circ} G & f \cdot g & \xrightarrow{T} & F \odot_{\circ} G & \partial f, \partial^{-1} f & \xrightarrow{T} & \partial_{\circ} F, \partial_{\circ}^{-1} F
 \end{array} \quad (3)$$

In passing we note that in order to avoid loss of order, in practice the derivations have the form  $\partial = h \cdot d/dx_i$ , where  $h$  is a function with  $h(0) = 0$ . As a first consequence, it allowed to construct integration techniques to any order that for a given accuracy demand are substantially faster than conventional methods [30]. Subsequently, it was realized that the differential algebraic operations are useful for a whole variety of other questions connected to the analytic properties of the transfer map [29]. It was possible to determine arbitrary order generating function representations of maps [30, 32]; factorizations into Lie operators [33] could be carried out for the first time to arbitrary order [30]; normal form methods [34, 35] could be performed to arbitrary order [30, 36]. And last but not least, the complicated PDEs for the fields and potentials stemming from the representation of Maxwell’s equations in particle optical coordinates could be solved to any order in finitely many steps [1].

Of course the question of what constitutes “information deemed relevant” for functions does not necessarily have a unique answer. Formula manipulators, for example, attack the problem from a different perspective by attempting to algebraically express functions in terms of certain elementary functions linked by algebraic operations and composition. In practice the Achilles heel of this approach is the complexity that such representations can take after only a few operations. But compared to the mere Taylor expansion, they have the advantage of rigorously representing the function under consideration. Below we will show how such rigor can be maintained without the computational expense of formula manipulation by a suitable augmentation of the Taylor approach.

### 3. The Treatment of Remainders

Compared to techniques of formula manipulation and to other rigorous mathematical efforts on computers, the Taylor DA methods do not make any statements about the remainder of Taylor’s formula. By extending the theory, it is possible to obtain rigorous bounds for the remainder terms. In this endeavour, we demand to be fully mathematically rigorous in that no approximations are

allowed. All this is achieved by keeping the idea of providing commuting diagrams for elementary operations; however, the objects on which these operations are to be carried out are not mere truncated Taylor series any more, but rather new objects called Taylor models [2, 3].

Furthermore, in order to keep the mathematical rigor for the solution of the differential equations defining the maps of the systems, we had to derive a new method to perform integration [5]. As in many other automated approaches for integration of functions and differential equations on computers, we utilize differential algebraic techniques for this purpose. While in the conventional computation of Taylor maps, in principle also conventional integrators can be used (although the ones that come for free in the differential algebraic approach are usually superior in speed and accuracy), this is not the case here, and one is more or less forced to develop new techniques.

Our method relies on an inclusion of the remainder term of a Taylor expansion in an interval. However, to quell misunderstandings from the beginning, it is important to note that our approach is not equivalent to interval methods that have been applied extensively for many types of verified calculations [6, 7, 37, 38]. The careful reader will realize that our method provides remainder bounds with an accuracy that does not scale merely linear with the domain interval, but rather as a high power of the domain interval; this feature is essential if high accuracy is required over an extended range of arguments, as is the case with the transfer map. Furthermore, it alleviates the so-called dependency problem [39], which among other things entails that extended conventional interval computations sometimes have a danger to “blow up” and yield rather pessimistic and sometimes even useless bounds.

#### 4. Computation of Remainder Bounds for Functional Dependencies

We begin our study of the rigorous computational treatment of the remainder with the definition of a Taylor Model. Let  $f$  be  $C^{(n+1)}$  on  $D_f \subset R^v$ , and  $\vec{B} = [a_1, b_1] \times \dots \times [a_v, b_v] \subset D_f$  an interval box containing the point  $\vec{x}_0$ . Let  $T$  be the Taylor polynomial of  $f$  around the point  $\vec{x}_0$ . We call the interval  $I$  an  $n$ th order Remainder Bound of  $f$  on  $\vec{B}$  if

$$f(\vec{x}) - T(\vec{x}) \in I \text{ for all } \vec{x} \in \vec{B}.$$

In this case, we call the pair  $(T, I)$  an  $n$ th order Taylor Model of  $f$ . It is clear that a given function  $f$  can have many different Taylor models, as with  $(T, I)$ , also  $(T, \bar{I})$  with  $\bar{I} \supset I$  is a Taylor model. Furthermore, we see that low-order polynomials have trivial remainder bounds; since every polynomial of order not exceeding  $n$  agrees with its  $n$ th order Taylor polynomial, the interval  $[0, 0]$  is a remainder bound.

For practical purposes, it is important that if the original interval box  $\vec{B}$  decreases in size, then according to the various formulas of the Taylor remainder [40], the remainder bounds can decrease in size with a power of  $n + 1$  and hence will become small quickly. In particular, this entails that the knowledge of a good Taylor model of a function on an interval box  $\vec{B}$  allows a rather accurate estimate of the range of the function.

Now we want to study to what extent it is possible to define arithmetic operations  $\oplus$ ,  $\odot$ , and  $\partial_{\odot}$  on Taylor models. In this case, the operation “ $T$ ” that turns a function into its Taylor polynomial has to be replaced by the inclusion operation  $\subset$ . So we must craft new adjoint operations on Taylor models that make the diagram

$$\begin{array}{ccc} f, g \in C^{n+1} & \xrightarrow{\subset} & (T_f, I_f), (T_g, I_g) \\ \downarrow * & & \downarrow \otimes \\ f * g & \xrightarrow{\subset} & (T_f, I_f) \otimes (T_g, I_g) \end{array}$$

commute in a similar way as in the case of the Differential Algebra on Truncated Power Series in Equation (3).

Let  $(T_f, I_f)$  and  $(T_g, I_g)$  be  $n$ th order Taylor models of the functions  $f$  and  $g$  on the interval box  $\vec{B}$ . Clearly, the Taylor polynomial of  $(f + g)$  is simply  $T_f + T_g$ ; on the other hand, we know that on  $\vec{B}$ ,  $f(\vec{x}) \in T_f(\vec{x}) + I_f$  and  $g(\vec{x}) \in T_g(\vec{x}) + I_g$ . Then obviously,

$$(f + g)(\vec{x}) \in (T_f + T_g)(\vec{x}) + (I_f + I_g) \text{ for all } \vec{x} \in \vec{B},$$

and so  $(T_f + T_g, I_f + I_g)$  is a Taylor model for  $(f + g)$  on  $\vec{B}$ . And for practical purposes, it is also important to note that if  $I_f, I_g$  are “fine of order  $\vec{B}^{n+1}$ ”, i.e. their size scales with the size of  $\vec{B}$  to the  $(n + 1)$ st power, so is  $I_{f+g} = I_f + I_g$ . In the same way we see that  $(T_f - T_g, I_f - I_g)$  is a Taylor model for  $(f - g)$ . So by simply defining

$$(T_f, I_f) \oplus (T_g, I_g) = (T_f + T_g, I_f + I_g),$$

we are able to close the commuting diagram for addition.

In order to study multiplication, let  $(T_f, I_f)$  and  $(T_g, I_g)$  be  $n$ th order Taylor models of the functions  $f$  and  $g$  on the interval box  $\vec{B}$ . As pointed out before, the Taylor polynomial  $T_{f \cdot g}$  of  $f \cdot g$  can then be obtained by multiplication of  $T_f$  and  $T_g$  and subtraction of the polynomial  $\bar{T}_{f \cdot g}$  consisting of the terms whose order exceeds  $n$ . For any  $\vec{x} \in \vec{B}$ , there are values  $e_f \in I_f$  and  $e_g \in I_g$  such that  $f(\vec{x}) = T_f(\vec{x}) + e_f$  and  $g(\vec{x}) = T_g(\vec{x}) + e_g$ . So we obtain

$$\begin{aligned} (f \cdot g)(\vec{x}) &= (T_f(\vec{x}) + e_f) \cdot (T_g(\vec{x}) + e_g) = T_f(\vec{x}) \cdot T_g(\vec{x}) + T_f(\vec{x}) \cdot e_g + T_g(\vec{x}) \cdot e_f + e_f \cdot e_g \\ &= T_{f \cdot g}(\vec{x}) + \{ \bar{T}_{f \cdot g}(\vec{x}) + T_f(\vec{x}) \cdot e_g + T_g(\vec{x}) \cdot e_f + e_f \cdot e_g \}. \end{aligned}$$

The first term is the Taylor polynomial of  $f \cdot g$ . The term in curly brackets describes the behavior of the remainder; it is a polynomial in the  $v + 2$  variables  $(\vec{x}, e_f, e_g) \in \vec{B} \times I_f \times I_g$  and is denoted by  $R(\vec{x}, e_f, e_g)$ . So by bounding  $R(\vec{x}, e_f, e_g)$  [2, 3, 40] with an interval  $I_R$ , we are able close the diagram with the definition

$$(T_f, I_f) \odot (T_g, I_g) = (T_{f \cdot g}, I_R).$$

We note that the necessary computation of  $T_{f \cdot g}$  from  $T_f$  and  $T_g$  is of course the standard multiplication within TPSA.

Besides providing the operations  $\oplus$  and  $\odot$  for Taylor models such that the diagrams in Equation (2) commute, there are a variety of other operations that have to be ported to the Taylor models, especially the intrinsic functions, the composition of functions, and several operations derived from these. For reasons of space, we have to restrict ourselves here to a referral to more detailed references about the matter [2, 3]. A complete set of standard functions on computers was implemented in COSY INFINITY [3, 4].

Altogether, the operations  $\oplus$  and  $\odot$  enable us to determine mathematically rigorous bounds for the remainder of any function that can be represented on a computer, and is hence of great help for problems of optimization [41]. In itself, it is also already useful for several problems in Beam Physics, in particular for the notoriously difficult bounding of approximate invariants of nonlinear motion [42].

## 5. Computation of Remainder Bounds for Flows of Differential Equations

Our goal is now to establish a Taylor model for the transfer map  $\mathcal{M}(\vec{r}_0, t)$  in eq. (1), and thus in particular a rigorous bound for the remainder term of the flow of the differential equation describing the motion over a domain  $(\vec{r}_{01}, \vec{r}_{02}) \times (t_0, t_2)$ . As pointed out before, this need precludes us from the direct use of conventional numerical integrators, as they cannot provide rigorous bounds for the integration error but only approximate estimates. Rather, we have to start from scratch from the foundations of the theory of differential equations [5].

As a first step it is necessary to introduce the inverse derivation operation  $\partial_{\odot}^{-1}$  on Taylor models. Given an  $n$ -th order Taylor model  $(P_n, I_n)$  of a function  $f$ , we can determine a Taylor model for the indefinite integral  $\partial_i^{-1} f = \int f dx'_i$  with respect to variable  $i$ . The Taylor polynomial part is obviously just given by  $\int P_{n-1} dx'_i$ , and a remainder bound can be obtained as  $(B(P_n - P_{n-1}) + I_n) \cdot B(x_i)$ , where  $B(x_i)$  is an interval bound for the variable  $x_i$  obtained from the range of definition

of  $x_i$ , and  $B(P_n - P_{n-1})$  is a bound for the part of  $P_n$  that is of exact order  $n$ . We thus define the operator  $\partial_{\circ,i}^{-1}$  on the space of Taylor models as

$$\partial_{\circ,i}^{-1}(P_n, I_n) = \left( \int P_{n-1} dx'_i, (B(P_n - P_{n-1}) + I_n) \cdot B(x_i) \right).$$

The careful reader may perhaps wonder about the introduction of the operator  $\partial_{\circ,i}$ ; this is also possible, however at an additional effort, since from the knowledge of a remainder bound of a function, no conclusions can be drawn regarding a remainder bound for its derivative (for example, the function can oscillate very quickly inside even a narrow interval). With a further extension of the concept of Taylor models that also describes the asymptotic behavior of coefficients, this problem can be solved, but since it is not required for our purposes, we will not discuss the matter in detail here.

We will use Taylor models for the solution of the initial value problem

$$\frac{d}{dt} \vec{r}(t) = \vec{F}(\vec{r}(t), t), \quad \vec{r}(t_0) = \vec{r}_0,$$

where  $\vec{F}$  is continuous and bounded. We are interested in both the case of a point initial condition  $\vec{r}_0$ , and the case in which the initial condition  $\vec{r}_0$  is a variable. In the latter case, our interest is in the flow of the ODE

$$\vec{r}(t) = \mathcal{M}(\vec{r}_0, t),$$

describing the values of final coordinates in terms of initial coordinates and time.

The solutions should be fully rigorous for all initial conditions  $\vec{r}_0$  and times  $t$  that satisfy

$$\vec{r}_0 \in [\vec{r}_{01}, \vec{r}_{02}], \quad t \in [t_0, t_1].$$

In particular,  $\vec{r}_0$  itself may be a Taylor model, as long as its range is known to lie in  $[\vec{r}_{01}, \vec{r}_{02}]$ .

As is commonly done, we re-write the ODE as an integral equation

$$\vec{r}(t) = \vec{r}_0 + \int_{t_0}^t \vec{F}(\vec{r}(t'), t') dt',$$

and introduce the operator  $A : \vec{C}^0[t_0, t_1] \rightarrow \vec{C}^0[t_0, t_1]$  on the space of continuous functions from  $[t_0, t_1]$  to  $R^v$  via

$$A(\vec{f})(t) = \vec{r}_0 + \int_{t_0}^t \vec{F}(\vec{f}(t'), t') dt'.$$

Then the problem of finding a solution to the ODE is transformed to a fixed-point problem on the space of continuous functions

$$\vec{r} = A(\vec{r}).$$

We apply Schauder's fixed point theorem to rigorously obtain a Taylor model for the flow.

**Theorem (Schauder):** *Let  $A$  be a continuous operator on the Banach Space  $X$ . Let  $M \subset X$  be compact and convex, and let  $A(M) \subset M$ . Then  $A$  has a fixed point in  $M$ , i.e. there is an  $\vec{r} \in M$  such that  $A(\vec{r}) = \vec{r}$ .*

In our specific case,  $X = \vec{C}^0[t_0, t_1]$ , the Banach space of continuous functions on  $[t_0, t_1]$ , equipped with the maximum norm, and the integral operator  $A$  is continuous on  $X$ . The process to apply Schauder's theorem consists of the following steps:

- Determine a family  $Y$  of subsets of  $X$ , the Schauder Candidate Sets. Each set in  $Y$  should be compact and convex, it should be contained in a suitable Taylor model, and its image under  $A$  should be in  $Y$ .
- Using Differential Algebraic (DA) methods on Taylor models, determine an initial set  $M_0 \in Y$  that satisfies the inclusion property  $A(M_0) \subset M_0$ . Then all requirements of Schauder's theorem are satisfied, and  $M_0$  contains a solution.

- Iteratively generate the sequence  $M_i = A(M_{i-1})$  for  $i = 1, 2, 3, \dots$ . Each  $M_i$  also satisfies  $A(M_i) \subset M_i$ , and we have  $M_1 \supset M_2 \supset \dots$ . We continue the refinement iteration until the size stabilizes sufficiently.

The first step can be fulfilled from the mathematical properties of Taylor models and the right hand side of the ODE,  $\vec{F}$ . The second step can be simplified greatly by choosing the optimal polynomial  $\vec{P}$  for the initial set  $M_0$ ; choose the  $n$ -th order flow  $\mathcal{M}_n(\vec{r}_0, t)$  for  $\vec{P}$  using the Differential Algebraic (DA) fixed point algorithm [1, 5]. Since  $\mathcal{M}_n(\vec{r}_0, t)$  is the DA fixed point, the remaining task for the inclusion requirement and the refinement iteration boils down to a mere comparison task of two involved intervals, which is computationally easy [5].

The method turned out to be extremely successful for validated initial value problems [43, 44]. As mentioned earlier, the interval method is prone to blow-up, making mere interval solutions hard to be practical. In the case of multidimensional systems, a further source of overestimation arises from the need of geometric repackaging of the solution at each integration time step, called “wrapping effect” [6, 7, 8]. This phenomenon makes the conventional interval based integration schemes difficult to obtain verified solutions for any practical problems [6, 45]. Addition to the fact that remainder bounds in Taylor models are sharp, our scheme allows the initial condition  $\vec{r}_0$  to be variables, and this helps to eliminate the wrapping effect optimally.

## 6. Examples of Verified Computation

In this section we provide examples of verified solutions of differential equations for beam optics via the Taylor model computation via the integration scheme discussed in the previous section.

As a first example of the verified transfer map computation, we analyze the motion of a charged particle in a magnet with constant magnetic field over an extended phase space. Since the motion in the dipole can be solved analytically based on simple geometrical arguments related to intersections of circles and straight lines, this represents a useful check of the practical validity of the remainder bounds. For our example, we chose a magnet with a deflection radius  $R = 1\text{m}$ . The integration was carried out over a deflection angle of 36 degrees with a fixed step size of 4 degrees. The initial conditions are within the domain intervals

$$[-.02, .02] \times [-.02, .02] \times [-.02, .02] \times [-.02, .02],$$

and the Taylor polynomial describing the dependence of the four final coordinate values on the four initial coordinate values was determined. The order in time and initial conditions was chosen to be 12, and the step size was estimated so as to ascertain an overall accuracy below  $10^{-9}$ ; since no automatic step size control was utilized, the estimate proved conservative and the actual resulting remainder bounds were somewhat smaller:

$$\begin{aligned} &[-0.4496880372277553\text{E} - 09, +0.3888593417126594\text{E} - 09] \\ &[-0.1301070602141642\text{E} - 09, +0.1337099965985420\text{E} - 09] \\ &[-0.3417079805637740\text{E} - 10, +0.3417079805637740\text{E} - 10] \\ &[-0.0000000000000000\text{E} + 00, +0.0000000000000000\text{E} + 00]. \end{aligned}$$

The resulting Taylor polynomials describing the dependence of final on initial coordinates were compared with those obtained by the code COSY INFINITY [13], and agreement was found. Furthermore, a program was written that solves the geometry for individual rays, and its results were compared for a large collection of rays with the results of the flow calculated by the verified integrator. For all rays studied, the difference between the final coordinates determined geometrically and those predicted by the twelfth order Taylor polynomial were within the calculated remainder bounds.

The next example is to verify the mapping functions for a more complicated beam optics system, a typical FODO cell of an accelerator lattice. The cell is set up consisting of the following sequence of elements: drift, defocusing quadrupole superimposed with a sextupole, drift, dipole, drift, defocusing quadrupole superimposed with a sextupole, and drift. The defocusing quadrupoles have the same strength  $k = -0.0085$  and the sextupole strength is  $h = 0.06$ . The lengths are 1m

for the drifts and 0.5m for the magnets; the dipole's curvature radius is 2.5m and the reference particle is a proton with an energy of 1 MeV.

We performed the verified integration through the cell using the 17th order Taylor models on the initial condition domain

$$[-0.1, 0.1] \times [-0.1, 0.1] \times [-0.1, 0.1] \times [-0.1, 0.1].$$

Different from the previous example, an automatic step size control was applied, keeping the growth of the remainder bound suppressed optimally. Integration of the system yielded a Taylor model containing the true solution of the corresponding differential equations. The following is the first ten terms of the Taylor model containing the  $x$ -component of the flow, which is the function mapping the initial conditions  $x_0$ ,  $a_0$ ,  $y_0$ , and  $b_0$  to the  $x$  position at the end of the cell.

RDA VARIABLE: NO= 17, NV= 4			
I	COEFFICIENT	ORDER	EXPONENTS
1	0.1398389113940111	1	1 0 0 0
2	0.1038317686361456	1	0 1 0 0
3	-.2447944264979660E-01	2	2 0 0 0
4	-.1183394850192213E-01	2	1 1 0 0
5	-.2119694344941219E-02	2	0 2 0 0
6	0.2361409770673162E-01	2	0 0 2 0
7	0.1212766097410308E-01	2	0 0 1 1
8	0.2185093364668458E-02	2	0 0 0 2
9	0.9944830763540945E-03	3	3 0 0 0
10	0.8715481705011164E-03	3	2 1 0 0

and the remainder bound was found as follows.

$$R \quad [-.2157121190249145E-012, 0.2178948979195422E-012]$$

It should be noted that the Taylor model encloses the flow with a relative overestimation of only  $10^{-10}$ , underscoring the ability of the Taylor model approach to integrate for a long time with a large size domain for the initial condition.

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