SUPPRESSION OF THE WRAPPING EFFECT BY
TAYLOR MODEL- BASED VERIFIED INTEGRATORS:
THE SINGLE STEP

Kyoko Makino[1][†] , Martin Berz[2][§]

[1]Department of Physics
University of Illinois at Urbana-Champaign
1110 W. Green Street, Urbana IL 61801-3080, USA

[2]Department of Physics and Astronomy
Michigan State University
East Lansing, MI 48824, USA
e-mail: berz@msu.edu

Abstract: The verified integration of ranges of initial conditons through ODEs faces two major challenges, namely the precise representation of the flow over the short term, and the avoidance of unfavorable buildup of errors in the long term. In this paper we show how the former question can be treated within the framework of Taylor model methods, in which the dependence on initial conditions is expressed by a high-order multivariate polynomial and a remainder bound. Numerous examples of the performance of the method and comparisons to other approaches are given.

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[†]Currently at Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA. e-mail: makino@msu.edu.

[§]Correspondence author

1. Introduction

The verified integration of differential equations is one of the important applications of interval- and related verified methods; in fact, the desire to integrate the dynamics of objects in the solar system has served as one of the original motivations for their development. Compared to other uses of verified methods, verified integration is particularly difficult because of the quite extended number of arithmetic operations and the fact that often similar operations repeat a great number of times.

While the problem of repeated application of similar operations manifests itself very clearly in verified integration, it is also affecting conventional integration, although in this case the effects are often more difficult to assess rigorously. Within the framework of conventional integration, the problems are usually tackled by using sufficiently small step size and methods of sufficient order for the step size under consideration, and optimizing the parameters of the algorithms as for example the coefficients in Runge Kutta and other frequently used tools.

However, the long-term control of these errors is much more difficult and represents a fundamental problem, in particular for nonlinear motion. This fact manifests itself particularly clearly in the frequent use of integration schemes that preserve certain known symmetries of the system like geometric constraints or symplecticity, because it is observed that conventional integrators do not satisfy these constraints well enough. It is hoped, then, that imposing the constraints leads to higher computational accuracy, an approach that is indeed often successful, but also often difficult to quantitatively assess.

Within the context of verified integration, the two primary concerns are that on the one hand, it is necessary to not only transport points, but rather regions, since even starting with points quickly leads to the need to treat regions due to the unavoidable overestimation. Already in his 1966 book[39] and in an earlier paper[38], Moore describes this fundamental problem of the verified solution of differential equations of dimension 2 and higher, the need for re-packaging of the flow of the ODE with as little loss as possible, to avoid what is usually called the wrapping effect. On the other hand, there is less room for empirical approaches for the long term since they often do not lend themselves to obtaining rigorous tighter enclosures. Thus verified integration is faced with the need to address the following issues:

- Representing the flow accurately, i.e. providing a tight enclosure for the action of the differential equation on an extended region for a time

step Δt

- Preventing local errors from accumulating in an unfavorable way when integrating over longer times.

To address the re-packaging or wrapping problem, which as observed by Moore [39], [38] leads to an error that scales linearly with the step size Δt and hence cannot be controlled by merely refining the step size, Moore proposes to express the differential equations and its solution in a moving coordinate system, which entails that in this system, the solution set will always be nearly "upright" and thus is expected to be encloseable with intervals at much reduced loss. The coordinate system originally chosen by Moore is an approximation of the linearized solution that is first order in time and has the form

$$M_n = I + \Delta t_n \cdot f'(x_{n-1}, t_{n-1})$$

where I is the identity and f is the right hand side of the differential equation. The local coordinate system after step n is obtained recursively as

$$A_n = M_n \cdot A_{n-1}$$

and the enclosure of the solution is given by

$$r_n = A_n[r_0]$$

which is the linear transformation under the matrix A_n of the original box enclosing the set of initial conditions. Moore observed that if the solution is expressed in terms of the matrix A_n, the overestimation due to the need for re-packaging grows with Δt^2, and thus a reduction of the step size can effectively reduce the wrapping problem.

The method was further extended by Eijgenraam [16], who instead of M_n chooses matrices of the form

$$S_n = I + \sum_{i=1}^{k} \frac{\Delta t_n^i}{i!} f^{(i)}(x_{n-1}, t)$$

where again the local coordinate system after step n is given by $A_n = S_n \cdot A_{n-1}$. For larger Δt, the matrices S_n represents a better approximation of the linear transformation describing the propagation by the step Δt of the linearized ODE. The f_i are defined recursively as $f_i = f'_{i-1} \cdot f(x)$ and are also known as the Lie derivatives of the ODE, and k is a suitably large fixed

value. This approach is often also referred to as the parallelepiped (PE) method.

In his ground breaking work on verified integration, Lohner [25], [26], [24], [27], [28], [29] added another variant based on an orthogonal coordinate system that is obtained by using the QR-decomposition of the matrix A_n. Specifically, the columns of A_n are sorted in descending order by Euclidean length, and the transformation matrix is chosen as the orthogonal part Q_n of the QR decomposition of the matrix A_n. While seemingly providing a less accurate approximation of the linearization than the propagation of S_n, the method has the significant advantage that the matrix Q_n is always well-conditioned by virtue of being orthogonal; thus the inversions necessary in propagating to the next time step can always be executed reliably, and propagation of interval vectors through the matrix does not lead to significant overestimation. In situations where integration over sufficiently large times is required and in which case the A_n can easily become ill-conditioned, this QR method offers a significant advantage.

An enhancement of the conventional QR method for large initial domain boxes is the combination of a parallelepiped to describe the bulk of the flow and a remainder expressed by the QR method as proposed by Lohner [26]. In our future study, this PEQR method will often serve as a reference for comparison.

While it is very difficult to assess the relative merits of these approaches in the general setting, for the special case of linear time-independent ODEs it is possible to provide a quantitative analysis of the behavior of the approaches. This work was pioneered by Nedialkov and Jackson [41], [42], and it was seen through an eigenvalue analysis similar to what is done in the study of stability of conventional ODE solvers that the asymptotic behavior of the QR method is essentially the same as that of conventional non-verified integration schemes. Many practical examples also support this assessment, and [42] contains a rather representative collection of them.

However, for non-autonomous systems, the situation is different even in the linear case; for example, Kühn [23] provides a rather elementary example consisting of a sequence of n matrices that when applied repeatedly lead to exponential growth in the QR method, while the product of the n matrices is actually unity. We will revisit this topic again in [31].

Other enclosures for the flows of the ODEs besides the parallelepipeds of the PE and QR methods have also been studied. It seems natural to consider structures that are invariant under linear transformations, which aside from numerical inaccuracies allows to at least represent the solution sets of linear

ODEs. The natural choices are ellipses, which appear in the work of Jackson [19], [20], [21], Kahan[22] and Neumaier[43], and convex polygons [45] as well as the related zonotopes [23]. The latter are linear transformations from $R^{m \cdot n}$ into R^n, where the higher dimensions are populated successively by assigning a new dimension to any error term that reaches a certain minimum size; apparently the approximation becomes better and better the larger the parameter m is chosen.

From a formal point of view, the zonotope methods are interesting because not only are they invariant under linear transformation, but also under addition, which facilitates the use of the objects in arithmetic. The latter methods have the advantage that using proper strategies of how new faces are added and others removed from the object, error growth can be substantially slowed. Particularly fruitful approaches seem to be the attempts at finding the "smallest" polygon including an interval box in [45] and the cascade algorithm presented in [23].

Other methods of avoiding potential exponential error growth for linear systems are developed by Gambill and Skeel [17] using odd-even reduction of the $(Mn) \times (Mn)$ matrix propagating the M initial and intermediate conditions in the n-dimensional system, as well as the intuitive approach by Barbarosie[2] based on propagating boundaries of sets instead of sets themselves, which can be beneficially applied to two-dimensional problems.

Various aspects of the above mentioned approaches to validated DE solvers are also studied and summarized in [14], [15].

All methods based on families of invariants of linear transformations discussed above, namely the PE, QR, PEQR, ellipsoid, and zonotope methods, have the following properties:

- the enclosure sets for the flow are convex, while nonlinear problems may require non-convex sets

- the accuracy of the enclosure, measured by the interval remainder bound, scales at most quadratically with size for nonlinear problems

- the families are not invariant under nonlinear transformations.

The Taylor model-based integrator introduced in [30], [7], further studied in [35], [10], and applied in [12], [18], [13], [9], [37] overcomes these three difficulties: Relationships between the coordinates $x(t)$ and initial coordinates x_i are expressed in terms of a Taylor model [30], [32], [34], [36] (P, I) consisting of a polynomial with floating point coefficients $P : R^n \to R^n$ and an n-dimensional interval I, both of which depend on t, such that $x(t) \in P(x_i) + I$.

The representation of final coordinates in terms of initial coordinates in terms of Taylor models has the properties

- the enclosure sets can be either convex or concave

- the accuracy of the enclosure scales with order $n + 1$, where n is the order of the Taylor models being used

- the family of Taylor models is invariant under nonlinear transformations

So the Taylor model method [32], [30] combines interval methods for validation and high order Taylor methods for efficient modeling of local functional behavior. The approach to express flows via Taylor models in the initial conditions generalizes the differential algebraic methods [3], [4], [5], which represent the first method that allows systematic determination of high order dependence on initial conditions, albeit without a rigorous remainder treatment.

The Taylor model method represents a multivariate functional dependence f in the domain B by a high order multivariate Taylor polynomial P and the remainder bound interval I as

$$f(x) \in P(x - x_R) + I \text{ for all } x \in B, \tag{1}$$

where x_R is the reference point of the Taylor expansion. The nth order Taylor polynomial P is expressed by floating point coefficients, and it captures the bulk of functional dependency. Because the manipulation of those polynomials can be performed by operations on the coefficients where the minor errors due to their floating point nature are moved into the remainder bound, the major source of interval overestimation is removed, and overestimation only occurs in the remainder bound, the size of which scales with order n of the width of the domain[36].

The standard binary operations and intrinsic functions on Taylor models were implemented in the code COSY Infinity [30], [6]. For the treatment of ODEs, it is of particular significance that the antiderivation operation ∂^{-1} can be treated as an intrinsic function in the Taylor model structure [30], [8]. This formally removes the difference between the solution of ODEs and merely algebraic equations based on fixed point methods.

When applied to the verified integrations of ODEs [7], the following advantages have been observed.

- The inclusion requirement asserting existence of a solution reduces to a mere inclusion of the remainder intervals, and different from conventional methods based on two separate algorithms for initial validation by an Euler step and subsequent higher order execution, the entire steps is performed in one algorithm. There is also no need to utilize additional ODEs for derivatives of the flow with respect to initial conditions.

- The direct availability of the antiderivation on Taylor models allows to treat the Picard operator like any other function, avoiding the need to explicitly bound error terms of integration formulas and leading to a rather straightforward verified fixed point problem.

- The explicit dependency on initial variables is carried through the whole integration process. This controls the bulk of the dependency problem very efficiently and hence the main source of wrapping effect is eliminated to order $n + 1$.

The results of the methods developed in [7] can be summarized in the following theorem.

Theorem 1. (Continuous Dynamical System with Taylor Models) Let $P + I$ be an n-dimensional Taylor model describing the flow of the ODE at the time t; i.e. for all initial conditions x_0 in the original domain region $B \subset R^n$, we have

$$x(x_0, t) \in I + \bigcup_{x_0 \in B} P(x_0).$$

Let $P^*(x_0, t)$ be the invariant polynomial depending on x_0 and t obtained in [7], and assume that the self-inclusion step of the Picard Operator mapping described there is satisfied over the interval $[t, t + \Delta t]$ by the remainder bound I^*. Then for all $x_0 \in B$, we have

$$x(x_0, t + \Delta t) \in I^* + \bigcup_{x_0 \in B} P^*(x_0, t + \Delta t).$$

Furthermore, if even $x(x_0, t) \in P(x_0) + I$, then $x(x_0, t + \Delta t) \in P^*(x_0, t + \Delta t) + I^*$.

By induction over the individual steps, we obtain a relationship between initial conditions and final conditions at time t. Thus formally, the continuous

case is made equivalent to the discrete case, for which the respective property follows immediately from the respective enclosure properties of Taylor models, as described for example in [36].

Theorem 2. *(Discrete Dynamical System with Taylor Models)*
Let $P+I$ be an n-dimensional Taylor model describing the flow of the discrete dynamical system $x_{n+1} = f(x_n, n)$, i.e. for all initial conditions x_0 in the original domain region $B \subset R^n$, we have

$$x_n(x_0) \in I + \bigcup_{x_0 \in B} P(x_0).$$

Let $P^* + I^*$ be the Taylor model evaluation of $f(P + I, n)$. Then for all $x_0 \in B$, we have

$$x_{n+1}(x_0) \in I^* + \bigcup_{x_0 \in B} P^*(x_0).$$

Furthermore, if even $x_n(x_0, t) \in P(x_0) + I$, then $x_{n+1}(x_0) \in P^*(x_0) + I^*$.

The two theorems thus allows the verified study of continuous and discrete dynamical systems, provided that the Taylor model arithmetic is performed in a verified manner. In the case of the implementation in COSY, all errors in the floating point coefficients are fully accounted for [36], [44].

For the purpose of practical efficiency, it is important that the treatment of the coefficients arithmetic supports sparsity, i.e. only coefficients that are nonzero (or more specifically, above a pre-specified accuracy threshold [36], [44]) contribute to computational effort. Finally, for high dimensional systems and high expansion order n in time, one often observes that the expansion in the initial conditions does not need to be executed to the same order unless the dimensions of the original domain box is of a comparable size as the time step. This can be exploited simply by not setting the initial Taylor model to a linear form $P(x_0) = A \cdot x_0$ describing the original box, but rather choose $P(x_0) = A \cdot x_0^w$ for some suitable odd integer power w. In this way, throughout the computation, only powers of x_0 that are multiples of w appear, which effectively limits the expansion in initial conditions to the largest m that satisfies $m \cdot w \leq n$. Combined with sparsity methods, this can drastically reduce computational expense and storage requirements.

Definition 3. (Transversal Weighting) Let the continuous dynamical system under consideration have v variables, and let the time expansion be executed to order n. Assume the initial box of interest is described by the Taylor model $P(x_0) = Ax_0^w$ where $w < n$ is an odd integer; then w is called the weighting of the transversal expansion.

In a typical nonlinear problem one often finds that, already expansion order 3 or 5 in initial conditions allows the treatment of rather large initial domain boxes, while an expansion order of $n = 17$ in time may be desirable; an example of this can be seen below in figure 4. This can be achieved by setting $w = 5$ or $w = 3$, respectively. Furthermore, in the case of linear ODEs where the dependency of final conditions on initial conditions is always linear, one can choose w in such a way that $2 \cdot w > n$, and thus only first order is retained. For the example case of $n = 17$, one may for example choose $w = 9$.

The method also has the interesting side effect that the effective expansion order in time of the higher order terms in the initial conditions is reduced, which because of their reduced importance and leads to additional computational savings without loss of accuracy. For example, in the $n = 17$ and $w = 5$ case, the first order dependence in initial condition is expanded to order 12, while the third order dependencies, of which there are many, are expanded only to order 2. From the combinatorial arguments in [5] it follows that the number of possible coefficients of order n in v initial conditions with weighting factor w is given by

$$N(n, v, w) = \sum_{j=0}^{[n/j]} \frac{(j + v - 1)!}{j! \cdot (v - 1)!} \cdot (n - w \cdot j + 1)$$

where $[x]$ denotes the Gauss bracket of x, the smallest integer not exceeding x. On the other hand, the number of floating point numbers necessary in a code like AWA that solves the ODE for the flow of the reference point and the first partials using polynomials with interval coefficients is $(n+1) \cdot (v+1) \cdot 2$.

For the purpose of providing some examples, we list in table 1 the number of floating point coefficients in a Taylor model of order n in v variables and with weighting w under the assumption of lack of any sparsity, i.e. all coefficients appear and lie above the accuracy threshold. The quantity n_i is the order of expansion in initial conditions. For comparison, the number of coefficients necessary to store all interval endpoints of the $n_i = 1$ representation used in AWA is also given. The first four rows show the situation for the case most similar to the performance of the $n_i = 1$ case of AWA; the smaller number of COSY coefficients is due to the fact that on the one hand, instead of interval coefficients only real numbers are stored, and on the other hand that the expansion order in time for the dependence on initial conditions is reduced. The other rows show the situation for other choices of weights, which of course is more expensive; yet in the COSY scheme third order n_i

n Order	v Dimension	w Weighting	n_i Order	Coefs Cosy	Coefs AWA
17	3	9	1	41	144
17	5	9	1	57	216
17	10	9	1	97	396
17	20	9	1	177	756
17	3	5	3	135	144
17	5	5	3	308	216
17	10	5	3	1248	396
17	20	5	3	6578	756
13	5	3	4	504	168
13	10	3	4	3094	308
15	5	3	5	882	192
15	10	3	5	7098	352

Table 1: Number of floating point coefficients necessary to store all appearing partial derivaties in COSY to order n_i in initial conditions, and in the first order code AWA

at least for low dimensions can still be achieved with a similar number of coefficients of AWA.

In the following section and in subsequent papers [11], [31], we will study in detail the two fundamental questions of verified integration, the accurate representation of flows of ODEs, and methods to prevent growth of the remainder bound, and illustrate the behavior with a large number of examples.

2. Faithful Representation of Flows by Taylor Models

As discussed in the previous section, the successful use of verified methods requires on the one hand the accurate representation of the solution sets over short time scales, and on the other hand the ability to suppress the long-term build up of errors. In this section we study the behavior of the Taylor model method with respect to the first question, which is directly connected to and characteristic of the mathematical behavior of the ODE being studied. We observe that for linear systems, this first source of errors is particularly easy to control, since the flows of linear ODEs are merely linear transformations of the initial coordinates. However, as simple as the matter is for linear ODEs, as complicated it is for nonlinear ODEs. In this case, except for special cases there is no simple representation of the dependency of final conditions on

initial conditions. This is the prime reason why nonlinear ODEs represent the real challenge in the verified integration of differential equations, and results obtained for the purely linear case are often not characteristic for the behavior in nonlinear cases.

In the following, we illustrate the behavior of the Taylor model based integration scheme[7] and compare it to other methods, specifically the code AWA [24] as a representative of the conventional methods. We compare with COSY-VI, the (V)alidated (I)ntegrator based on the COSY language system [6] that is using the Taylor model arithmetic discussed in [36], [6].

The ODEs under consideration are the Volterra equations governing the growth of two conflicting populations, modeling a predator-prey relation, which are frequently used in the study of ODE solvers [1], [40]. The solution trajectories obey the constraint

$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{Constant},$$

as can be seen by simple differentiation and insertion of the ODE, and thus the solutions follow the contour lines of the function C. In the quadrant characterized by $x_{1,2} > 0$, the constant is positive, which entails that contour lines of C cannot cross the x_1 or x_2 axis, and so contour lines originating in this quadrant stay in it. Furthermore, within this quadrant the function asymptotically approaches zero as x_1 or x_2 become large, and so contour lines are bounded and follow closed curves. Figure 1 illustrates the shape of C and a few of its contour lines. The period of one cycle of the solution depends on the initial condition, and outer orbits take longer.

The Volterra equations are a frequently cited example for the numerical verification of ODE solvers. For verified ODE solvers, their nonlinearity combined with their periodicity allows for a particularly transparent study of the wrapping effect.

We take the same model discussed by Ames and Adams [1] and by Moore [40], and have the initial condition interval vector centered around the point values used in their discussions. We aim, in such a way, to provide a good comparison between our approach and other approaches. The ODEs and initial conditions for the Volterra equations are

$$\frac{dx_1}{dt} = 2x_1(1 - x_2), \quad \frac{dx_2}{dt} = -x_2(1 - x_1)$$
$$x_{01} \in 1 + [-0.05, 0.05], \quad x_{02} \in 3 + [-0.05, 0.05] \quad \text{at } t = 0. \qquad (2)$$

The right hand side of the ODEs has the form of a "single use expression" (SUE), so it has no source of overestimation of arithmetic nature; this makes
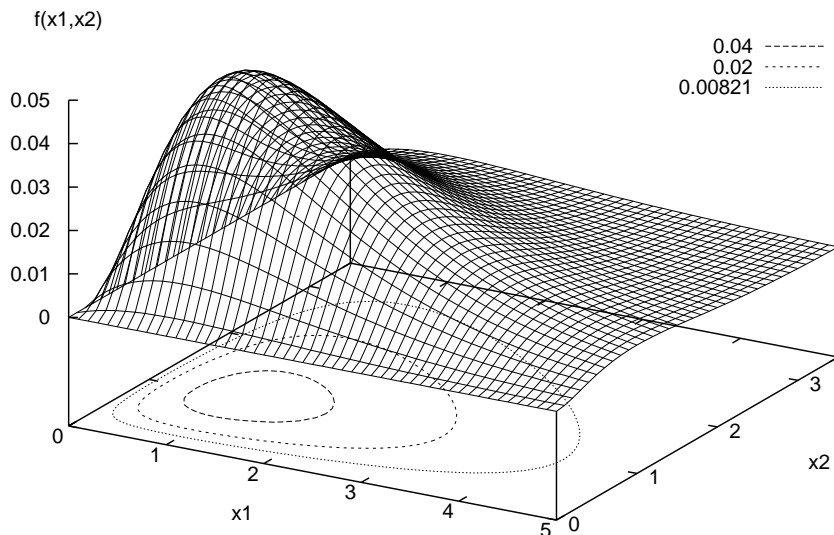
Figure 1: The solution trajectories of the Volterra equations, $f(x_1, x_2) \equiv x_1 x_2^2 e^{-x_1 - 2x_2} = c$(onstant). $f(x_1, x_2)$ is shown by mesh, and the contour lines for various values of c's are shown. The initial condition $(x_{01}, x_{02}) = (1, 3)$ corresponds to $c = 9e^{-7} \simeq 0.00821$.

any overestimation due to the wrapping effect more clearly visible and separates this effect from the ability of the Taylor models to significantly reduce any dependency problem that may be present in the right hand side[33].

The solution trajectory for the point initial values $(x_{01}, x_{02}) = (1, 3)$ is a closed orbit with a period of about $T \simeq 5.488138468035$. We attempted to carry out the integration of the system with AWA and COSY-VI for one period T. As will be shown, the system starts to exhibit noticeable nonlinearity around $t \sim 4$. We used AWA in its standard mode; namely we use the enclosure method 4 based on an intersection of interval-vector and QR-decomposition [24], [26], [41]. AWA's error tolerances E_a and E_r, the absolute and the relative accuracy of the solution used for the step size control, are set at 10^{-12} each. However, those accuracy requirements are not necessarily achieved [24], as we will see later. The computational order has to be pre-set in both AWA and COSY-VI, and the same order was used to facilitate comparison. Both AWA and COSY-VI have automatic step size control, and it was observed that their choices of step sizes for different

times t were similar. We performed the integration of the Volterra equations by AWA and COSY-VI with various computational orders, demanding the completion of one period T.

The pictures in Figure 2 show the solution regions $R(t)$ at various characteristic times, as they are enclosed by Taylor models. They are made based on the observation that flows of ODEs are bijective and thus the outer edges of the original box are mapped into the outer edges of the result after application of the ODE. Hence it is only necessary to draw four curves, two for which x_1 is fixed at the positive and negative values and x_2 varies, and two for which x_2 is fixed at the positive and negative values and x_1 moves. The remainder bounds are so small that they are insignificant to printer resolution.

Initially nonlinearity is not very significant, and until the nonlinearity becomes noticeable around $t \sim 4$, the solution regions $R(t)$ are still well represented by parallelepipeds. After that, the nonlinearity becomes larger and larger, and the solution region $R(t = 4.85)$ shows clear limitations to any attempt to accurately model the region by a parallelepiped or any other convex object. The nonlinearity temporarily decreases afterwards, but the strong nonlinearity returns just before the completion of the period as observed in $R(t = 5.45)$.

The solution enclosures at each time step of the 18th order Taylor model computation by COSY-VI are placed along the center point trajectory in Figure 3. Since COSY-VI completes the whole integration period without noticeable overestimation, it tightly keeps the closed orbit structure of the ODE trajectory. An elongation of the solution region $R(t)$ along the trajectory is observed, which is the result of different cycle periods for the various closed orbits. The dashed boxes are the solution enclosure interval vectors obtained by AWA, showing the beginning of breakdown before $t = 4$. The last solution interval box by AWA in Figure 3 is at time $t \simeq 4.634$. In the case of AWA, despite of the error tolerance demand, a quick error growth is clearly observed after $t = 4$, and eventually integration cannot proceed despite drastic attempts at decreasing the step size. Eventually the box size reaches more than 10^{14} at time $t \simeq 4.93115$ and execution terminates. The dramatic growth in solution interval box size shows a clear correlation to the strong nonlinearity, which becomes apparent at $t = 4.85$ in Figure 2.

On the other hand, COSY-VI continues the computation during the period of strong nonlinearity by keeping the step size smaller; once the nonlinearity becomes weak again, the step size increases again. When the step size control is done only connected to the local error, the step size progress
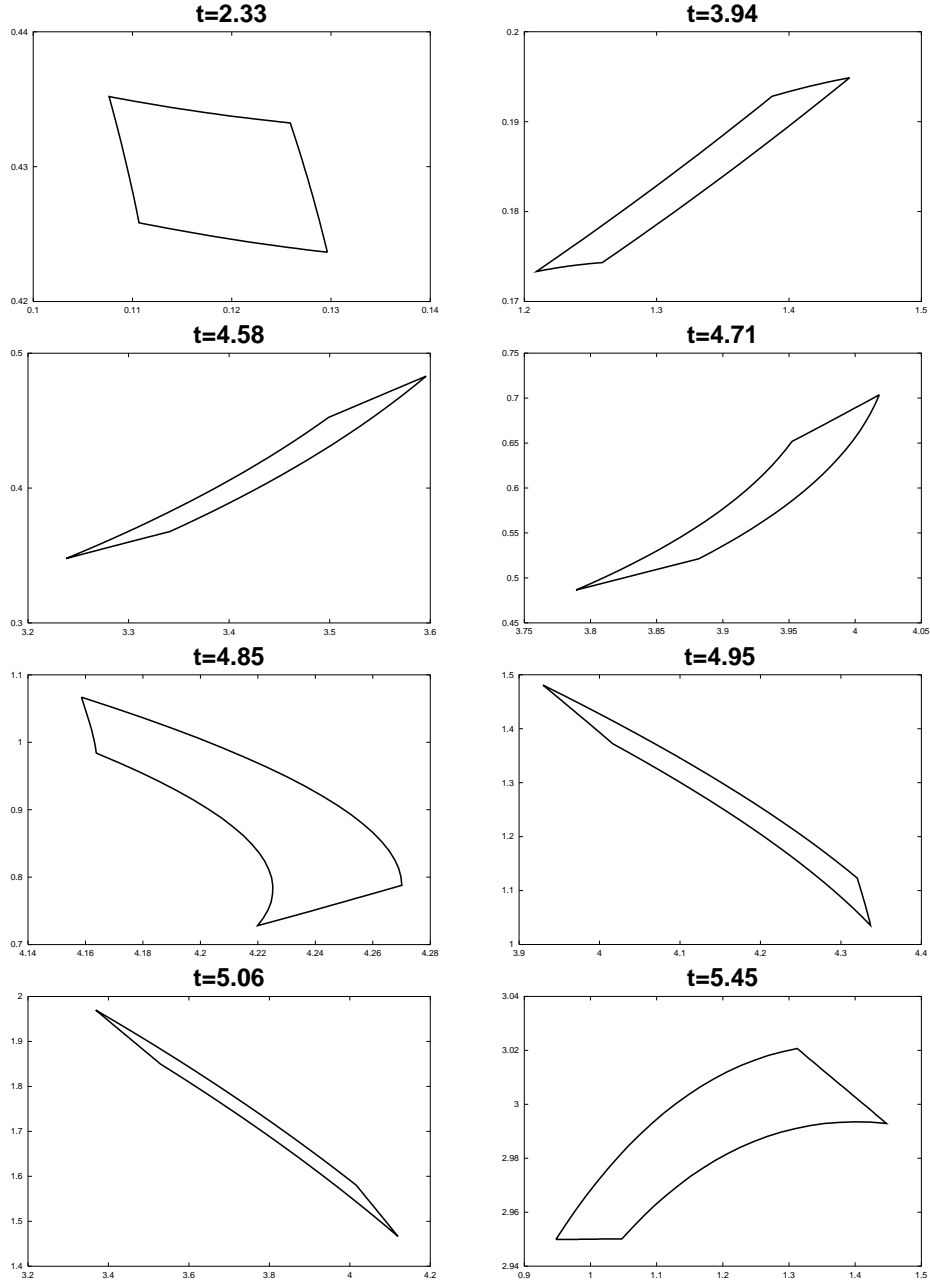
Figure 2: Solution enclosures at characteristic times, obtained by COSY-VI with computation order 18.
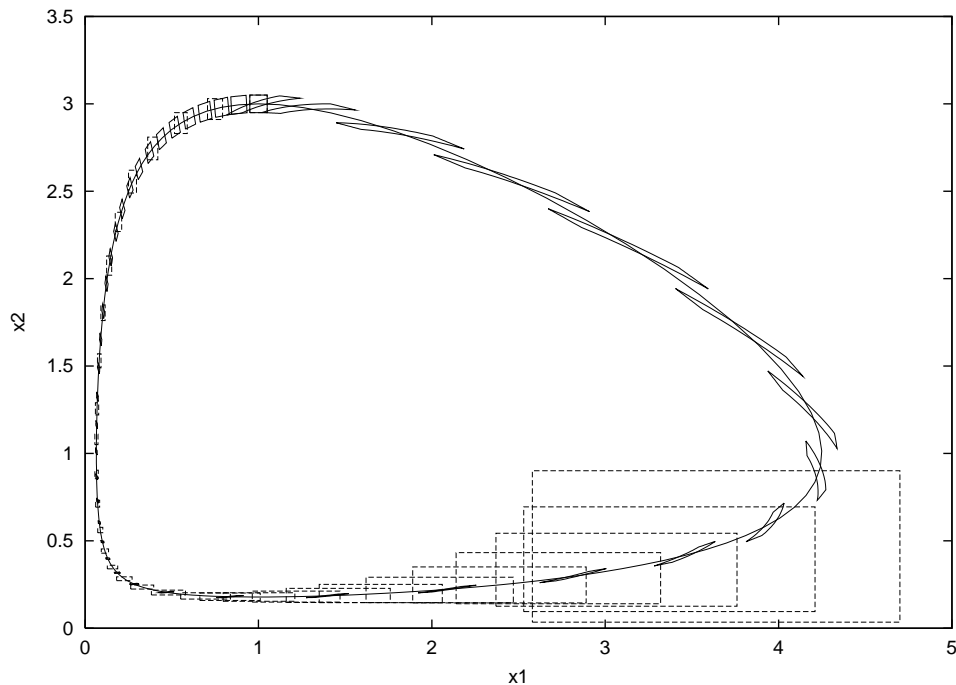
Figure 3: Solution enclosures of the Volterra eqs. at each time step by Taylor models (solid regions) and AWA (dashed boxes) in an 18th order computation.

directly reflects the difficulty of integration due to the strength of nonlinearity.

The performance was studied with different computation orders for the system, but AWA terminated prematurely at nearly the same time regardless of the integration order; a typical consequence of the wrapping effect, which cannot be controlled by increasing the order. COSY-VI completed the whole demanded integration period T without difficulty when the expansion order in time was sufficiently high. For lower time expansion order, it was necessary to keep the step size small as mentioned earlier.

Also listed in Table 2 is the CPU time comparison, using a 450 MHz Pentium III PC running Linux; the weighting w was chosen to be 1. Since AWA did not complete the period, we also listed the breakdown time t in the ODE system.

To illustrate the performance of the computation with COSY-VI, we now

Order	COSY-VI	AWA	
	CPU time	CPU time	Breakdown time t
12	3.2 sec	13.6 sec	5.06039
18	13.6sec	10.7 sec	4.93115

Table 2: CPU time. COSY-VI completed the whole integration period $T = 5.488138468035$, but AWA broke down at time t.

list the resulting Taylor model for the variables x_1 after the completion of one full cycle at $t = 5.488138468035000$. Shown are the floating point coefficients for each monomial, as well as its order and the exponents of the expansion in the initial conditions. Note that there is a third column for exponents, which during the integration step is used to describe the dependence on time, but which does not appear at the end since the final value of t is plugged in. We show all terms up to order 4, as well as the end of the expansions which contain terms of order 12, as well as the remainder bounds.

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 I   COEFFICIENT          ORDER EXPONENTS
 1    1.000000000415308      0    0 0  0
 2   0.5000000002077984E-01  1    1 0  0
 3   0.1593548597307891      1    0 1  0
 4   0.2987903619745317E-02  2    2 0  0
 5   0.7967742985213962E-02  2    1 1  0
 6   0.1745863785938967E-01  2    0 2  0
 7   0.4979839364267220E-04  3    3 0  0
 8   0.5551021323566726E-03  3    2 1  0
 9   0.6348634118140111E-03  3    1 2  0
10   0.1191291279313411E-02  3    0 3  0
11   0.3258832737600261E-05  4    4 0  0
12   0.3241341493295573E-06  4    3 1  0
13   0.3862783708476137E-04  4    2 2  0
14   0.2689662801524732E-05  4    1 3  0
15   0.3564904350045831E-04  4    0 4  0
...
79   0.2264828694386490E-15 12   12 0  0
80  -.1070762043111673E-14  12   11 1  0
81   0.3189161647800073E-14 12   10 2  0
82   0.1429170282664684E-14 12    9 3  0
83   0.1168048490492948E-13 12    8 4  0
84   0.6197159510359881E-13 12    7 5  0
85   0.6886774467995614E-13 12    6 6  0
86   0.2141863127503214E-12 12    5 7  0
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87   0.1915198148620145E-12  12    4 8   0
88   0.2264491972426495E-12  12    3 9   0
89   0.1788727621438823E-12  12    210   0
90   0.5499818896261770E-13  12    111   0
91   0.6996138986393415E-13  12    012   0
R       [-.1481801093188394E-008,0.1490922875566877E-008]
```

To understand the meaning of the terms, consider some examples. After one revolution, the center point of the first variable is mapped back to a value near 1, as expected. The coefficient describing the linear dependence of the final first variable on the initial first variable is around 0.05, corresponding to the original box width. There is also a linear dependence on the second variable of about 0.16, describing a substantial shearing of the end result, which is also clearly visible in figure 3. Furthermore, there are many higher order contributions; for example the second order dependence on $x_1 x_2$ is around -0.00597, indicating an appreciable curvature, which is also noticeable in figure 3. The terms of order 12 are smaller than 10^{-12}, illustrating that the expansion of final conditions on initial conditions does indeed converge. The remainder bound has a width of about $3 \cdot 10^{-9}$, which is more than seven orders of magnitude less than the dependence on linear terms.

For the purpose of a more quantitative study of the behavior of the integrators, let us now consider in detail the execution of a single step of the integration process. We choose a region in which nonlinearity is sufficiently strong so that the effects can be noticed in one step. We choose as initial condition the linear part of the Taylor model at $t = 4.85$. Since AWA can not treat in detail the nonlinear solution set produced by COSY for this time, we delete its nonlinear terms and obtain an approximation of the solution set at the time of interest that has the form of a parallelepiped.

Then we use this parallelepiped to perform a single time step by the time Δt. We execute the step with COSY so that as a result, nonlinear terms are being populated. To simulate the behavior of AWA, all the resulting nonlinearities as well as the $(n + 1)$st order remainder interval produced by COSY are bounded into an interval, which is a measure of the one-step accuracy of a linear code like AWA. It is likely that this estimation is somewhat optimistic since it ignores any possible dependency in the iterative process of the solution of the ODE.

Figure 4 shows the width of the resulting higher order terms as a function of the expansion order for various different time steps, where T is the time step recommended by COSY's step size controller. As can be seen, at order
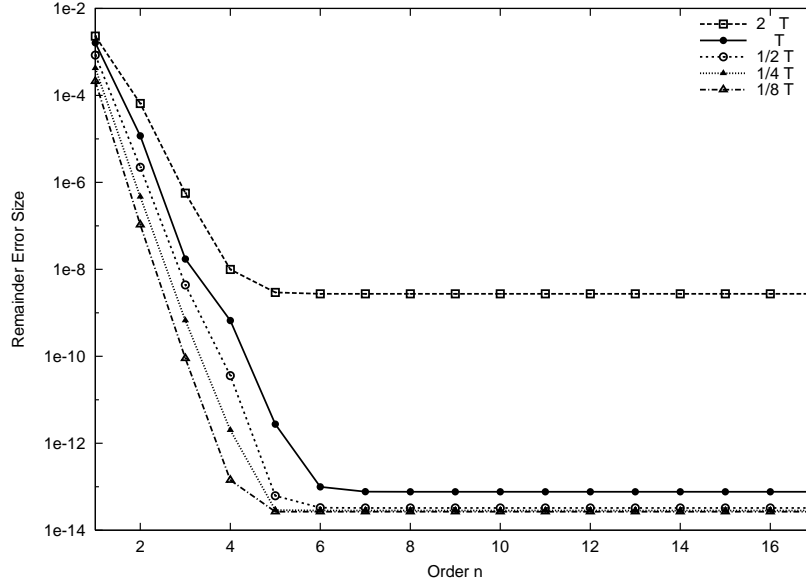
Figure 4: Remainder errors for a single step as a function of order and step size

1 the one-step error is around 10^{-3}, while for the smaller step sizes, between orders 4 to 6 the one-step error can be suppressed below 10^{-13}. Because of the high order dependence of the integration error on step size, the error at twice the recommended step size reaches only around 10^{-8}. Thus for a suitable step size, the one-step integration error produced by COSY's Taylor model method is 10 orders of magnitude less than that for a linear method.

It is also illuminating to study the behavior of the error as a function of the size of the parallelepiped. For this purpose we execute a step at the recommended step size for parallelepipeds scaled by various factors and observe the behavior at different orders. Figure 5 shows the resulting widths of the remainder bounds. All boxes up to the original size of the box can be integrated to an accuracy below 10^{-13} for sufficiently high orders between 4 and 6; the larger box allows integration only to an error of 10^{-12}. On the other hand, a linear method similar to the one used in AWA can produce a one-step error only in the range of 10^{-2} to 10^{-5}. So altogether, again the Taylor model approach leads to a reduction of the one-step error by 7 to 10
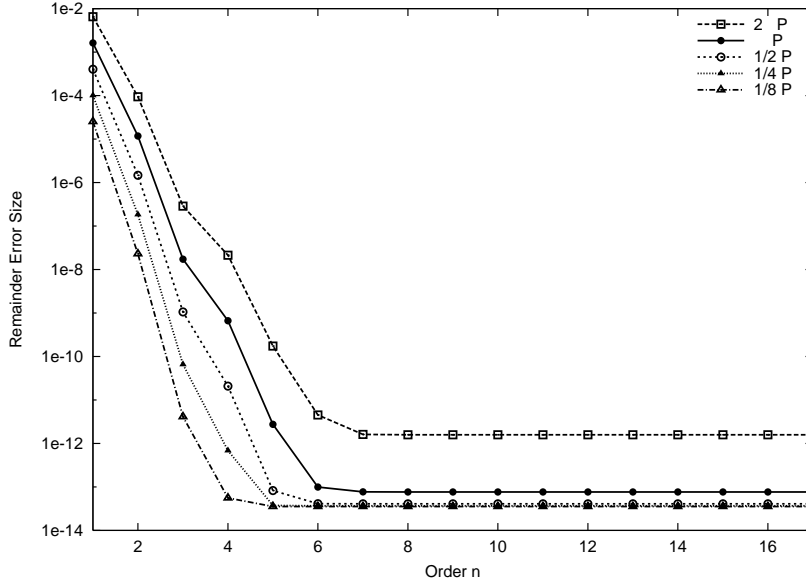
Figure 5: Remainder errors for a single step as a function of order and box size

orders of magnitude. Overall we observe that the Taylor model method has the ability to represent the solution set very accurately up to the error of the remainder bound, the size of which at a fixed time can be affected by the order of expansion in the transversal variable, as well as of course by the step size and as necessary the floating point accuracy. In fact, under the assumption of expandability of the flow in time and transversal variables, and under the assumption of arbitrary precision arithmetic, for a fixed t, the Taylor model method allows to represent the flow to any pre-specified accuracy. In [11], [31] we show how the local accuracy can be preserved under long-term integration.

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