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Shrink wrapping for Taylor models revisited

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Abstract Taylor models have been used successfully to calculate verified inclusions of the solutions of initial value problems for ordinary differential equations. In this context, Makino and Berz introduced an accompanying method called *shrink wrapping*. This method aims to reduce the wrapping effect which occurs during repeated forward integration of Taylor models.

We review shrink wrapping as proposed by Makino and Berz, state examples that point to a flaw in their theorem and concept of proof, and present a new, corrected version of shrink wrapping.

Keywords shrink wrapping, wrapping effect, Taylor models, ordinary differential equations

Mathematics Subject Classification (2010) 65L05 · 65L70 · 65G40

1 Introduction

Let $\mathbb{N} := \{1, 2, \dots\}$, $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and for $n \in \mathbb{N}$ let

$$\mathbb{IR}^n := \{[a, b] := [a_1, b_1] \times \cdots \times [a_n, b_n] \mid a, b \in \mathbb{R}^n,\ a \leq b \text{ componentwise}\}$$

denote the set of interval vectors in $\mathbb{R}^n$. If $n = 1$, than simply $\mathbb{IR} := \mathbb{IR}^1$ is written.

First, we recall the definition of Taylor models. Let $m \in \mathbb{N}_0$, $n \in \mathbb{N}$, $D \in \mathbb{IR}^n$ and $x_0 \in D$ be fixed. For a real, multivariate polynomial $p \in \mathbb{R}[x_1, \dots, x_n]$ in n unknowns $x_1, \dots, x_n$ of degree less or equal m and an interval $I \in \mathbb{IR}$, an m-th order Taylor model $p + I$ can be defined as

$$p + I := \{f \in C^0(D, \mathbb{R}) \mid f(x) \in p(x - x_0) + I \text{ for all } x \in D\}. \quad (1)$$

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The plus sign in $p + I$ on the left-hand side has only a suggestive meaning. It does not implicitly define some obscure summation of the polynomial part p and the remainder interval part I. Contrary to that, for fixed $x \in D$, the notation

$$p(x - x_0) + I := \{p(x - x_0) + y \mid y \in I\}$$

appearing on the right-hand side stands for a well-defined, commonly used set sum. Recall that, as usual, $C^0(D, \mathbb{R})$ denotes the set of all continuous functions $f : D \to \mathbb{R}$.[1] The idea of definition (1) is to consider p as the Taylor polynomial of order m with evaluation point x_0 of an $m + 1$-times differentiable function $f \in C^{m+1}(D, \mathbb{R})$ such that the remainder term $R(x) := f(x) - p(x - x_0)$ is enclosed in I for all $x \in D$. In that case $p + I$ is also called an m-th order Taylor model for $f \in C^{m+1}(D, \mathbb{R})$. This point of view explains the name "Taylor model", although definition (1) on its own does not necessitate any Taylor expansion of some unknown function f in the background. Taylor model vectors are analogously denoted by $p + I$ where now

$$p = (p_1, \ldots, p_k) \in (\mathbb{R}[x_1, \ldots, x_n])^k$$

is a k-vector of multivariate polynomials and $I = I_1 \times \cdots \times I_k \in \mathbb{IR}^k$ is an interval vector so that $p_i + I_i$ is a Taylor model as defined in (1) for all $i = 1, \ldots, k$. The range of $p + I$ is then given by

$$p(D - x_0) + I = \{p(x - x_0) + y \mid x \in D, y \in I\} \subseteq \mathbb{R}^k. \tag{2}$$

Now, arithmetic operations $+, -, \times, \div$, standard functions like exp, log, sin, cos, etc., and also integration with respect to one of the n variables can be defined on the set of all m-th order Taylor models with fixed D and x_0. Based on Taylor model arithmetic an explicit method for enclosing all solutions of an interval initial value problem for an ordinary differential equation (ODE) can be formulated in terms of Taylor models. See, for example, [5] or [2] for details. Suppose that such a k-dimensional ODE with interval initial conditions is given:

$$\begin{aligned} y' &= f(y, t) \in \mathbb{R}^k, \quad t \in (t_0, t_e) \\ y(t_0) &\in Y_0 \in \mathbb{IR}^k \end{aligned} \tag{3}$$

The Taylor model method proceeds by stepwise solving the ODE on appropriately chosen subintervals $[t_i, t_{i+1}]$ where $t_0 < t_1 < \cdots < t_N = t_e$, $N \in \mathbb{N}$. For each $i \in \{0, \ldots, N\}$, the method supplies a Taylor model k-vector $p^{(i)} + I^{(i)}$ such that for each $y_0 \in Y_0$ the solution $\tilde{y}$ of (3) with point initial value $\tilde{y}(t_0) = y_0$ fulfills

$$\tilde{y}(t_i) \in p^{(i)}(D - x_0) + I^{(i)}, \tag{4}$$

[1] In general $C^k(D, \mathbb{R})$, $k \in \mathbb{N}_0$, denotes the set of all k-times continuously differentiable functions $f : D \to \mathbb{R}$.

i.e., $\tilde{y}(t_i)$ is contained in the range of $p^{(i)} + I^{(i)}$.[2] In this context the domain D and the evaluation point x_0 for $p^{(i)} + I^{(i)}$ are usually taken as

$$D := B := [-1, 1]^n \quad \text{and} \quad x_0 := 0 \in \mathbb{R}^n, \tag{5}$$

where $n := k$ equals the dimension of the underlying ODE. This standard domain B with the origin as evaluation point will from now on be kept for all Taylor models considered in this paper.

The range $p^{(i)}(B) + I^{(i)}$, which is only implicitly given by $p^{(i)} + I^{(i)}$, is formally taken as the set of possible initial conditions for the next integration step from t_i to t_{i+1}. During the stepwise integration procedure the remainder interval vectors $I^{(i)}$, $i = 0, \ldots, N$, which cover all numerical and rounding errors may strongly increase in diameter due to the well-known wrapping effect of interval arithmetic.

The shrink wrapping technique invented by Makino and Berz [6], [7] aims to reduce/eliminate the remainder interval vectors $I^{(i)}$ as follows. The coefficients of the polynomials $p_j^{(i)}$, $j = 1, \ldots, n$, are slightly perturbed so that the range of the resulting perturbation $\tilde{p}^{(i)}$ fulfills

$$p^{(i)}(B) + I^{(i)} \subseteq \tilde{p}^{(i)}(B),$$

i.e., the range of $p^{(i)} + I^{(i)}$ is contained in that of $\tilde{p}^{(i)} + J$ where $J := [0, 0]^n \in \mathbb{IR}^n$ is the zero interval.[3] At first glance it seems contradictory that replacing the smaller set of initial values $p^{(i)}(B) + I^{(i)}$ for the integration step from t_i to t_{i+1} by the larger set $\tilde{p}^{(i)}(B)$ can diminish the wrapping effect and supply tighter inclusions in the end. Until now, the sometimes tremendous efficiency of shrink wrapping is only belayed by numerical evidence. A complete error analysis that fully explains the advantages of shrink wrapping is still missing in the literature and we want to state clearly that this is also not done here. Still, the following simple example may give an impression how shrink wrapping takes better care of inner dependencies. Take $m \geq 2$, $B := [-1, 1]$, and consider the two identical one-dimensional m-th order Taylor models $p_1 + I$ and $p_2 + I$ with $p_1(x) := x =: p_2(x)$ and $I := [-\delta, \delta]$ for some $\delta > 0$. Without further ado we state that, since $m \geq 2$, the product of both Taylor models computes as $(p_1 + I)(p_2 + I) = x^2 + J$, where

$$J := p_2(B)I + (p_1(B) + I)I = \delta(2 + \delta)[-1, 1].$$

Thus, the range of the product is

$$R := B^2 + J = [0, 1] + \delta(2 + \delta)[-1, 1] = [-\delta(2 + \delta), (1 + \delta)^2].$$

[2] We remark that the Taylor model method also supplies verified enclosures at all intermediate points $t \in (t_i, t_{i+1})$, $i = 0, \ldots, N - 1$, but shrink wrapping is only performed at the grid points wherefore we focus on them.

[3] In practical implementations small rounding errors might still have to be considered in J so that it is not exactly the zero interval, but close to.

Taking $q := 1 + \delta$ as a simplified shrink wrap factor and $\tilde{p}_i(x) := qx$, $i = 1, 2$, as shrink wrapped Taylor models (with zero remainder intervals) the desired inclusion of ranges

$$p_i(B) + I = [-1 - \delta, 1 + \delta] = qB = qp_i(B) = \tilde{p}_i(B)$$

holds true with equality in this case. Since $m \geq 2$, the product of the shrink wrapped Taylor models is $\tilde{p_1}\tilde{p_2} = q^2x^2$ having the range

$$S := q^2B^2 = q^2[0, 1] = [0, (1 + \delta)^2] \subsetneq [-\delta(2 + \delta), (1 + \delta)^2] = R.$$

Here, especially the lower bound of S is better than that of R since the inner dependencies of squaring is better resolved by the $\tilde{p}_i$ than by the p_i+I, $i = 1, 2$.

The paper is organized as follows. In Section 2 shrink wrapping as proposed by Makino and Berz is precisely stated and reviewed. We point to a flaw in their theorem and proof and give two illustrating counterexamples. In Section 3 we propose a new shrink-wrapping version and prove its correctness. A corresponding algorithm is sketched. Finally, in Section 4, we present some numerical results of our verified ODE-solver `verifyode` (implemented in MATLAB/INTLAB[10]) that uses the new shrink wrapping method. These results are compared to those obtained by Eble[2] with the following other verified ODE-solvers:
- AWA, developed by Lohner[4]
- COSY-VI, developed by Berz and his group [1]
- RIOT, developed by Eble [2] in his dissertation

2 Shrink Wrapping by Makino and Berz

In [6], Definition 2, Theorem 3, and also in [7], Definition 3, Theorem 6, Makino and Berz state the following definition and theorem which build the theoretical basis of their shrink wrapping method. The meaning and slightly different (original) notation will be explained afterwards in detail.

Definition 1 (Makino and Berz [6], Definition 2)
Let $\mathcal{M} = \mathcal{I} + \mathcal{S} + I$, where $\mathcal{S}$ is a polynomial and I is a small interval. We include I into the interval box $d \cdot [-1, 1]^v$. We pick numbers s and t satisfying

$$s \geq |\mathcal{S}_i(x)| \quad \forall x \in B,\ 1 \leq i \leq v, \tag{6}$$

$$t \geq \left| \frac{\partial \mathcal{S}_i(x)}{\partial x_j} \right| \quad \forall x \in B,\ 1 \leq i, j \leq v. \tag{7}$$

We call a map $\mathcal{M}$ shrinkable if

$$(1 - vt) > 0 \quad \text{and} \quad (1 - s) > 0; \tag{8}$$

both of which can be achieved if $\mathcal{S}$ (and since it is a polynomial, also its derivative) is sufficiently small in magnitude. Then we define q, the so-called shrink wrap factor, as

$$q = 1 + d \cdot \frac{1}{(1 - (v - 1)t) \cdot (1 - s)}\ . \tag{9}$$

Theorem 1 (Makino and Berz [6], Theorem 3, Shrink Wrapping) *Let $\mathcal{M} = \mathcal{I} + \mathcal{S}(x)$, where $\mathcal{I}$ is the identity. Let $I = d \cdot [-1, 1]^v$, and*

$$R = I + \bigcup_{x \in B} \mathcal{M}(x)$$

be the set sum of the interval $I = [-d, d]^v$ and the range of $\mathcal{M}$ over the original domain box B. Let q be the shrink wrap factor of $\mathcal{M}$; then we have

$$R \subseteq \bigcup_{x \in B} (q\mathcal{M})(x) \tag{10}$$

and hence multiplying $\mathcal{M}$ with the number q allows to set the remainder bound to zero.

We start with explaining the notation of Definition 1. First, $v \in \mathbb{N}$ denotes a fixed dimension which corresponds to n used in the introduction and $B := [-1, 1]^v$ is the v-dimensional unit cube which is the standard domain of all Taylor models considered here. Next, $d \in \mathbb{R}_{>0}$ is a radius such that the "interval" I, which is meant to be an interval vector in $\mathbb{IR}^v$, is contained in $d \cdot B = d \cdot [-1, 1]^v = [-d, d]^v$. Furthermore, $\mathcal{I}, \mathcal{S} \in (\mathbb{R}[x_1, \ldots, x_v])^v$ are a v-vectors of multivariate polynomials where $\mathcal{I}$ stands for "identity":

$$\mathcal{I}(x_1, \ldots, x_v) := (x_1, \ldots, x_v).$$

Thus,

$$\mathcal{M} = \mathcal{I} + \mathcal{S} + I \tag{11}$$

is the Taylor model vector with polynomial part $\mathcal{P} := \mathcal{I} + \mathcal{S}$ and remainder interval vector I. The slight notational difference compared to our introduction is that Makino and Berz use upper case calligraphic letters to denote the polynomial part.

The shrink wrapping strategy described in [6], p.15 ff., starts with transforming an arbitrary Taylor model to a normalized form (11) such that the following condition holds true:

$$\mathcal{S}(0) = 0 \text{ and } \mathcal{S} \text{ has relatively small linear coefficients in magnitude.} \tag{12}$$

This additional condition is not included in Definition 1 and also not used in the proof of Theorem 1.

We will give two counterexamples to Theorem 1. For the first, condition (12) is not satisfied, while the second fulfills condition (12) in the strong way that not only the constant coefficient but also all linear coefficients of $\mathcal{S}$ are zero, see Examples 1 and 2 below.

Now, the notation and meaning of Theorem 1 are considered. In contrast to Definition 1 where $\mathcal{M} = \mathcal{I} + \mathcal{S} + I$ is a Taylor model, here $\mathcal{M} = \mathcal{I} + \mathcal{S}$ denotes only its its polynomial part. The remainder interval vector $I = [-d, d]^v$ is now taken as the superset that included the remainder interval vector I of Definition 1. The conclusion of Theorem 1 says that

$$\mathcal{M}(B) + I \subseteq (q\mathcal{M})(B),$$

i.e., the range of the Taylor model $\mathcal{M} + I$ is contained in the range of the shrink wrapped Taylor model

$$q\mathcal{M} := (q\mathcal{M}_1, \ldots, q\mathcal{M}_v),$$

where q is the shrink wrap factor as in (9) of Definition 1, and the remainder interval vector of the shrink wrapped Taylor model is the zero interval which is simply omitted.

This result, known as shrink wrapping, is used by Makino and Berz in the procedure of computing verified enclosures of solutions of ordinary initial value problems. Its purpose is to get rid of the constant remainder interval vector I of a Taylor model that serves as initial condition of a single integration step as explained in the introduction. The effect is that the so-called wrapping effect is reduced so that difficult long term integration becomes possible up to a certain degree. Shrink wrapping was implemented in the software package COSY INFINITY[1].

The first counterexample to Theorem 1 is stated now. Although condition (12) is not satisfied, it will clearly show where the error in the proof of Makino and Berz is located.

Example 1 Let $v := 2$, $\mathcal{S}_1 :\equiv 0$, $\mathcal{S}_2(x_1, x_2) := 0.24x_1^2 - 0.99$, and $d := 0.0052$. Then $s := 0.99$ and $t := 0.48$ fulfill the conditions (6), (7), (8) of Definition 1, and

$$q := 1 + \frac{d}{(1-(v-1)t)(1-s)} = 1 + \frac{d}{(1-t)(1-s)} = 1 + \frac{0.0052}{0.52 \cdot 0.01} = 2$$

is the corresponding shrink wrap factor according to (9). For $\mathcal{M} := \mathcal{I} + \mathcal{S}$ we have $\mathcal{M}(B) \nsubseteq (q\mathcal{M})(B)$ so that also $\mathcal{M}(B) + I \nsubseteq (q\mathcal{M})(B)$ where $I := [-d, d]^2$. This contradicts (10) of Theorem 1.

Proof: For $x \in B$ we have

$$|\mathcal{S}_1(x)| = 0 < 0.99 = s, \quad |\mathcal{S}_2(x)| = 0.99 - 0.24|x_1|^2 \le 0.99 = s,$$

$$\left|\frac{\partial \mathcal{S}_2(x)}{\partial x_1}\right| = 0.48|x_1| \le 0.48 = t, \quad \left|\frac{\partial \mathcal{S}_i(x)}{\partial x_j}\right| = 0 < 0.48 = t$$

for $(i, j) \in \{(1, 1), (1, 2), (2, 2)\}$, $1 - s > 0$, and $1 - vt > 0$. Therefore conditions (6), (7), and (8) of Definition 1 are fulfilled. Take $\hat{x} := (1, 1)^T \in B = [-1, 1]^2$. Then

$$y := \mathcal{M}(\hat{x}) = (1, 1 + 0.24 - 0.99)^T = (1, 0.25)^T.$$

We show that $y \notin (q\mathcal{M})(B) = (2\mathcal{M})(B)$. In order to derive a contradiction we assume that $y = 2\mathcal{M}(\tilde{x})$ for some $\tilde{x} \in B$. Then $1 = y_1 = 2\mathcal{M}_1(\tilde{x}) = 2\tilde{x}_1$ so that $\tilde{x}_1 = 0.5$ and therefore

$$0.25 = y_2 = 2\mathcal{M}_2(\tilde{x}) = 2(\tilde{x}_2 + 0.24\tilde{x}_1^2 - 0.99) = 2(\tilde{x}_2 - 0.93).$$

Hence, $\tilde{x}_2 = 0.125 + 0.93 = 1.055 > 1$ contradicting $\tilde{x} \in B = [-1, 1]^2$. □

The left picture in Figure 1 illustrates the sets $\mathcal{M}(B)$ and $(q\mathcal{M})(B) = (2\mathcal{M})(B)$ of Example 1 and shows that $\mathcal{M}(B)$ is not contained in $(q\mathcal{M})(B)$.The assumptions of Theorem 1 imply that $\mathcal{M} : B \to \mathbb{R}^v$ is injective, see [6], p.17, Lemma 1, third inequality. Thus Brouwer's invariance of domain theorem yields that $\partial\mathcal{M}(B) = \mathcal{M}(\partial B)$, where ∂X denotes the boundary of a set $X \subseteq \mathbb{R}^v$. Therefore the boundaries of $\mathcal{M}(B)$ and $(q\mathcal{M})(B)$ are simply obtained by mapping the four edges of B.

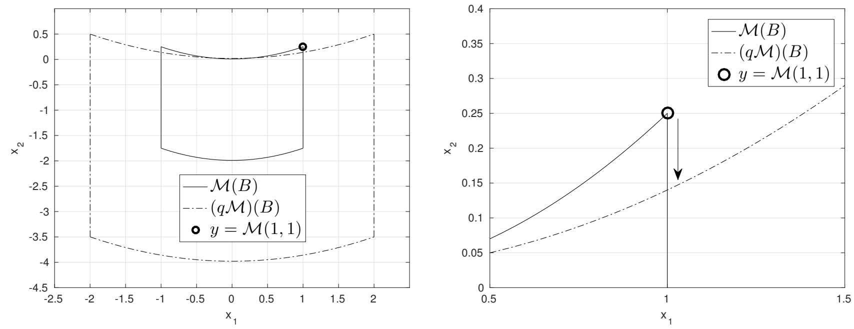

Fig. 1 Example 1

The main flaw in the proof of Theorem 1 given in [6] is located in the last paragraph at the bottom of page 19. There the following intuitive argument is given:

> "To complete the proof, we observe that because of the bound s on $\mathcal{S}$, the box $(1-s)[-1,1]^v$ lies entirely in the range of $\mathcal{M}$. Thus multiplying the map $\mathcal{M}$ with any factor $q > 1$ entails that the edges of the box $(1-s)[-1,1]^v$ move out by the amount $(1-s)(q-1)$ in all directions. Since the box is entirely inside the range of $\mathcal{M}$, this also means that the border of the range of $\mathcal{M}$ moves out by at least the same amount in any direction i. ..."

It is true that the box $(1-s)[-1,1]^v = (1-s)B$ lies inside $\mathcal{M}(B)$. In Example 1 this is the tiny box $[-0.01, 0.01]^2$. It is also true that the edges of a box centered at zero "move out" in all axis parallel directions when multiplied with a factor $q > 1$. However, this is a property of boxes (interval vectors) containing zero in their interior and not of arbitrary sets containing zero in their interior. The Example 1 is chosen extreme in the sense that the upper edge of $\mathcal{M}(B)$ does not "move out" in vertical direction when multiplied with the factor $q = 2$. This can be seen for the upper right corner point $y = \mathcal{M}(1,1) = (1, 0.25)^T$. At that point, the boundary of $(q\mathcal{M})(B)$ actually "moves in" in vertical direction and not "out" compared to the boundary of $\mathcal{M}(B)$. This is illustrated in the right picture of Figure 1. (Of course y is radially stretched by the factor $q = 2$ and becomes the upper right corner point $qy = 2y = (2, 0.5)^T$ of $(q\mathcal{M})(B)$; however different from this is axis parallel movement of the boundary.)

The counterexample to Theorem 1 satisfying condition (12) is such that $\mathcal{S}$ has zero constant and linear coefficients. This shows that Theorem 1 cannot be rescued by simply adding this condition to the assumptions.

Example 2 Let $v := 2$, $\alpha \in (0, 1/4)$, $\mathcal{S}_1 :\equiv 0$, $\mathcal{S}_2(x_1, x_2) := \alpha(x_1^2 - x_2^2)$, and $d \in (0, 1/20]$. Then $s := \alpha$ and $t := 2\alpha$ fulfill the conditions (6), (7), (8) of Definition 1, and

$$q := 1 + \frac{d}{(1-(v-1)t)(1-s)} = 1 + \frac{d}{(1-2\alpha)(1-\alpha)}$$

is the corresponding shrink wrap factor according to (9). For $\mathcal{M} := \mathcal{I} + \mathcal{S}$ and $I := [-d, d]^2$ we have $\mathcal{M}(B) + I \nsubseteq (q\mathcal{M})(B)$. This contradicts (10) of Theorem 1.

Proof: For $x \in B$ we compute $|\mathcal{S}_1(x)| = 0 < \alpha = s$, $|\mathcal{S}_2(x)| = \alpha|x_1^2 - x_2^2| \leq \alpha = s$,

$$\left|\frac{\partial \mathcal{S}_1(x)}{\partial x_i}\right| = 0 < 2\alpha = t, \left|\frac{\partial \mathcal{S}_2(x)}{\partial x_i}\right| = 2\alpha|x_i| \leq 2\alpha = t \quad \text{for } i \in \{1, 2\},$$

$1 - s > 0$, and $1 - vt > 0$. Therefore conditions (6), (7), and (8) of Definition 1 are fulfilled. Take $\hat{x} := (1, 1)^T \in B = [-1, 1]^2$ and $e := (-d, d)^T \in I$. Then $y := \mathcal{M}(\hat{x}) = (1, 1)^T = \hat{x}$ so that $z := y + e = (1 - d, 1 + d)^T \in \mathcal{M}(B) + I$. We show that $z \notin (q\mathcal{M})(B)$. In order to derive a contradiction we assume that $z = q\mathcal{M}(\tilde{x})$ for some $\tilde{x} \in B$. Then, $1 - d = z_1 = q\mathcal{M}_1(\tilde{x}) = q\tilde{x}_1$ so that $\tilde{x}_1 = (1 - d)/q$ and therefore

$$1 + d = z_2 = q\mathcal{M}_2(\tilde{x}) = q(\tilde{x}_2 + \alpha(\tilde{x}_1^2 - \tilde{x}_2^2)) = -\alpha q\tilde{x}_2^2 + q\tilde{x}_2 + \alpha(1 - d)^2/q.$$

Solving this equation for $\tilde{x}_2$ yields

$$\tilde{x}_2 = \frac{1}{2\alpha} \pm \sqrt{\frac{1}{4\alpha^2} - \xi} \quad \text{with} \quad \xi := \frac{q(1 + d) - \alpha(1 - d)^2}{\alpha q^2} > 0.$$

Now, $\tilde{x}_2 \in [-1, 1]$ and $\frac{1}{2\alpha} > 2$ imply $\xi < \frac{1}{4\alpha^2}$ and

$$\tilde{x}_2 = \frac{1}{2\alpha} - \sqrt{\frac{1}{4\alpha^2} - \xi}\ . \tag{13}$$

We want to derive the contradiction $\tilde{x}_2 > 1$. For that, by (13), it suffices to show

$$\left(\frac{1}{2\alpha} - 1\right)^2 > \frac{1}{4\alpha^2} - \xi \quad \Leftrightarrow \quad \zeta := \alpha(\xi + 1) - 1 > 0. \tag{14}$$

A computation yields[4]

$$\frac{\zeta}{\alpha d} = \frac{(-4\alpha^4 + 12\alpha^3 - 13\alpha^2 + 8\alpha - 3)d + 8\alpha^4 - 20\alpha^3 + 18\alpha^2 - 7\alpha + 1}{d^2 + (4\alpha^2 - 6\alpha + 2)d + 4\alpha^4 - 12\alpha^3 + 13\alpha^2 - 6\alpha + 1} =: f(\alpha, d).$$

For $\alpha \in (0, 1/4)$ and $d \in (0, 1/20]$ the numerator and the denominator of $f(\alpha, d)$ are positive so that also $\zeta = \alpha d \cdot f(\alpha, d) > 0$ which proves the right-hand side of (14). □

[4] The computation was done with the MATLAB 2016a Symbolic Math Toolbox.

Example 2 shows that for arbitrary small perturbation bounds s, t, and d (in absolute value) there exist counterexamples to Theorem 1. In Figure 2 we chose $\alpha := 0.1$ and $d := 0.005$ for illustration. The left picture shows that for these parameters the difference between $\mathcal{M}(B)$ and $(q\mathcal{M})(B)$ is below plotting resolution. The right picture shows these sets in the neighborhood of the upper right corner $y = \mathcal{M}(1,1) = (1,1)^T$ of $\mathcal{M}(B)$. It can be seen that the point

$$z = y + (-d, d)^T = (1-d, 1+d)^T \in \mathcal{M}(B) + I$$

is not contained in $(q\mathcal{M})(B)$.

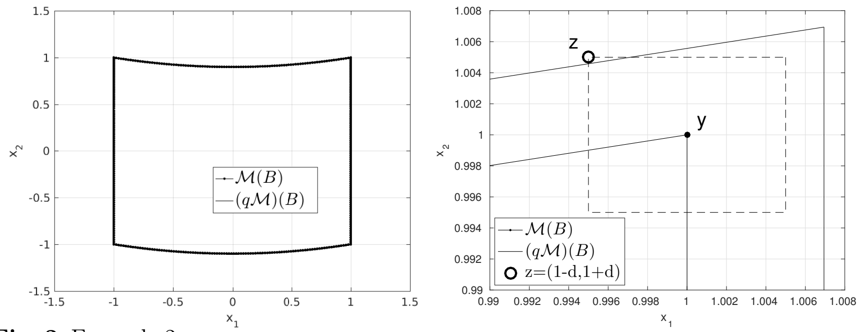

Fig. 2 Example 2

3 A new shrink wrapping version

In this section a new shrink wrapping version is presented. The difference compared to shrink wrapping by Makino and Berz is that the domain B is stretched by some new shrink wrap factor q in advance before $\mathcal{M}$ is applied, i.e., the range of the new shrink wrapped Taylor model will be $\mathcal{M}(qB)$ and not $q\mathcal{M}(B)$.

For didactic reasons the new shrink wrapping method is firstly presented in a simple form in Lemma 1 where, similar to Definition 1, all partial derivatives are uniformly bounded by one single constant $t > 0$. Also the remainder interval I is simply taken as $I := rB$, $r > 0$. These simplifications make the concept and proof clearer. The lemma is formulated for arbitrary continuously differentiable multivariate functions instead of multivariate polynomials.

Lemma 1 *Let $n \in \mathbb{N}$, $B := [-1,1]^n$, $r \in \mathbb{R}_{\geq 0}$ and $t \in [0, 1/n)$. Define $q := 1 + \frac{r}{1-nt}$ and suppose that a continuously differentiable function $f : qB \to \mathbb{R}^n$ is given such that $g(x) := f(x) - x$ satisfies $\left|\frac{\partial g_i(x)}{\partial x_j}\right| \leq t$ for all $x \in qB$ and all $i, j \in \{1, \dots, n\}$. Then $f(B) + rB \subseteq f(qB)$.*

Proof: Take $\hat{x} \in B$ and $v \in rB$. Note that $\hat{x} + (q-1)B \subseteq qB$. Define

$$h : \hat{x} + (q-1)B \to \mathbb{R}^n, \; x \mapsto f(\hat{x}) - g(x) + v.$$

Using the mean value theorem we compute for an arbitrary $\overline{x} \in \hat{x} + (q-1)B$:

$$\|h(\overline{x}) - \hat{x}\| = \|g(\hat{x}) - g(\overline{x}) + v\| \leq nt\|\hat{x} - \overline{x}\| + \|v\| \leq nt(q-1) + r = q-1,$$

where $\|\cdot\| := \|\cdot\|_\infty$ denotes the maximum norm on $\mathbb{R}^n$. Hence,

$$h(\hat{x} + (q-1)B) \subseteq \hat{x} + (q-1)B$$

so that Brouwer's fixed point theorem supplies an $\tilde{x} \in \hat{x} + (q-1)B \subseteq qB$ such that $\tilde{x} = h(\tilde{x}) = f(\hat{x}) - g(\tilde{x}) + v$, i.e., $f(\hat{x}) + v = \tilde{x} + g(\tilde{x}) = f(\tilde{x}) \in f(qB)$. □

Translated to Taylor models $p+I$, $p \in (\mathbb{R}[x])^n$ and $I := rB$, this means that the shrink wrapped Taylor model $\hat{p}(x) := p(qx)$ (attached with zero remainder interval vector) fulfills $p(B) + I \subseteq \hat{p}(B)$.

The general form of the new shrink wrapping method is formulated in Lemma 2. There, restrictions on partial derivatives are more separately imposed for each of the n distinct components. Also the remainder interval vector is now taken more carefully as zero-symmetric with possibly distinct component radii. On the one hand these refinements make the notation and proof a little bit more involved, but on the other hand they supply much better numerical results than the rough version given in Lemma 1.

The Jacobian matrix of a differentiable function $g : \mathbb{R}^n \to \mathbb{R}^m$, $m, n \in \mathbb{N}$, is denoted by $g'(x) := \left(\frac{\partial g_i}{\partial x_j}(x)\right)_{\substack{i=1,\dots,m \\ j=1,\dots,n}}$. The absolute value $|A|$ of a matrix A, or $|b|$ of a vector b, is meant componentwise. For a set $X \subseteq \mathbb{R}^n$ and a column vector $a \in \mathbb{R}^n$ we use the abbreviation

$$aX := \operatorname{diag}(a)X = \{\operatorname{diag}(a)x | x \in X\}, \tag{15}$$

where $\operatorname{diag}(a)$ is the diagonal matrix of order n with diagonal a. Moreover, $\mathbb{1} \in \mathbb{R}^n$ denotes the vector having 1 in each component.

Lemma 2 *Let $n \in \mathbb{N}$, $B := [-1,1]^n$, $r, s \in \mathbb{R}^n_{\geq 0}$, and $q := \mathbb{1} + r + s$. Suppose that a continuously differentiable function $f : qB \to \mathbb{R}^n$ is given such that $g(x) := f(x) - x$ satisfies*

$$|g'(x)|(q - \mathbb{1}) \leq s \quad \textit{for all } x \in qB \tag{16}$$

which means componentwise

$$\sup_{x \in qB} |g_i'(x)|(q - \mathbb{1}) = \sup_{x \in qB} \sum_{j=1}^{n} \left|\frac{\partial g_i}{\partial x_j}(x)\right| (q_j - 1) \leq s_i \quad \textit{for all } i \in \{1, \dots, n\}. \tag{17}$$

Then we have $f(B) + rB \subseteq f(qB)$.

Proof: Take $\hat{x} \in B$ and $v \in rB$. Note that $\hat{x} + (q - \mathbb{1})B \subseteq qB$. Define

$$h : \hat{x} + (q - \mathbb{1})B \to \mathbb{R}^n, \; x \mapsto f(\hat{x}) - g(x) + v.$$

For $\overline{x} \in \hat{x} + (q - \mathbb{1})B$ and $i \in \{1, \dots, n\}$ there is, according to the mean value theorem, a ξ on the line between $\hat{x}$ and $\overline{x}$ such that $g_i(\hat{x}) - g_i(\overline{x}) = g_i'(\xi)(\hat{x} - \overline{x})$. Using (17) we compute

$$|h_i(\overline{x}) - \hat{x}_i| = |g_i(\hat{x}) - g_i(\overline{x}) + v_i| \leq |g_i'(\xi)||\hat{x} - \overline{x}| + |v_i| \leq s_i + r_i = q_i - 1.$$

Hence $h(\hat{x} + (q - \mathbb{1})B) \subseteq \hat{x} + (q - \mathbb{1})B$ so that Brouwer's fixed point theorem supplies an $\tilde{x} \in \hat{x} + (q - \mathbb{1})B \subseteq qB$ such that $\tilde{x} = h(\tilde{x}) = f(\hat{x}) - g(\tilde{x}) + v$, i.e., $f(\hat{x}) + v = \tilde{x} + g(\tilde{x}) = f(\tilde{x}) \in f(qB)$. □

In practical applications the shrink wrap vector $q = \mathbb{1} + r + s$ defined in Lemma 2 is aimed to be close to $\mathbb{1}$, i.e., r and especially s shall be small. Therefore, it is somewhat clear that the quite restrictive condition (16) requires $|g'(x)|$ to be appropriately small also. This becomes more likely if $f(x) \approx x$ is close to the identity.

To achieve that in practice, f is first shifted by subtracting $f(0)$ and then it is multiplied (preconditioned) with an approximate inverse R of $f'(0)$, where $0 \in \mathbb{R}^n$ is the center of the standard domain B. This corresponds to the normalization (11) and (12) by Makino and Berz. The final preconditioning with R is formulated in the following corollary.

Corollary 1 *Let $n \in \mathbb{N}$, $B := [-1, 1]^n$, $r, \tilde{r}, s \in \mathbb{R}^n_{\geq 0}$, and $q := \mathbb{1} + \tilde{r} + s$. Furthermore, let $R \in \mathbb{R}^{n,n}$ be an invertible matrix with $|R|r \leq \tilde{r}$. Suppose that $f : qB \to \mathbb{R}^n$ is a continuously differentiable function such that $g(x) := Rf(x) - x$ satisfies*

$$|g'(x)|(q - \mathbb{1}) \leq s \quad \textit{for all } x \in qB.$$

Then $f(B) + rB \subseteq f(qB)$.

Proof: Lemma 2 applied to $\tilde{f} := Rf$ yields $\tilde{f}(B) + \tilde{r}B \subseteq \tilde{f}(qB)$. By assumption on $\tilde{r}$ we have $R(rB) \subseteq \tilde{r}B$ so that $Rf(B) + R(rB) \subseteq Rf(qB)$. Applying R^{-1} to both sides yields the assertion. □

As mentioned before, in practical applications shrink wrapping is most effective if the shrink wrap vector q is close to $\mathbb{1}$. If this is not achievable, other, more simple fallback strategies can sometimes still be applied to reduce the wrapping effect. For example, the image $p(B) + I$ of the given Taylor model $p + I$ can be enclosed into a shifted parallelotope $p(0) + \tilde{A}B$ where $\tilde{A} \in \mathbb{R}^{n,n}$ is an appropriate invertible matrix.

The following lemma formalizes this parallelotope enclosure. Like before, more general functions of the form $f(x) = Ax + h(x)$ with invertible matrix $A \in \mathbb{R}^{n,n}$ and continuous, supposedly small perturbation function h are considered instead of shifted multivariate polynomials $p - p(0)$. A simplified shrink wrap vector $q = \mathbb{1} + r$ is introduced such that $\tilde{A} := A \cdot \mathrm{diag}(q)$ is the desired matrix that generates the enclosing parallelotope $\tilde{A}B$.

Lemma 3 *Let $n \in \mathbb{N}$, $B := [-1,1]^n$, $I \in \mathbb{IR}^n$, $r \in \mathbb{R}^n_{\geq 0}$, and $q := \mathbb{1} + r$. Furthermore, let $f : B \to \mathbb{R}^n$, $x \mapsto Ax + h(x)$ where $A \in \mathbb{R}^{n,n}$ is an invertible matrix and h is a function such that $|A^{-1}(h(x)+e)| \leq r$ for all $x \in B$ and all $e \in I$. Then $f(B) + I \subseteq A(qB) = (A \cdot \mathrm{diag}(q))B$.*

Proof: For $x \in B$ and $e \in I$ we have

$$|x + A^{-1}(h(x)+e)| \leq |x| + |A^{-1}(h(x)+e)| \leq \mathbb{1} + r = q.$$

Hence, $v := x + A^{-1}(h(x)+e) \in qB$ and $f(x) + e = Av \in A(qB)$. □

3.1 Outline of a shrink wrapping algorithm

In this subsection main points of an algorithm implementing shrink wrapping according to Lemma 2 and Corollary 1 are listed. Note that for a verified implementation many standard aspects of correctly directed rounding must be regarded in addition. Since they are common knowledge in this area, we do not explicitly describe them in the sketched algorithm. Also possible fallback strategies like a parallelotope enclosure according to Lemma 3 that might be used if shrink wrapping is not applicable are not explained in detail.

The main challenge is to determine $s \in (\mathbb{R}_{\geq 0})^n$ such that (16) (respectively, (17)) is fulfilled. The problem is that s occurs somewhat implicitly twice in this condition, first as an upper bound on the right-hand side, and second in the definition of the extended domain $qB = [-(\mathbb{1}+r+s), (\mathbb{1}+r+s)]$ on which the bound shall be valid. We use a straight forward iteration based on (17) to estimate $s_1, \ldots, s_n$ one after another. This key part is stated in step 7 below in MATLAB-like pseudocode. Afterwards this estimate is relaxed by some factor slightly greater than one. Finally, the resulting shrink wrap vector q must be verified a posteriori.

Input: A Taylor model n-vector $p + I$ which shall be shrink wrapped.

1. Set $c := p(0)$ and $p := p - c$ so that $p(0) = 0$ is valid in the sequel.
2. Decompose $p(x) = Ax + h(x)$, $x := (x_1, \ldots, x_n)^T$, with matrix $A \in \mathbb{R}^{n,n}$ and h having zero constant and linear terms, i.e., $h(0) = 0 = h'(0)$.
3. If A is not invertible or if its condition number is too large, then shrink wrapping is not applicable. Then, try other fallback strategies or return $p + I$ unchanged.
4. Compute an approximate inverse R of A.
5. Determine $r \in (\mathbb{R}_{\geq 0})^n$ such that $I \subseteq rB = [-r, r] \in \mathbb{IR}^n$ and set $\tilde{r} := |R|r$.
6. Compute $g(x) := Rp(x) - x$ and its Jacobian matrix $g'(x)$.
7. Estimate the shrink wrap vector q as follows with `rs`$:= \tilde{r}$, `dgi_dxj`$:= \frac{\partial g_i}{\partial x_j}$:

```
q_max = 1.01;  % heuristic bound for shrink wrap factors
q_tol = 1E-12; % heuristic minimum rate of change
iter_max = 3;  % heuristic upper bound for iterations
q = 1+rs;
improve = true;
```

```
iter = 0;
while improve && iter < iter_max
  s = zeros(size(rs));
  q_old = q;
  for i = 1:n
    for j = 1:n
      compute upper bound t of |dgi_dxj([-q,q])|
      s(i) = s(i) + t * (q(j)-1);
    end
    q(i) = 1 + rs(i) + s(i);
    if q(i) > q_max shrink wrapping seems not promising
                    -> try other fallback strategies
  end
  improve = any((q-q_old)./q > q_tol);
  iter = iter + 1;
end
```

8. Relax s by multiplication with a factor slightly greater 1 and set $q := \mathbb{1} + \tilde{r} + s$.
9. Verify the new shrink wrap vector q a posteriori. If this is not successful, other fallback strategies might be used again.
10. Compute $\tilde{p}(x) := p(q_1 x_1, \ldots, q_n x_n) + c$.

Output: The shrink wrapped Taylor model n-vector $\tilde{p} + J$ with an almost zero remainder $J \in \mathbb{IR}^n$ that originates from rounding errors only.

4 Numerical examples

Based on [2] and [5] we implemented a verified ODE-solver `verifyode` using Taylor models in MATLAB/INTLAB[10]. The new shrink wrapping method presented in Section 3 was successfully tested for several standard problems stated in [2], Chap. 5. Here we show results for computing

I) the motion of the Asteroid 1997 XF11 in the solar system,
II) the Lotka-Volterra equations.

As stated in the introduction our results are compared to those obtained by Eble[2] with the following other verified ODE-solvers:

- AWA, developed by Lohner [4]
- COSY-VI, developed by Berz and his group [1]
- RIOT, developed by Eble [2] in his dissertation

Like COSY-VI also RIOT (always) uses shrink wrapping as specified by Makino and Berz, see Section 2. Thus, according to our counterexamples, also RIOT may not produce correct, verified results. But anyway we considered it as interesting to compare results of COSY-VI and RIOT to those of `verifyode`.

We start with test case I). For greater details and astrophysical explanations we refer to [3] and [2], Chap. 5, Sec. 5.5. The differential equation reads:

$$\begin{aligned} y_1' &= y_4 \\ y_2' &= y_5 \\ y_3' &= y_6 \\ y_4' &= -\gamma \frac{y_1}{d} \\ y_5' &= -\gamma \frac{y_2}{d} \\ y_6' &= -\gamma \frac{y_3}{d} \\ d &:= (y_1^2 + y_2^2 + y_3^2)^{3/2} \\ \gamma &:= 0.9986 \end{aligned} \tag{18}$$

The interval initial conditions at $t_0 := 0$ are:

$$\begin{aligned} y_1(0) &\in -1.77269098191512 && \pm 0.5 \cdot 10^{-7} \\ y_2(0) &\in 0.1487214852342955 && \pm 0.5 \cdot 10^{-7} \\ y_3(0) &\in -0.07928350462244194 && \pm 0.5 \cdot 10^{-7} \\ y_4(0) &\in 0.2372031916516237 && \pm 0.5 \cdot 10^{-6} \\ y_5(0) &\in 0.612524538758628 && \pm 0.5 \cdot 10^{-6} \\ y_6(0) &\in 0.04583217572165624 && \pm 0.5 \cdot 10^{-6} \end{aligned} \tag{19}$$

The components y_1, y_2, y_3 are the (x, y, z)-coordinates of the asteroid in the solar system with the sun in its center. The remaining components $y_{3+i} = y_i'$, $i = 1, 2, 3$, are their velocities.

Eble[2] computed enclosures for all y_i at $t_e = 5.5\pi$ and at $t_e = 11\pi$. This corresponds to time periods of 2.75 years and 5.5 years, respectively. Table 1 shows the parameter settings that he used for AWA, COSY-VI, and RIOT, see [2], p.162, 163. Our parameter settings for `verifyode` are stated at the end of the table. They are comparable to those of RIOT and COSY-VI with no preconditioning and activated shrink wrapping which is abbreviated by 'None/On'.

COSY-VI 'QR/Blunting' means that the QR-method is used for preconditioning as described in [6] and [8] and that shrink wrapping is done with additional 'blunting' of ill-conditioned matrices as described in [6], p.20-22. This setting seems very stable and very well-suited for long term integration.

AWA	t_0	t_e	order p	step size	enclosure method	error tolerances	
	0	5.5π 11π	18	$h_0 = 0.0001$	4	$\epsilon_{abs} = $ 1E-16	$\epsilon_{err} = $ 1E-16

COSY-VI	t_0	t_e	order n	step size			local error tolerance
	0	5.5π 11π	10	$h_0 = 0.1$	$h_{min} = 0.001$	$h_{max} = 1$	1E-11

preconditioning	shrink wrapping	weighted order
None/QR	On/Blunting	None

RIOT	t_0	t_e	order n	sparsity tolerance	step size control		
	0	5.5π 11π	10	1E-20	AUTO	$h_0 = 0.1$	$h_{min} = 0.001$

local error tolerance	order check	bounder
1E-11	TotalDegree	LDB

`verifyode`	t_0	t_e	order n	sparsity tolerance	step size control	
	0	5.5π 11π	10	1E-20	$h_0 = 0.1$	$h_{min} = 0.001$

local error tolerance	bounder	shrink wrapping	relative ϵ-inflation
1E-11	NAIVE	On	1E-1

Table 1 Parameter settings test case I)

The computed results are displayed in Table 2. There, for all six components y_i the enclosure intervals and their diameters at the end of integration at $t_e = 5.5\pi$ (2.75 years) and $t_e = 11\pi$ (5.5 years), respectively, are stated.

According to [2] COSY-VI 'QR/Blunting' integrates the initial value problem (18), (19) up to $t_e = 46\pi$ (23 years) without problems while AWA with enclosure method 4 breaks down at $t_e \approx 46.7549$ (7.44 years). COSY-VI 'None/On' managed $t_e = 5.5\pi$ (2.75 years) but could not deal with $t_e = 11\pi$ (5.5 years). We mention that `verifyode` with the stated parameter settings integrates up to round about $t_e = 48$ (7.64 years). This clearly shows the impact of preconditioning on long term integration. Preconditioning is not yet implemented in `verifyode`.

For the first integration period of 2.75 years Riot computes the tightest interval enclosures followed by `verifyode`, AWA and COSY-VI 'QR/Blunting'. COSY-VI 'None/On' produces the widest intervals. For the second integration period of 5.5 years `verifyode` computes the tightest interval enclosures followed by COSY-VI 'QR/Blunting' and AWA. Riot produces the widest intervals and, as said before, COSY-VI 'None/On' could not deal with this integration period.

	AWA	COSY-VI None/On	COSY-VI QR/Blunting	RIOT	`verifyode`
years	2.75	2.75	2.75	2.75	2.75
[y1]	$-5.67^{0\,980}_{1\,439}$E-1	$-5.67^{0\,240}_{2\,180}$E-1	$-5.67^{0\,966}_{1\,453}$E-1	-5.671^{006}_{413}E-1	$-5.67^{0\,992}_{1\,427}$E-1
[y2]	$1.838\,7^{40}_{32}$	$1.838\,7^{47}_{24}$	$1.838\,73^{9}_{2}$	$1.838\,73^{9}_{3}$	$1.838\,73^{9}_{3}$
[y3]	$-1.318\,2^{13}_{63}$E-1	-1.318^{134}_{343}E-1	$-1.318\,2^{14}_{63}$E-1	$-1.318\,2^{16}_{61}$E-1	$-1.318\,2^{13}_{63}$E-1
[y4]	$-5.867\,5^{03}_{52}$E-1	-5.867^{444}_{612}E-1	$-5.867\,5^{06}_{50}$E-1	$-5.867\,5^{11}_{45}$E-1	$-5.867\,5^{09}_{47}$E-1
[y5]	$4.99^{8\,817}_{6\,838}$E-2	$^{5.001\,823}_{4.993\,833}$E-2	$4.99^{8\,851}_{6\,810}$E-2	$4.99^{8\,686}_{6\,969}$E-2	$4.99^{8\,755}_{6\,900}$E-2
[y6]	-2.628^{649}_{789}E-2	-2.628^{441}_{997}E-2	-2.628^{648}_{790}E-2	-2.628^{660}_{778}E-2	-2.628^{652}_{786}E-2
d([y1])	4.581 125E-5	1.938 527E-4	4.856 704E-5	4.063 959E-5	4.338 834E-5
d([y2])	6.982 230E-6	2.204 949E-5	6.316 541E-6	4.990 423E-6	5.023 891E-6
d([y3])	4.919 242E-6	2.081 581E-5	4.863 480E-6	4.448 172E-6	4.864 552E-6
d([y4])	4.791 893E-6	1.670 766E-5	4.245 541E-6	3.361 500E-6	3.715 201E-6
d([y5])	1.977 308E-5	7.989 099E-5	2.040 883E-5	1.716 141E-5	1.854 481E-5
d([y6])	1.393 621E-6	5.554 181E-6	1.414 084E-6	1.168 779E-6	1.335 963E-6
time [s]	3.01[4]	2 454.26	1 702.76	34 336.20	3 401.02[5]
years	5.5	5.5	5.5	5.5	5.5
[y1]	$-9.1^{83\,529}_{92449}$E-1		$-9.18^{7\,245}_{8\,739}$E-1	$-9^{144\,781}_{231\,145}$E-1	$-9.18^{7\,382}_{8\,596}$E-1
[y2]	$-7.4^{27\,962}_{32\,376}$E-1		$-7.4^{29\,834}_{30\,500}$E-1	$-7.4^{11\,222}_{49\,016}$E-1	$-7.4^{29\,899}_{30\,439}$E-1
[y3]	$7.6^{80\,225}_{20470}$E-3		$7.6^{55\,686}_{44\,973}$E-3	$7^{961\,098}_{339\,076}$E-3	$7.6^{54\,741}_{45\,954}$E-3
[y4]	$9.13^{9\,898}_{4\,469}$E-1		$9.13^{7\,633}_{6\,730}$E-1	$9.1^{61\,645}_{12\,709}$E-1	$9.13^{7\,552}_{6\,815}$E-1
[y5]	$-4.04^{2\,339}_{7\,165}$E-1		$-4.04^{4\,378}_{5\,129}$E-1	$-4.0^{15\,455}_{63\,907}$E-1	$-4.04^{4\,447}_{5\,057}$E-1
[y6]	$6.03^{5\,479}_{4\,566}$E-2		$6.03^{5\,094}_{4\,952}$E-2	$6.03^{7\,988}_{1\,965}$E-2	$6.03^{5\,085}_{4\,960}$E-2
d([y1])	8.918 362E-4		1.492 804E-4	8.636 351E-3	1.213 813E-4
d([y2])	4.412 134E-4		6.645 066E-5	3.779 277E-3	5.382 371E-5
d([y3])	5.975 463E-5		1.071 215E-5	6.220 211E-4	8.785 532E-6
d([y4])	5.427 170E-4		9.014 262E-5	4.893 542E-3	7.363 283E-5
d([y5])	4.824 878E-4		7.501 268E-5	3.845 040E-3	6.088 643E-5
d([y6])	9.119 810E-6		1.413 859E-6	6.021 407E-5	1.236 146E-6
time [s]	5.26	-	3 427.04	111 640.48	7 466.79

Table 2 Asteroid 1997 XF11 orbit calculation

[4] Although it is not in the focus of this paper, it is amazing how fast AWA runs. After a few seconds it is finished while the other solvers need several thousand seconds. Up to a great amount this is due to the very expansive high order Taylor model arithmetic, which, compared to AWA, does not yet pay off for both considered, still quite short integration periods.

[5] The results for AWA, COSY-IV, and RIOT were computed by Eble[2] using a 1.83 GHz AMD Sempron 2600+ Processor under Ubuntu Linux 5.10. The results for `verifyode` were computed with a 3.60GHz Intel Xeon E5-1620 Processor under openSUSE Linux 13.1 and MATLAB 2016a (Prerelease). Therefore the computing times of the latter are only vaguely comparable to those of the former. Having in mind that COSY-VI is compiled Fortran code while `verifyode` is interpreted MATLAB code, the performance of `verifyode` seems acceptable and competitive.

In test case II) the following special kind of Lotka-Volterra equations is considered:

$$\begin{aligned} y_1' &= 2y_1(1 - y_2) \\ y_2' &= y_2(y_1 - 1) \end{aligned} \tag{20}$$

Interval initial conditions at $t_0 := 0$ are taken as:

$$\begin{aligned} y_1(0) &\in [0.95, 1.05] \\ y_2(0) &\in [2.95, 3.05] \end{aligned} \tag{21}$$

The length of one predator-pray cycle of (20) with point initial value $y(0) := (1, 3)$ is approximately $T := 5.4888138468035$. It turns out that AWA cannot integrate up to $t_e := T$ with interval initial conditions (21). In contrast COSY-VI and RIOT can deal with them quite easily. This is discussed in detail in [6], p.8 ff, and [2], Sec. 5.2. Like for test case I), the parameter settings for COSY-VI, RIOT, and `verifyode` are listed in Table 3, see also [2], p.147, 148.

COSY-VI	t_0	t_e	order n	step size			local error tolerance
	0	T	18	$h_0 = 0.03$	$h_{min} = 0.003$	$h_{max} = 1$	1E-11

preconditioning	shrink wrapping	weighted order
None/None/QR	On/Blunting/Blunting	None

RIOT	t_0	t_e	order n	sparsity tolerance	step size control		
	0	T	18	1E-20	AUTO	$h_0 = 0.03$	$h_{min} = 0.003$

local error tolerance	order check	bounder
1E-11	TotalDegree	LDB

`verifyode`	t_0	t_e	order n	sparsity tolerance	step size control	
	0	T	18	1E-20	$h_0 = 0.03$	$h_{min} = 0.003$

local error tolerance	bounder	shrink wrapping	relative ϵ-inflation
1E-11	NAIVE	On	1E-2

Table 3 Parameter settings test case II)

Table 4 lists the computed enclosure intervals for y_1 and y_2 and their diameters at $t_e = T$. As mentioned before the results of `verifyode` (and RIOT) are best comparable to COSY-VI 'None/on'. It can be seen that except COSY-VI 'None/Blunting', which gives significantly wider intervals, all other enclosures produced by COSY-VI 'None/On' and 'QR/Blunting', RIOT, and `verifyode` are of similar quality.

	COSY-VI			RIOT	`verifyode`
	None/On	None/Blunting	QR/Blunting		
[y1]	1.240 265 0.816 719	1.454 922 0.718 909	1.240 265 0.816 719	1.240 280 0.798 904	1.243 906 0.776 616
[y2]	3.045 759 2.935 927	3.077 687 2.873 835	3.045 759 2.935 927	3.054 377 2.933 777	3.058 869 2.931 524
d([y1])	0.424	0.737	0.424	0.442	0.468
d([y2])	0.110	0.204	0.110	0.121	0.128
time [s]	23.36	42.88	7.17	696.49	10.79[6]

Table 4 Lotka-Volterra equations

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[6] Recall that, as mentioned in a footnote to Table 2, the results for COSY-VI and RIOT were calculated with a different computer than those of `verifyode` so that performance cannot be compared one-to-one.

[7] For some unknown reason the article cannot be found in the online archive of the *International Journal of Differential Equations and Applications* available from `www.ijpam.eu/en/index.php/ijdea/issue/archive` but it is available from the authors' web page `www.bt.pa.msu.edu/pub/` .