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An Application of Taylor Models to the Nakao Method on ODEs

Nobito YAMAMOTO* and Takashi KOMORI

** Department of Computer Science*
The University of Electro-Communications
Fax: 042–443–5349
E-mail: yamamoto@im.uec.ac.jp

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The authors give short survey on validated computaion of initial value problems for ODEs especially Taylor model methods. Then they propose an application of Taylor models to the Nakao method which has been developed for numerical verification methods on PDEs and apply it to initial value problems for ODEs with some numerical experiments.

Key words: Taylor model, Nakao method, validated computation, ODEs

1. Introduction

In the present paper, we discuss validated computation methods to initial value problems for ODEs. In this field, the method based on Taylor expansion and QR factorization by Lohner has been most widely used. Recently, Taylor model method has been developed as a powerful method which includes formula manipulation processes of polynomials, and it is applied to many kinds of different problems [2]. On the other hand, the Nakao method which is developed for numerical verification of partial differential equations is also applicable to ODEs [14].

Our goal is understanding Taylor model method in the context of Nakao method, and we present new formulations of validated computation to initial value problems for ODEs with an application of Taylor models.

In Chapter 2, we outline validated computation of initial value problems for ODEs and describe effects of error expansions due to wrapping effect and countermeasures against the error expansions including Lohner's method.

In Chapter 3, a short survey for Taylor models is presented. We start with the concept and the arithmetic of Taylor models, and then describe application to initial value problems for ODEs.

In Chapter 4, we apply the Nakao method to initial value problems for ODEs, and combine Taylor models and the Nakao method in Chapter 5. In Chapter 6, some numerical examples and consideration of the effect of Taylor models are shown.

2. Validated computation of initial value problems for ODEs

We consider methods for validated computation to an initial value problem of the following equation in a vector form.

$$\begin{cases} \dfrac{d}{dt}\boldsymbol{u}(t) = \boldsymbol{f}(t, \boldsymbol{u}), \quad 0 < t < T, \\ \boldsymbol{u}(0) = \boldsymbol{u}_0. \end{cases}$$

Here $\boldsymbol{u}(t)$, $\boldsymbol{f}$ are vectors in $\mathbf{R}^m$. If the function $\boldsymbol{f}(t, \boldsymbol{u})$ in the right-hand side is Lipschitz continuous w.r.t. $\boldsymbol{u}$, then the solution to this equation uniquely exists. Therefore main problem in validated computation on ODEs is not verification of existence or uniqueness of the solutions but how we can get bounds, as tight as the least upper bound if possible, of the computational errors to the approximate solutions. Estimation of truncation error (or discretization error) is determined by each method of computation of the approximate solutions. In validated computation we use this estimation and interval arithmetic which takes account of the effect of round-off error. However if we naively introduce the interval arithmetic, overestimation of the widths of intervals may occur. There are two main reasons why those things happen.

The first one is interval inflation due to the fact that the distributive law does not hold for interval variables. Especially an enclosure of the range of a nonlinear function by intervals often causes a large overestimation (these phenomina are called dependency problems). The mean-value form [13] and its variants have been used to reduce the overestimations, and Taylor model is another effective method.

The second is wrapping effect. As an example of wrapping effect, we consider the following equations with the initial conditions given by intervals.

$$\begin{cases} \dfrac{d}{dt}u_1 = u_2, \\ \dfrac{d}{dt}u_2 = -u_1, \\ u_1(0) = [-0.5, 0.5], \\ u_2(0) = [3.5, 4.5]. \end{cases} \tag{1}$$

The solution to this system revolves around the origin along a circle on the u_1-u_2 plane. Now we compute the solution by a finite difference method. The initial condition is a square whose edges are parallel to u_1-axis or u_2-axis. For the next step $t = t_1$, the true solution is a rotated square. But so long as we adopt interval arithmetic, our approximate solution is a square whose edges are parallel to u_1-axis or u_2-axis, which encloses the square of the true solution. When we repeat this process, the size of the interval increases exponentially on each step. This shows a typical example of wrapping effect.

The principle part of wrapping effect actually arises through iteration of matrix-vector products for interval vectors in discretized computation of the equations. Since so many kinds of problems can be attributed to matrix-vector iteration,

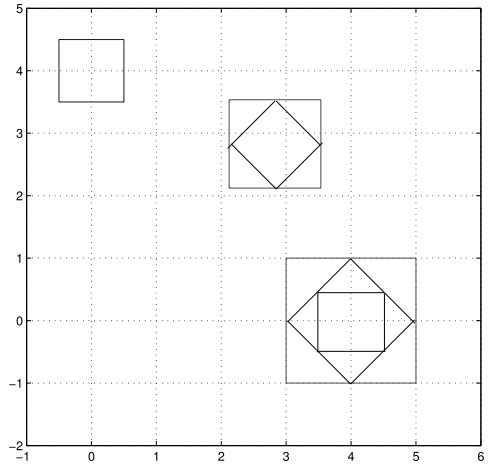

Fig. 1. The wrapping effect caused by (1)

wrapping effect is the difficulty to avoid not only for initial value problems for ODEs but also for a lot of problems in other fields [5].

As countermeasures against wrapping effect, we can apply several kinds of methods [5]:

- Rearranging expression evaluation (e.g., calculating matrix-matrix product before matirx-vector product in matrix-vector iteration)
- Coordinate transformations (e.g., parallelpipeds [1], QR factorization [4] etc.)
- Using enclosures by ellips (ellipsoids [15])
- Using enclosures by convex polygons (zonotopes [3])
- Taylor models [8]

These methods are applied to various problems in many fields. On validated computation of ODEs, the seeds of wrapping effect are the following.

- The interval widths when the initial values are given by intervals
- The truncation error and round-off error in the computation processes

The Lohner's method adopts two countermeasures against wrapping effect.

1. For initial intervals, extracting the linear part of the transformation of the initial interval vector from the computation of ODEs, use rearranging expression evaluation.
2. For the truncation error and round-off error, use coordinate transformation based on QR factorization.

Let us discuss these methods [17, 4].

Set the initial value problem as follows.

$$\begin{cases} \dfrac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(t, \boldsymbol{u}), \quad 0 < t < T, \\ \boldsymbol{u}(0) = \boldsymbol{u}_0 \in [\boldsymbol{u}_0], \end{cases} \tag{2}$$

$\boldsymbol{u}, \boldsymbol{u}_0, \boldsymbol{f} \in R^m$,

$\boldsymbol{f}$: $C^p[0,T]$ w.r.t. t and $C^p(D)$ w.r.t. $\boldsymbol{u} \in D \subset R^m$,

where initial value $\boldsymbol{u}_0$ is an arbitrary point in an initial box (i.e., an interval vector) $[\boldsymbol{u}_0]$.

We use Taylor expansion method for the approximate solutions. In order to calculate the derivatives, computer programs adopting automatic differentiation are often used.

Take time steps $0 = t_0 < t_1 < \cdots < t_n = T$. Let h be the step size and $[\boldsymbol{u}_j]$ be an interval including the true solution $\boldsymbol{u}_j$ at $t = t_j$. We intend to get an interval $[\boldsymbol{u}_{j+1}]$ using Taylor expansion method. To estimate the truncation error of Taylor expansion, we need an interval vector $[\boldsymbol{u}]$ which includes the true solution between the steps $[t_j, t_{j+1}]$.

Now find an interval constant vector $[\boldsymbol{u}]$ such that

$$[\boldsymbol{u}] \supset [\boldsymbol{u}_j] + [0, h]\boldsymbol{f}([t_j, t_{j+1}], [\boldsymbol{u}])$$

holds. Then $[\boldsymbol{u}]$ contains the solution between $[t_j, t_{j+1}]$, which can be proved by Schauder's fixed point theorem [17]. Using $[\boldsymbol{u}]$, we obtain more tight interval vector $[\boldsymbol{u}_{j+1}]$ than $[\boldsymbol{u}]$ which includes the solution $\boldsymbol{u}_{j+1}$ at t_{j+1} by the following form which comes from the Taylor expansion of $\boldsymbol{u}(t)$ at $t = t_j$.

$$[\boldsymbol{u}_{j+1}] = [\boldsymbol{u}_j] + \sum_{k=1}^{p-1} h^k \boldsymbol{f}^{(k)}(t_j, [\boldsymbol{u}_j]) + h^p \boldsymbol{f}^{(p)}([t_j, t_{j+1}], [\boldsymbol{u}]), \tag{3}$$

where $h = t_{j+1} - t_j$, and

$$\begin{aligned} \boldsymbol{f}^{(1)} &= \boldsymbol{f}, \\ \boldsymbol{f}^{(k+1)} &= \frac{1}{k+1}\left(\frac{\partial \boldsymbol{f}^{(k)}}{\partial t} + \frac{\partial \boldsymbol{f}^{(k)}}{\partial \boldsymbol{u}}\boldsymbol{f}\right). \end{aligned}$$

At each step in Taylor expansion method we carry out the computation using the mean-value form with $[\boldsymbol{u}_j]$ as an argument, which is defined as follows.

Let $[g([\boldsymbol{u}])]$ be an interval which includes the range of a function g for an interval $[\boldsymbol{u}]$, i.e.,

$$g([\boldsymbol{u}]) = \{g(\boldsymbol{u}) \mid \boldsymbol{u} \in [\boldsymbol{u}]\}.$$

One of such intervals is obtained by the right-hand side of the next expression.

$$g([\boldsymbol{u}]) \subset g(\hat{\boldsymbol{u}}) + [g'([\boldsymbol{u}])]([\boldsymbol{u}] - \hat{\boldsymbol{u}}),$$

where $\hat{\boldsymbol{u}}$ can be taken any vector in $[\boldsymbol{u}]$ and g' is the derivative of g. The inclusion is called the mean-value form of $g([\boldsymbol{u}])$ at $\hat{\boldsymbol{u}} \in [\boldsymbol{u}]$.

Let $\hat{\boldsymbol{u}}_j$ be the center and $[\boldsymbol{r}_j]$ be the diameter interval of the interval vector $[\boldsymbol{u}_j]$. We write the right-hand side of (3) as a vector function $\boldsymbol{g}([\boldsymbol{u}_j])$ and apply the mean-value form at $\hat{\boldsymbol{u}}_j$. Then we can represent the calculation of $\hat{\boldsymbol{u}}_{j+1}$ and $[\boldsymbol{r}_{j+1}]$ as follows.

$$\begin{aligned} \hat{\boldsymbol{u}}_{j+1} &= \boldsymbol{g}(\hat{\boldsymbol{u}}_j), \\ [\boldsymbol{r}_{j+1}] &= [A_j][\boldsymbol{r}_j] + [\boldsymbol{z}_{j+1}]. \end{aligned}$$

Here $[A_j]$ denotes an interval matrix which is derived from the mean-value form of the Taylor expansion method, and $[\boldsymbol{z}_{j+1}]$ denotes an interval vector which includes higher order terms w.r.t. $[\boldsymbol{r}_j]$, the remainder term of the Taylor expansion, and the round-off error caused by the calculation.

When we carry out the above calculation, interval inflation arises because of wrapping effect which is mainly caused by the matrix-vector iteration $[A_j][\boldsymbol{r}_j]$.

Now we intend to reduce some part of the wrapping effect which is attributed to the diameter of the initial box. For

$$[\boldsymbol{r}_0] = [\boldsymbol{u}_0] - \hat{\boldsymbol{u}}_0$$

let us write

$$[\boldsymbol{r}_j] = B_j[\boldsymbol{r}_0] + [\bar{\boldsymbol{r}}_j].$$

Here B_j denotes an $m \times m$ matrix which is defined for each j with B_0 as an identity matrix. Then we calculate as follows [4].

$$\begin{aligned}
[\boldsymbol{r}_{j+1}] &= B_{j+1}[\boldsymbol{r}_0] + [\bar{\boldsymbol{r}}_{j+1}], \\
[\bar{\boldsymbol{r}}_{j+1}] &= [A_j][\bar{\boldsymbol{r}}_j] + [\boldsymbol{z}_{j+1}], \\
B_{j+1} &= \text{the center matrix of the interval matrix } [A_j]B_j.
\end{aligned}$$

Using this manner, a kind of rearranging expression evaluation, we can avoid the wrapping effect from the initial box in a certain degree.

Higher order terms, truncation error, and round-off error will propagate to the next step through $[\bar{\boldsymbol{r}}_j]$, and then again the wrapping effect arises. In order to reduce this, we use a coordinate transformation based on QR factorization. Take an expression

$$[\bar{\boldsymbol{r}}_j] = C_j[\tilde{\boldsymbol{r}}_j].$$

Then $[\bar{\boldsymbol{r}}_{j+1}]$ is calculated by

$$\begin{aligned}
[\tilde{\boldsymbol{r}}_{j+1}] &= \left(C_{j+1}^{-1}[A_j]C_j\right)[\tilde{\boldsymbol{r}}_j] + C_{j+1}^{-1}[\boldsymbol{z}_{j+1}], \\
[\bar{\boldsymbol{r}}_{j+1}] &= C_{j+1}[\tilde{\boldsymbol{r}}_{j+1}].
\end{aligned}$$

Since we know a major reason of wrapping effect is rotation, C_{j+1} is defined so that the matrix $\left(C_{j+1}^{-1}[A_j]C_j\right)$ in the right-hand side of the first expression causes as less rotation as possible. One of the ways for that is to choose $C_{j+1} = Q$ where the matrix Q is obtained from QR factorization of U which is the center matrix of $[A_j]C_j$. In actual computation it has to be done to calculate the matrix product $\left(C_{j+1}^{-1}[A_j]C_j\right)$ before matrix-vector product. Data propagation from step to step is carried out through $[\tilde{\boldsymbol{r}}_j]$, and the calculation of $[\boldsymbol{r}_j]$ is done only when it is necessary.

In addition, it is more effective to sort the columns of U before the QR factorization. See Lohner's papers [4, 5] together with the software package for the Lohner's method, so called AWA.

3. Outline of Taylor model

A Taylor model [6, 7] is defined for a multivariable function by a set of a Taylor polynomial with coefficients of floating point numbers and an interval which includes the remainder. Recently Taylor models have been applied to many different kinds of problems and suceeded in getting good results.

Taylor models have two kinds of usefulness such as

- giving sharp bounds to the ranges of multidimensional nonlinear functions against the dependency problem,
- reducing the wrapping effect caused not only by matrix-vector iterations but also by nonlinear operations on interval vectors.

Let us see the definition [2].

DEFINITION 1 (TM for enclosure). *Let $D \subset \mathbf{R}^m$ be a box with $\boldsymbol{x}_0 \in D$. Let $P^{(\nu)}\colon D \to \mathbf{R}^k$ be a polynomial of degree ν w.r.t. $\boldsymbol{x} - \boldsymbol{x}_0$, $\boldsymbol{x} \in D$, and $I \subset \mathbf{R}^k$ be an open non-empty set. Then the quadruple $(P^{(\nu)}, \boldsymbol{x}_0, D, I)$ is called a Taylor model of order ν with expansion point $\boldsymbol{x}_0$ over D.*

Let $S = (P^{(\nu)}, \boldsymbol{x}_0, D, I)$ be a Taylor model. We regard S as the set of functions $\boldsymbol{f} \in C^{n+1}(D, \mathbf{R}^k)$ that satisfy $\boldsymbol{f}(\boldsymbol{x}) - P^{(\nu)}(\boldsymbol{x} - \boldsymbol{x}_0) \in I$, $\forall \boldsymbol{x} \in D$ and the ν-th order Taylor expansion of $\boldsymbol{f}$ around $\boldsymbol{x}_0 \in D$ equals $P^{(\nu)}(\boldsymbol{x} - \boldsymbol{x}_0)$. Then we have another definition.

DEFINITION 2 (TM for functions). *Let $P^{(\nu)}$, $\boldsymbol{x}_0$, D and I be defined as in* Definition 1. *Consider a set $S \subset C^{n+1}(D, \mathbf{R}^k)$ defined by*

$$S := \{\boldsymbol{f} \in C^{n+1}(D, \mathbf{R}^k) \mid \boldsymbol{f}(\boldsymbol{x}) - P^{(\nu)}(\boldsymbol{x} - \boldsymbol{x}_0) \in I,\ \forall \boldsymbol{x} \in D\}.$$

For a given function $\boldsymbol{g} \in C^{n+1}(D, \mathbf{R}^k)$, if

$$\boldsymbol{g} \in S,$$

then S is called a Taylor model for $\boldsymbol{g}$.

It can be said that Definition 1 prepares an enclosure of a nonlinear transformation of the box D, and Definition 2 gives a good estimation of the range of the nonlinear function $\boldsymbol{g}(D)$. We define

$$\mathcal{U} = P^{(\nu)}(\boldsymbol{x} - \boldsymbol{x}_0) + I, \quad \boldsymbol{x} \in D$$

from the Taylor model S, which is a nonconvex domain with the boundary represented by the polynomial. The domain $\mathcal{U}$ can be used as an enclosure of the transformed box of D, and can be taken as a bound for the range of the function $\boldsymbol{g}$ such that $\boldsymbol{g}(\boldsymbol{x}) \in P^{(\nu)}(\boldsymbol{x} - \boldsymbol{x}_0) + I$ holds for all $\boldsymbol{x} \in D$. Hereinafter $\mathcal{U}$ is also called Taylor model.

TM arithmetic. Let us define addition and multiplication of Taylor models. For

$$\begin{aligned}\mathcal{U}_1 &= P_1^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_1, \quad \boldsymbol{x}\in D,\\ \mathcal{U}_2 &= P_2^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_2, \quad \boldsymbol{x}\in D,\end{aligned}$$

we define

$$\begin{aligned}\mathcal{U}_1+\mathcal{U}_2 &= P_1^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+P_2^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_1+I_2, \quad \boldsymbol{x}\in D,\\ \mathcal{U}_1\cdot\mathcal{U}_2 &= P_{12}^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_{12}, \quad \boldsymbol{x}\in D,\end{aligned}$$

where

$$\begin{aligned}P_{12}^{(\nu)} &:= \text{the part of } P_1^{(\nu)}\cdot P_2^{(\nu)} \text{ up to degree } \nu,\\ I_{12} &:= [P_e^{(2\nu)}]+[P_1^{(\nu)}]I_2+[P_2^{(\nu)}]I_1+I_1\cdot I_2,\\ P_e^{(2\nu)} &:= \text{the part of } P_1^{(\nu)}\cdot P_2^{(\nu)} \text{ of degrees } \nu+1 \text{ to } 2\nu,\end{aligned}$$

and

$$[P(\boldsymbol{x})] := \text{a box which contains the set } \{\boldsymbol{y}\mid \boldsymbol{y}=P(\boldsymbol{x}),\ \boldsymbol{x}\in D\}$$

for a polynomial $P(\boldsymbol{x})$. We use $[\mathcal{U}]$ for a Taylor model $\mathcal{U}$ by similar meaning.

Functions of Taylor models are defined using their Taylor expansions. In order to operate $g(\boldsymbol{y})\in\mathbf{R}$ ($\boldsymbol{y}\in\mathbf{R}^k$) on

$$\mathcal{U}=P^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I, \quad \boldsymbol{x}\in D,$$

we take $\boldsymbol{c}\in I$ and suppose that $g\in C^p([P^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I])$. Then we define

$$\begin{aligned}g(\mathcal{U}) := g(\boldsymbol{c}) &+ \sum_{s=1}^{(p-1)}\frac{1}{s!}g^{(s)}(\boldsymbol{c})(\mathcal{U}-\boldsymbol{c})^s\\ &+\frac{1}{p!}g^{(p)}([P^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I])(\mathcal{U}-\boldsymbol{c})^p,\end{aligned}$$

where $g^{(s)}$ denotes a tensor of order s corresponding to the s-th differential of g w.r.t. $\boldsymbol{y}$, and then $g^{(s)}(\boldsymbol{c})(\mathcal{U}-\boldsymbol{c})^s$ means a tensor operation which is calculated using addition and multiplication of Taylor models. The last (remainder) term $g^{(p)}([P^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I])$ can be bounded by use of interval arithmetic. In case that $g(\boldsymbol{y})$ is a vector function, the similar definition is applied to each element. The resulting Taylor model is written by

$$g(\mathcal{U})=P_g^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_g, \quad \boldsymbol{x}\in D.$$

In actual computation, we have to use interval coefficients for the polynomials in order to take account of the round-off errors [9, 16]. Take $P_g^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)$ the center of the interval polynomial and $P_E^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)$ a polynomial whose coefficients are the diameter interval caused by the round-off errors, then the Taylor model is defined by

$$\begin{aligned} g(\mathcal{U}) &= P_g^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I'_g, \\ I'_g &= I_g+\left[P_E^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)\right], \quad \boldsymbol{x}\in D. \end{aligned}$$

Let us consider compositions of Taylor models. Take Taylor models for functions $\boldsymbol{f}\colon \mathbf{R}^m \to \mathbf{R}^m$ and $\boldsymbol{g}\colon \mathbf{R}^m \to \mathbf{R}^k$ by

$$\mathcal{F} = P_f^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_f, \quad \boldsymbol{x}\in D_1$$

and

$$\mathcal{G} = P_g^{(\nu)}(\boldsymbol{y}-\boldsymbol{y}_0)+I_g, \quad \boldsymbol{y}\in D_2,$$

respectively. If

$$\left[P_f^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_f\right] \subset D_2 \tag{4}$$

holds, then the Taylor model for the composition $g\circ f$ written by

$$\mathcal{GF} = P_{gf}^{(\nu)}(\boldsymbol{x}-\boldsymbol{x}_0)+I_{gf}, \quad \boldsymbol{x}\in D_1$$

can be defined through the computation of $g(\mathcal{F})$ by the Taylor models' arithmetic. Note that we do not obtain a correct enclosure of the range of the composition in case the condition (4) does not hold.

In the software package COSY Infinity [10] the arithmetic of Taylor models is installed and many intrinsic functions are ready for high order Taylor models.

TM for verified integration of ODEs. Taylor models are expected to have the following advantages in validated computation of the solutions to ODEs.

- Reduction of the wrapping effect caused by linear and nonlinear operations on the diameter of the initial data
- Tight enclosing of the range of the function in the right-hand side

However note that the wrapping effect caused by discretization error is not reduced by naive Taylor models. We need some preconditioning (e.g., QR factorization) to reduce it [11, 12].

The initial data contained in the box $[\boldsymbol{u}_0]$ is dealt with in a form

$$\boldsymbol{u}(0) = \boldsymbol{u}_0 + \boldsymbol{x},$$

where $\boldsymbol{u}_0 \in [\boldsymbol{u}_0]$, $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)^{\mathrm{T}}$, $-\eta_i \le x_i \le \eta_i$, and η_i $(i = 1, \ldots, m)$ give the radii of the initial box.

Take nodal points $0 = t_0 < t_1 < \cdots < t_n = T$ and transform (2) into an integral equation using the solution at $t = t_j$.

$$\boldsymbol{u}(t) = \boldsymbol{u}(t_j) + \int_{t_j}^{t} \boldsymbol{f}(\tau, \boldsymbol{u})\, d\tau, \quad t_j < t < t_{j+1}.$$

We assume that we have a Taylor model for $\boldsymbol{u}(t_j)$

$$\mathcal{U}_j = P_j(\boldsymbol{x}) + I_j.$$

Take $\boldsymbol{u}(\tau)^{(0)} := P_j(\boldsymbol{x})$ and iterate the following procedure which is based on the Picard's successive approximation. Integrate $\boldsymbol{f}(\tau, \boldsymbol{u}(\tau)^{(k-1)})$ by

$$\boldsymbol{z}(t)^{(k)} = \boldsymbol{u}(t_j) + \int_{t_j}^{t} \boldsymbol{f}(\tau, \boldsymbol{u}(\tau)^{(k-1)})\, d\tau,$$

and compute $P_z(t, \boldsymbol{x})^{(k)}$ which appears in the Taylor model for $\boldsymbol{z}(t)^{(k)}$ w.r.t. $\boldsymbol{x}$

$$\mathcal{Z}^{(k)} = P_z(t, \boldsymbol{x})^{(k)} + I_z^{(k)}.$$

Take

$$\boldsymbol{u}(t)^{(k)} := P_z(t, \boldsymbol{x})^{(k)},$$

then it is seen that the right-hand side is a k-th degree polynomial w.r.t. t. Here we do not compute $I_z^{(k)}$ actually.

After the iteration until $k = \nu$, find an interval vector I_{j+1} such that

$$\boldsymbol{u}(t_j) + \int_{t_j}^{t} \boldsymbol{f}(\tau, P_z(\tau, \boldsymbol{x})^{(\nu)} + I_{j+1})\, d\tau \subset P_z(t, \boldsymbol{x})^{(\nu)} + I_{j+1}$$

holds for all $t_j < t < t_{j+1}$ and $\boldsymbol{x} \in [\boldsymbol{u}_0] - \boldsymbol{u}_0$.

Once we find I_{j+1}, the Taylor model for $\boldsymbol{u}_{j+1}$ is obtained by

$$\mathcal{U}_{j+1} = P_z(t_{j+1}, \boldsymbol{x})^{(\nu)} + I_{j+1}.$$

The proof is based on the Schauder's fixed point theorem [6].

Summing up the above, the verification method of ODEs using Taylor models has the following features.

- Reduction of the wrapping effect attributed to the initial box by Taylor models w.r.t. $\boldsymbol{x}$
- Tight estimation of the integrand $\boldsymbol{f}$ by Taylor model arithmetic
- Improvement of the accuracy by Picard iteration

4. Application of Nakao method to IVPs

In this section, we present a formulation of application of the Nakao method to initial value problems for ODEs (2).

Take nodal points $0 = t_0 < t_1 < \cdots < t_n = T$. Compute an approximate solution $\tilde{\boldsymbol{u}}_j$ to the solution $\boldsymbol{u}(t_j)$ on each point, and construct $\tilde{\boldsymbol{u}}(t)$ such that $\tilde{\boldsymbol{u}}(t_j) = \tilde{\boldsymbol{u}}_j$ holds using k-th degree piecewise polynomials.

Hereinafter we assume that $\boldsymbol{f}(t, \boldsymbol{u})$ has the 2nd order continuous partial derivatives w.r.t. $\boldsymbol{u}$, and each time step size $h = t_{j+1} - t_j$ is equal for simpilicity. Moreover we take $k = 1$ and write the approximate solution as follows.

$$\tilde{\boldsymbol{u}}(t) = \tilde{\boldsymbol{u}}_j l_0^j(t) + \tilde{\boldsymbol{u}}_{j+1} l_1^j(t), \quad t_j \le t \le t_{j+1},$$

where $l_0^j(t) := \frac{t_{j+1}-t}{h}$ and $l_1^j(t) := \frac{t-t_j}{h}$.

Let us transform (2) into an integral equation.

$$\boldsymbol{u}(t) = \boldsymbol{u}(0) + \int_0^t \boldsymbol{f}(\tau, \boldsymbol{u})\, d\tau, \quad 0 < t < T.$$

Using the approximate solution $\tilde{\boldsymbol{u}}(t)$, we write $\boldsymbol{u}(t) = \tilde{\boldsymbol{u}}(t) + \boldsymbol{\omega}(t)$. For the error $\boldsymbol{\omega}(t)$ we have

$$\begin{aligned} &\boldsymbol{\omega}(t) = \boldsymbol{\omega}_j + \int_{t_j}^t \boldsymbol{f}(\tau, \tilde{\boldsymbol{u}} + \boldsymbol{\omega})\, d\tau - (\tilde{\boldsymbol{u}}(t) - \tilde{\boldsymbol{u}}_j), \\ &t_j \le t \le t_{j+1},\ j = 0, \ldots, n-1, \end{aligned} \tag{5}$$

where $\boldsymbol{\omega}_j = \boldsymbol{\omega}(t_j)$.

Now we apply the Nakao method to (5). For $[t_j, t_{j+1}]$ define

$$\begin{aligned} &S_N := \{\boldsymbol{\omega}_N(t) \in R^m \mid \text{linear function on } t_j \le t \le t_{j+1}\}, \\ &P_N\colon \text{a projection from } \{C[t_j, t_{j+1}]\}^m \text{ to } S_N \end{aligned}$$

and divide the error $\boldsymbol{\omega}$ into 2 parts as $\boldsymbol{\omega} = \boldsymbol{\omega}_N + \boldsymbol{\omega}_\perp$ where $\boldsymbol{\omega}_N := P_N\boldsymbol{\omega}$ and $\boldsymbol{\omega}_\perp := (I - P_N)\boldsymbol{\omega}$. Note that the projection P_N gives the linear interpolation on $[t_j, t_{j+1}]$. Then we have

$$\boldsymbol{\omega}_N(t) = \boldsymbol{\omega}_j l_0^j(t) + \boldsymbol{\omega}_{j+1} l_1^j(t), \quad t_j \le t \le t_{j+1},$$

for $\boldsymbol{\omega}_j = \boldsymbol{\omega}_N(t_j)$, $\boldsymbol{\omega}_{j+1} = \boldsymbol{\omega}_N(t_{j+1})$.

According to the Nakao method, we will derive a fixed point equation w.r.t. $\boldsymbol{\omega}_N$ and $\boldsymbol{\omega}_\perp$, then apply the Schauder's fixed point theorem and construct the sufficient conditions to the theorem for a certain set W so called candidate set. The sufficient conditions are represented by a system of inequalities. Verifying these inequalities using validated computation, we prove the existence of $\boldsymbol{\omega}$ as a solution to the fixed point equation and obtain bounds for $\boldsymbol{\omega}$ which give the error bounds for the solution $\boldsymbol{u}(t)$ on $[t_j, t_{j+1}]$.

Fixed point equation. In order to derive a fixed point equation, we divide the equation (5) into 2 parts using P_N.

$$\boldsymbol{\omega}_N(t) = \boldsymbol{\omega}_j + P_N \int_{t_j}^{t} \{\boldsymbol{f}(\tau, \tilde{\boldsymbol{u}}(\tau) + \boldsymbol{\omega}_N(\tau) + \boldsymbol{\omega}_\perp(\tau)\}\, d\tau - (\tilde{\boldsymbol{u}}_{j+1} - \tilde{\boldsymbol{u}}_j), \tag{6}$$

$$\boldsymbol{\omega}_\perp(t) = (I - P_N) \int_{t_j}^{t} \{\boldsymbol{f}(\tau, \tilde{\boldsymbol{u}}(\tau) + \boldsymbol{\omega}_N(\tau) + \boldsymbol{\omega}_\perp(\tau)\}\, d\tau, \tag{7}$$

$$t_j < t < t_{j+1},\ j = 0, \ldots, n-1.$$

In this paper, we use a Taylor expansion of $\boldsymbol{f}(t, \boldsymbol{u})$ w.r.t. $\boldsymbol{u}$ for calculation of $\boldsymbol{\omega}_{j+1}$. The reasons are as follows.

- We intend to apply the device of rearranging expression evaluation for the initial box similar to the Lohner's method.
- We make calculation of the integration so simple that our computer programs can be applied to various $\boldsymbol{f}$ without much modification.

Now we take the 2nd order Taylor expansion for $\boldsymbol{f}(t, \boldsymbol{u})$ w.r.t. $\boldsymbol{u}$ which has terms of the 3rd order tensors. Indeed the expression seems rather involved, but we believe it is preferable to the expression of Taylor expansion method in (3) which includes $\boldsymbol{f}^{(k)}$.

$$\begin{aligned}\boldsymbol{\omega}_{j+1} = \boldsymbol{\omega}_j + \int_{t_j}^{t_{j+1}} \left\{ \boldsymbol{f}(\tau, \tilde{\boldsymbol{u}}_j) + \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j)\boldsymbol{\xi}_j(\tau) + \frac{1}{2}\boldsymbol{\xi}_j(\tau)^{\mathrm{T}}(\diamond \boldsymbol{f})\boldsymbol{\xi}_j(\tau) \right\} d\tau \\ - (\tilde{\boldsymbol{u}}_{j+1} - \tilde{\boldsymbol{u}}_j),\end{aligned} \tag{8}$$

where

$$\begin{aligned}\boldsymbol{\xi}_j(\tau) &:= \tilde{\boldsymbol{u}}(\tau) - \tilde{\boldsymbol{u}}_j + \boldsymbol{\omega}_N(\tau) + \boldsymbol{\omega}_\perp(\tau), \\ \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) &:= \text{the Jacobian of } \boldsymbol{f} \text{ w.r.t. } \boldsymbol{u} \\ &\qquad \text{at } \boldsymbol{u} = \tilde{\boldsymbol{u}}_j,\ t = \tau \text{ (we omit the argument } \tau \text{ for simplicity).}\end{aligned}$$

And $(\diamond \boldsymbol{f})$ is defined by the following. Take

$$\diamond f_i := \text{an } m \times m \text{ matrix whose } kl\text{-element is } \frac{\partial^2 f_i}{\partial u_k \partial u_l}(\Theta_{ijkl}).$$

Here

$$\Theta_{ijkl} = \tilde{\boldsymbol{u}}_j + s_{ijkl}\boldsymbol{\xi}_j(\tau),$$

for some $0 \le s_{ijkl} \le 1$ which is specified for each (i, j, k, l). Using $\diamond f_i$ we define

$$\boldsymbol{\xi}_j(\tau)^{\mathrm{T}}(\diamond \boldsymbol{f})\boldsymbol{\xi}_j(\tau) := (\boldsymbol{\xi}_j(\tau)^{\mathrm{T}} \diamond f_1 \boldsymbol{\xi}_j(\tau), \ldots, \boldsymbol{\xi}_j(\tau)^{\mathrm{T}} \diamond f_m \boldsymbol{\xi}_j(\tau))^{\mathrm{T}}.$$

Namely, $(\diamond \boldsymbol{f})$ is a tensor of the 3rd order.

Let us calculate

$$L_0^j := \int_{t_j}^{t_{j+1}} l_0^j(\tau)\,d\tau, \quad L_1^j := \int_{t_j}^{t_{j+1}} l_1^j(\tau)\,d\tau,$$
$$L_{00}^j := \int_{t_j}^{t_{j+1}} (l_0^j(\tau))^2\,d\tau, \quad L_{11}^j := \int_{t_j}^{t_{j+1}} (l_1^j(\tau))^2\,d\tau, \quad L_{01}^j := \int_{t_j}^{t_{j+1}} l_0^j(\tau) l_1^j(\tau)\,d\tau,$$

and

$$\overline{\diamond \boldsymbol{f}} := (\diamond \boldsymbol{f}) \quad \text{with } \Theta = \tilde{\boldsymbol{u}}_j.$$

Note that this is constant w.r.t. τ and the coorsponding $\diamond f_i$ are symmetric matrices. Moreover take

$$[D(\diamond \boldsymbol{f})] := [(\diamond \boldsymbol{f}) - \overline{\diamond \boldsymbol{f}}]$$

and $[\boldsymbol{\omega}_\perp]$. Here we define $[\boldsymbol{v}]$ for a tensor function $\boldsymbol{v}(t)$ by an interval tensor which is constant w.r.t. t such that

$$\boldsymbol{v}(t) \in [\boldsymbol{v}], \quad t_j \le t \le t_{j+1}$$

holds elementwise.

Now let us take

$$\hat{\boldsymbol{e}}_j := \tilde{\boldsymbol{u}}_{j+1} - \tilde{\boldsymbol{u}}_j.$$

Since $l_0^j(\tau) + l_1^j(\tau) = 1$ we have

$$\boldsymbol{\xi}_j = \hat{\boldsymbol{e}}_j l_1^j(\tau) + \boldsymbol{\omega}_j l_0^j(\tau) + \boldsymbol{\omega}_{j+1} l_1^j(\tau) + \boldsymbol{\omega}_\perp.$$

Using these quantities we define the following.

$$\begin{aligned}
\boldsymbol{r}_j &:= h\boldsymbol{f}(\tau, \tilde{\boldsymbol{u}}_j) - \left(I - \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_1^j\right)\hat{\boldsymbol{e}}_j + \frac{1}{2}\hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\, \hat{\boldsymbol{e}}_j L_{11}^j, \qquad (9)\\
\boldsymbol{r}(\boldsymbol{\omega}_N) &:= \left[I + \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_0^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{01}^j\right]\boldsymbol{\omega}_j + \left[\frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_1^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{11}^j\right]\boldsymbol{\omega}_{j+1}\\
&\quad + \frac{1}{2}\boldsymbol{\omega}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_j L_{00}^j + \boldsymbol{\omega}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_{j+1} L_{01}^j + \frac{1}{2}\boldsymbol{\omega}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_{j+1} L_{11}^j,\\
[\boldsymbol{r}(\boldsymbol{\omega}_\perp)] &:= \left\{\frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) h + \left(\hat{\boldsymbol{e}}_j L_1^j + \boldsymbol{\omega}_j L_0^j + \boldsymbol{\omega}_{j+1} L_1^j + \frac{h}{2}[\boldsymbol{\omega}_\perp]\right)^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\right\}[\boldsymbol{\omega}_\perp],\\
[\boldsymbol{r}_j'] &:= \frac{1}{2}\hat{\boldsymbol{e}}_j^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \hat{\boldsymbol{e}}_j L_{11}^j,\\
[\boldsymbol{r}(\boldsymbol{\omega}_N)'] &:= \hat{\boldsymbol{e}}_j^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \boldsymbol{\omega}_j L_{01}^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \boldsymbol{\omega}_{j+1} L_{11}^j\\
&\quad + \frac{1}{2}\boldsymbol{\omega}_j^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \boldsymbol{\omega}_j L_{00}^j + \boldsymbol{\omega}_j^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \boldsymbol{\omega}_{j+1} L_{01}^j + \frac{1}{2}\boldsymbol{\omega}_{j+1}^{\mathrm{T}} [D(\diamond \boldsymbol{f})] \boldsymbol{\omega}_{j+1} L_{11}^j,\\
[\boldsymbol{r}(\boldsymbol{\omega}_\perp)'] &:= \left(\hat{\boldsymbol{e}}_j L_1^j + \boldsymbol{\omega}_j L_0^j + \boldsymbol{\omega}_{j+1} L_1^j + \frac{h}{2}[\boldsymbol{\omega}_\perp]\right)^{\mathrm{T}} [D(\diamond \boldsymbol{f})][\boldsymbol{\omega}_\perp].
\end{aligned}$$

Then $\boldsymbol{\omega}_{j+1}$ can be written by

$$\boldsymbol{\omega}_{j+1} = \boldsymbol{r}_j + \boldsymbol{r}(\boldsymbol{\omega}_N) + \boldsymbol{\omega}', \tag{10}$$

where $\boldsymbol{\omega}'$ is a certain vector function such that

$$\boldsymbol{\omega}' \in [\boldsymbol{r}(\boldsymbol{\omega}_\perp)] + [\boldsymbol{r}'_j] + [\boldsymbol{r}(\boldsymbol{\omega}_N)'] + [\boldsymbol{r}(\boldsymbol{\omega}_\perp)'].$$

The right-hand side will be used to estimate the bound of $\boldsymbol{\omega}'$ in verification process.

We put the linear terms w.r.t. $\boldsymbol{\omega}_{j+1}$ in the right-hand side of (10) into the left-hand side and derive a quasi Newton formulataion as follows.

$$\boldsymbol{\omega}_{j+1} = A_j^{-1}\{\boldsymbol{r}_j + \boldsymbol{p}(\boldsymbol{\omega}_N) + \boldsymbol{\omega}'\}, \tag{11}$$

where

$$\begin{aligned} A_j &:= I - \left\{ \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j)L_1^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{11}^j \right\}, \\ \boldsymbol{p}(\boldsymbol{\omega}_N) &:= \left[I + \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j)L_0^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{01}^j \right] \boldsymbol{\omega}_j \\ &\quad + \frac{1}{2}\boldsymbol{\omega}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_j L_{00}^j + \boldsymbol{\omega}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_{j+1} L_{01}^j + \frac{1}{2}\boldsymbol{\omega}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{\omega}_{j+1} L_{11}^j. \end{aligned} \tag{12}$$

Let $\boldsymbol{N}(\boldsymbol{\omega})$ define the operator which gives $\boldsymbol{\omega}_N(t)$ for given $\boldsymbol{\omega} = \boldsymbol{\omega}_N + \boldsymbol{\omega}_\perp$ using $\boldsymbol{\omega}_{j+1}$ calculated by the above expressions (11).

Moreover define

$$H(\boldsymbol{\omega}) := \boldsymbol{N}(\boldsymbol{\omega}) + (I - P_N) \int_{t_j}^{t_{j+1}} \boldsymbol{f}(\tau, \tilde{\boldsymbol{u}}(\tau) + \boldsymbol{\omega}(\tau))\, d\tau,$$

then the equation (5) is equivalent to the following fixed point equation.

$$\boldsymbol{\omega} = H(\boldsymbol{\omega}).$$

Since H is a compact operator on $\{C^0[t_j, t_{j;1}]\}^m$, we can apply Schauder's fixed point theorem and obtain that if

$$H(W) \subset W,$$

then there exists $\boldsymbol{\omega} \in W$ such that $\boldsymbol{\omega} = H(\boldsymbol{\omega})$ holds.

Candidate set. A candidate set W is constructed as follows. Giving non negative constant vectors $\boldsymbol{\alpha}_{j+1}$ and $\boldsymbol{\beta}_j$, define

$$W_N := \{\boldsymbol{\omega}_N \in S_N \mid \boldsymbol{\omega}_N(t_j) = \boldsymbol{\omega}_j,\ |\boldsymbol{\omega}_N(t_{j+1})| \le \boldsymbol{\alpha}_{j+1}\}, \tag{13}$$

$$W_\perp := \{\boldsymbol{\omega}_\perp \in S_\perp \mid |\boldsymbol{\omega}_\perp|_{\infty(j)} \le \boldsymbol{\beta}_j\}, \tag{14}$$

where $S_\perp = (I - P_N)\{C[t_{j-1}, t_j]\}^m$, and $|\cdot|_{\infty(j)}$ is defined elementwise by

$$|\boldsymbol{v}|_{\infty(j)} := \sup_{t_j < t < t_{j+1}} |\boldsymbol{v}(t)|$$

for an arbitrary vector function $\boldsymbol{v}(t)$ on $[t_j, t_{j+1}]$.

The candidate set W is constructed by

$$W := W_N + W_\perp.$$

Then we derive sufficient conditions for

$$H(W) \subset W,$$

using interval estimation for the left-hand side. The sufficient conditions are represented by inequalities w.r.t. $\boldsymbol{\alpha}_j$, $\boldsymbol{\alpha}_{j+1}$ and $\boldsymbol{\beta}_j$. If we find $\boldsymbol{\alpha}_{j+1}$ and $\boldsymbol{\beta}_j$ which satisfy these inequalities for $\boldsymbol{\alpha}_j$ obtained in the previous step, then it is proved that the candidate set W surely includes the fixed point $\boldsymbol{\omega}$. In order to estimate $\boldsymbol{\omega}_\perp$, we use the following fact which is an elementary property of interpolation polynomials.

If $\boldsymbol{z} \in \{C[t_{j-1}, t_j]\}^m$ has its continuous second derivative $\frac{d^2\boldsymbol{z}}{dt^2}$,

$$|(I - P_N)\boldsymbol{z}|_{\infty(j)} \le \frac{h^2}{2} \left| \frac{d^2\boldsymbol{z}}{dt^2} \right|_{\infty(j)}$$

holds.

Then we estimate $\boldsymbol{\omega}_\perp = (I - P_N)H(\boldsymbol{\omega})$, $\boldsymbol{\omega} \in W$ by

$$|\boldsymbol{\omega}_\perp|_{\infty(j)} \le \frac{h^2}{2} \left| \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}} + \boldsymbol{\omega}) \boldsymbol{f}(\,\cdot\,, \tilde{\boldsymbol{u}} + \boldsymbol{\omega}) \right|_{\infty(j)}.$$

Estimation of the right-hand side needs interval arithmetic and the mean-value form may be applied if necessary.

Approximate solutions. Since we use triangular inequalities in the process of estimation of $\boldsymbol{\omega}_{j+1}$ it is preferable that the approximate solution $\tilde{\boldsymbol{u}}_{j+1}$ satisfies $\boldsymbol{r}_j \approx 0$. A computational scheme for $\tilde{\boldsymbol{u}}_{j+1}$ is obtained from (9).

$$h\boldsymbol{f}(t_j, \tilde{\boldsymbol{u}}_j) - \left(I - \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_1^j \right) \hat{\boldsymbol{e}}_j + \frac{1}{2} \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \hat{\boldsymbol{e}}_j L_{11}^j = 0.$$

From this, we have a Newton iteration formula w.r.t. $\hat{\boldsymbol{e}}_j$ as follows.

$$\begin{aligned} \hat{\boldsymbol{e}}_j &= \left(I - \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_1^j - \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{11}^j \right)^{-1} \left\{ h\boldsymbol{f}(t_j, \tilde{\boldsymbol{u}}_j) - \frac{1}{2} \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \hat{\boldsymbol{e}}_j L_{11}^j \right\} \\ &= A_j^{-1} \left\{ h\boldsymbol{f}(t_j, \tilde{\boldsymbol{u}}_j) - \frac{1}{2} \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \hat{\boldsymbol{e}}_j L_{11}^j \right\}. \end{aligned} \tag{15}$$

Using this iteration, we define $\tilde{\boldsymbol{u}}_{j+1} = \tilde{\boldsymbol{u}}_j + \hat{\boldsymbol{e}}_j$.

Treament of initial box. As is in the Lohner's method, treatment of the initial box should be based on rearranging expression evaluation w.r.t. the initial diameter $[\boldsymbol{\omega}_0] := [\boldsymbol{u}_0] - \tilde{\boldsymbol{u}}_0$. We extract the linear term of $\boldsymbol{\omega}_0$ from the expression of $\boldsymbol{\omega}_{j+1}$ and specify the coefficient matrix. Let

$$\boldsymbol{\omega}_j = Q_j \boldsymbol{\omega}_0 + \boldsymbol{y}_j \tag{16}$$

and

$$B_j := I + \frac{d\boldsymbol{f}}{d\boldsymbol{u}}(\tilde{\boldsymbol{u}}_j) L_0^j + \hat{\boldsymbol{e}}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} L_{01}^j.$$

Substitute them into (12), then we have

$$\begin{aligned}
\boldsymbol{\omega}_{j+1} \;=\; A_j^{-1} \Big\{ & B_j Q_j \boldsymbol{\omega}_0 + B_j \boldsymbol{y}_j + \frac{1}{2} \boldsymbol{\omega}_0^{\mathrm{T}} Q_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_j \boldsymbol{\omega}_0 L_{00}^j \\
& + \boldsymbol{\omega}_0^{\mathrm{T}} Q_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_{j+1} \boldsymbol{\omega}_0 L_{01}^j + \frac{1}{2} \boldsymbol{\omega}_0^{\mathrm{T}} Q_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_{j+1} \boldsymbol{\omega}_0 L_{11}^j \\
& + \big(\boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} (Q_j L_{00}^j + Q_{j+1} L_{01}^j) + \boldsymbol{y}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} (Q_j L_{01}^j + Q_{j+1} L_{11}^j) \big) \boldsymbol{\omega}_0 \\
& + \frac{1}{2} \boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_j L_{00}^j + \boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_{j+1} L_{01}^j + \frac{1}{2} \boldsymbol{y}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_{j+1} L_{11}^j + \boldsymbol{r}_j + \boldsymbol{\omega}' \Big\}.
\end{aligned}$$

From this the definitions of Q_{j+1} and $\boldsymbol{y}_{j+1}$ are obtained.

$$Q_{j+1} := A_j^{-1} B_j Q_j, \tag{17}$$

$$\begin{aligned}
\boldsymbol{y}_{j+1} := A_j^{-1} \Big\{ & B_j \boldsymbol{y}_j + \frac{1}{2} \boldsymbol{\omega}_0^{\mathrm{T}} Q_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_j \boldsymbol{\omega}_0 L_{00}^j \\
& + \boldsymbol{\omega}_0^{\mathrm{T}} Q_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_{j+1} \boldsymbol{\omega}_0 L_{01}^j + \frac{1}{2} \boldsymbol{\omega}_0^{\mathrm{T}} Q_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} Q_{j+1} \boldsymbol{\omega}_0 L_{11}^j \\
& + \big(\boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} (Q_j L_{00}^j + Q_{j+1} L_{01}^j) + \boldsymbol{y}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} (Q_j L_{01}^j + Q_{j+1} L_{11}^j) \big) \boldsymbol{\omega}_0 \\
& + \frac{1}{2} \boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_j L_{00}^j + \boldsymbol{y}_j^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_{j+1} L_{01}^j + \frac{1}{2} \boldsymbol{y}_{j+1}^{\mathrm{T}} \overline{\diamond \boldsymbol{f}} \boldsymbol{y}_{j+1} L_{11}^j + \boldsymbol{r}_j + \boldsymbol{\omega}' \Big\}.
\end{aligned} \tag{18}$$

Then we estimate $\boldsymbol{\omega}_{j+1} = Q_{j+1} \boldsymbol{\omega}_0 + \boldsymbol{y}_{j+1}$ by the right-hand side of (18).

For the verification process, we modify the definition of W_N as follows.

$$W_N := \{ \boldsymbol{\omega}_N \in S_N \mid \boldsymbol{\omega}_N(t_j) = \boldsymbol{\omega}_j,\ \boldsymbol{\omega}_N(t_{j+1}) = Q_{j+1} \boldsymbol{\omega}_0 + \boldsymbol{y}_{j+1},\ |\boldsymbol{y}_{j+1}| \leq \boldsymbol{\alpha}_{j+1} \},$$

and check whether the right-hand side of (18) is less than or equal to $\boldsymbol{\alpha}_{j+1}$.

Using this device, the wrapping effect from the linear transformation of the initial box $[\boldsymbol{u}_0]$ will be reduced. However, note that here we do not take any countermeasure against wrapping effect caused by truncation error and round-off error. To do this, besides the coordinate transformation based on QR factorization,

it may work to restart from some time point when the widths of intervals have become rather large.

The round-off error that arises in the calculation of Q_{j+1} is taken into the enclosure of $\boldsymbol{y}_{j+1}$ in a similar manner described in the Section 3, and Q_{j+1} itself is taken by point values, not intervals. Then the round-off error is dealt with by some devices against wrapping effect caused by $\boldsymbol{y}_{j+1}$ when such devices would be applied.

The reader may regard the method in this section as a Taylor model method of order 1 reading through the next section.

5. Application of TMs to Nakao method

Since the estimation of $\boldsymbol{\omega}_{j+1}$ is vulnarable to wrapping effect more than the estimation of $\boldsymbol{\omega}_{\perp}$ is, we apply Taylor models to $\boldsymbol{\omega}_{j+1}$.

In this paper we adopt Taylor models of order 2. Indeed higher order Taylor models (e.g., from 6th to 9th) are used for practical problems, however, we take such a low order TMs on purpose since we want to investigate actual process of computation of Taylor models in the Nakao method, in addition to the reason that the authors did not have opportunity to employ COSY Infinity.

Now let us take an initial value $\boldsymbol{\omega}_0$ from the initial box $[\boldsymbol{\omega}_0] = [\boldsymbol{u}_0] - \tilde{\boldsymbol{u}}_0$ and represent it by

$$\boldsymbol{\omega}_0 = \boldsymbol{x},$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)^{\mathrm{T}}$, $-\eta_i \le x_i \le \eta_i$. Note that η_i $(i = 1, \ldots, m)$ give the radii of the initial interval vector. For each $\boldsymbol{\omega}_j$, we define the Taylor model of order 2 by

$$\boldsymbol{\omega}_j = Q_j \boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j], \tag{19}$$

where Q_j is an $m \times m$ matrix and $[\boldsymbol{z}_j] \subset \mathbf{R}^m$ is a "zonotope" in our formulation, which we will see afterward. Here we do not take a constant term for the polynomial part because the center of $\boldsymbol{\omega}_j$ is almost 0 in actual computation, and the term $[\boldsymbol{z}_j]$ may include the constant term as a perturbation from 0. The term $\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}$ is defined as follows.

$$\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} := (\boldsymbol{x}^{\mathrm{T}} P_1^j \boldsymbol{x}, \ldots, \boldsymbol{x}^{\mathrm{T}} P_m^j \boldsymbol{x})^{\mathrm{T}}$$

where P_i^j $(i = 1, \ldots, m)$ are $m \times m$ matrices. Namely, $(\boldsymbol{P}_j)$ is a tensor of the 3rd order.

As is in the previous section, the formula to specify Q_{j+1} in

$$\boldsymbol{\omega}_{j+1} = Q_{j+1}\boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]$$

is obtained by substitution of (19) into (12). Comparing the both side of (11) after the substitution, we have (17) for Q_{j+1}. In order to obtain the formulae for $(\boldsymbol{P}_{j+1})$ and $[\boldsymbol{z}_{j+1}]$, we substitute

$$\boldsymbol{y}_j = \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]$$

into (18) and compare the both side.

For concrete calculation of $\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x}$, we review the matrix-tensor product. For an arbitrary $m \times m$ matrix M with M_{kl} for its kl-element and the vector $\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}$, the product is calculated by

$$M(\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}) = \left(\boldsymbol{x}^{\mathrm{T}}\left(\sum_l M_{1l}P_l^j\right)\boldsymbol{x}, \ldots, \boldsymbol{x}^{\mathrm{T}}\left(\sum_l M_{nl}P_l^j\right)\boldsymbol{x}\right)^{\mathrm{T}}.$$

Based on this calculation, we specify P_i^{j+1} $(i = 1, \ldots, m)$ which construct the tensor $(\boldsymbol{P}_{j+1})$. Taking

$$\overline{\diamond \boldsymbol{f}} = (\overline{\diamond f}_1, \ldots, \overline{\diamond f}_m)^{\mathrm{T}}$$

and

$$X_j := A_j^{-1}B_j$$

with X_{ik} for its ik-element, calculate P_i^{j+1} $(i = 1, \ldots, m)$ by

$$P_i^{j+1} = \sum_k \Bigg\{ X_{ik}P_k^j + \left(A_j^{-1}\right)_{ik} \Bigg(Q_j^{\mathrm{T}}\overline{\diamond f}_k Q_{j+1}L_{01}^j + \frac{1}{2}Q_j^{\mathrm{T}}\overline{\diamond f}_k Q_j L_{00}^j + \frac{1}{2}Q_{j+1}^{\mathrm{T}}\overline{\diamond f}_k Q_{j+1}L_{11}^j \Bigg) \Bigg\}. \quad (20)$$

For higher order terms than 2nd order w.r.t. $\boldsymbol{x}$, we take intervals which include the ranges of the terms and put them into $[\boldsymbol{z}_{j+1}]$. Define

$$[\boldsymbol{p}(\boldsymbol{x})]\text{: an interval which includes the range of } \boldsymbol{p}(\boldsymbol{x})$$

for any polynomial $\boldsymbol{p}(\boldsymbol{x})$. We may use $[\mathcal{U}]$ for a Taylor model $\mathcal{U}$ by similar definition. Then $[\boldsymbol{z}_{j+1}]$ is specified by

$$\begin{aligned}
[\boldsymbol{z}_{j+1}] \;=\; & A_j^{-1}B_j[\boldsymbol{z}_j] \\
& + A_j^{-1}\Bigg\{ \Big(\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\right]^{\mathrm{T}}\overline{\diamond \boldsymbol{f}}\left(Q_j L_{00}^j + Q_{j+1}L_{01}^j\right) \\
& \qquad + \left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\right]^{\mathrm{T}}\overline{\diamond \boldsymbol{f}}\left(Q_j L_{01}^j + Q_{j+1}L_{11}^j\right)\Big)[\boldsymbol{x}] \\
& \qquad + \left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\right]^{\mathrm{T}}\overline{\diamond \boldsymbol{f}}\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\right]L_{01}^j \\
& \qquad + \frac{1}{2}\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\right]^{\mathrm{T}}\overline{\diamond \boldsymbol{f}}\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\right]L_{00}^j \\
& \qquad + \frac{1}{2}\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\right]^{\mathrm{T}}\overline{\diamond \boldsymbol{f}}\left[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\right]L_{11}^j \\
& \qquad + \boldsymbol{r}_j + \boldsymbol{\omega}' \Bigg\}. \qquad (21)
\end{aligned}$$

Note that the fomulation described above is obtained by substituting the following into the Nakao method in the previous section.

$$\begin{aligned} \boldsymbol{\omega}_0 &= \boldsymbol{x}, \\ \boldsymbol{y}_j &= \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j], \\ \boldsymbol{y}_{j+1} &= \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]. \end{aligned}$$

In a similar way, we can obtain higher order Taylor models for the Nakao method by iterating such substitution.

As is mentioned before, $[\boldsymbol{z}_{j+1}]$ is stored in computer as a "zonotope," that is a convex polygonal domain. Take $[\boldsymbol{z}_0] = \boldsymbol{0}$ and treat $[\boldsymbol{z}_{j+1}]$ as a set by

$$[\boldsymbol{z}_{j+1}] = \bigl\{\boldsymbol{z} \in \mathbf{R}^m \bigm| \boldsymbol{z} = \bigl(A_j^{-1}B_j\bigr)\boldsymbol{z}_j + \boldsymbol{\eta}_{j+1}\bigr\},$$

where $\boldsymbol{z}_j \in [\boldsymbol{z}_j]$ and

$$\begin{aligned} \boldsymbol{\eta}_{j+1} \in A_j^{-1}\Bigl\{ & \Bigl(\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\bigr]^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\bigl(Q_j L_{00}^j + Q_{j+1}L_{01}^j\bigr) \\ & \quad + \bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\bigr]^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\bigl(Q_j L_{01}^j + Q_{j+1}L_{11}^j\bigr)\Bigr)[\boldsymbol{x}] \\ & + \bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\bigr]^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\bigr] L_{01}^j \\ & + \frac{1}{2}\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\bigr]^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x} + [\boldsymbol{z}_j]\bigr] L_{00}^j \\ & + \frac{1}{2}\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\bigr]^{\mathrm{T}} \overline{\diamond \boldsymbol{f}}\bigl[\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + [\boldsymbol{z}_{j+1}]\bigr] L_{11}^j \\ & + \boldsymbol{r}_j + \boldsymbol{\omega}'\Bigr\}. \end{aligned} \tag{22}$$

If an enclosure of $[\boldsymbol{z}_{j+1}]$ is necessary, we calculate $[\boldsymbol{z}'_{j+1}] = \bigl[\bigl(A_j^{-1}B_j\bigr)[\boldsymbol{z}_j] + \boldsymbol{\eta}_{j+1}\bigr]$ by interval arithmetic.

For the verification process, we modify the definition of W_N by

$$\begin{aligned} W_N := \bigl\{ & \boldsymbol{\omega}_N \in S_N \bigm| \boldsymbol{\omega}_N(t_j) = \boldsymbol{\omega}_j, \\ & \boldsymbol{\omega}_N(t_{j+1}) = Q_{j+1}\boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x} + \bigl(A_j^{-1}B_j\bigr)\boldsymbol{z}_j + \boldsymbol{\eta}_{j+1}, \\ & \boldsymbol{z}_j \in [\boldsymbol{z}_j],\ |\boldsymbol{\eta}_{j+1}| \le \boldsymbol{\alpha}_{j+1}\bigr\}, \end{aligned} \tag{23}$$

and check whether the right-hand side of (22) is less than or equal to $\boldsymbol{\alpha}_{j+1}$.

Summing up the above procedure, we present an algorithm to obtain an enclosure for the solution $\boldsymbol{u}(t)$ $(t_j \le t \le t_{j+1})$ as follows.

1. Compute an approximate solution $\tilde{\boldsymbol{u}}_{j+1}$ and the tensor $\overline{\diamond \boldsymbol{f}}$ for $\tilde{\boldsymbol{u}}_j$.
2. Give initial values for $\boldsymbol{\alpha}_{j+1}, \boldsymbol{\beta}_j \in \mathbf{R}^m$. Take $[\boldsymbol{\omega}_\perp] = [-\boldsymbol{\beta}_j, \boldsymbol{\beta}_j]$ and $[\boldsymbol{z}'_{j+1}]$ by

$$[\boldsymbol{z}'_{j+1}] := \bigl[\bigl(A_j^{-1}B_j\bigr)[\boldsymbol{z}_j] + [-\boldsymbol{\alpha}_{j+1}, \boldsymbol{\alpha}_{j+1}]\bigr]$$

using $[\boldsymbol{z}_j]$ which is obtained in the previous step. The enclosure $[\boldsymbol{z}'_{j+1}]$ is used for estimation of the right-hand side of (22).

3. Specify Q_{j+1}, $(\boldsymbol{P}_{j+1})$ by (17) and (20), respectively, and calculate an enclosure of $\boldsymbol{\omega}_{j+1}$ by

$$[\boldsymbol{\omega}_{j+1}] := [Q_{j+1}\boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_{j+1})\boldsymbol{x}] + [\boldsymbol{e}_{j+1}] + [\boldsymbol{z}'_{j+1}].$$

Here we take Q_{j+1} and $(\boldsymbol{P}_{j+1})$ by point values, not intervals. The round-off error arises in the calculation of Q_{j+1} and $(\boldsymbol{P}_{j+1})$ is taken into the set $[\boldsymbol{e}_{j+1}]$ in a similar manner described in the Section 3.

4. Define the interval vector $[\Theta]$ using the minimum and the maximum vectors in $(\tilde{\boldsymbol{u}}_j + [\boldsymbol{\omega}_j]) \cup (\tilde{\boldsymbol{u}}_{j+1} + [\boldsymbol{\omega}_{j+1}]) + [\boldsymbol{\omega}_\perp]$ which includes $\Theta(\tau)$ $(t_j \le \tau \le t_{j+1})$, and compute $D(\diamond \boldsymbol{f})$.
5. Calculate $[\boldsymbol{\eta}_{j+1}]$:= the right-hand side of (22) $+[\boldsymbol{e}_{j+1}]$.
6. Take $[\boldsymbol{u}] = [\Theta]$ and estimate $\boldsymbol{\omega}_\perp$ by

$$|\boldsymbol{\omega}_\perp|_{\infty(j)} \le \frac{h^2}{2}\left|\frac{d\boldsymbol{f}}{d\boldsymbol{u}}([\boldsymbol{u}])\boldsymbol{f}([\boldsymbol{u}])\right|_{\infty(j)}.$$

7. If $|[\boldsymbol{\eta}_{j+1}]| \le \boldsymbol{\alpha}_{j+1}$ and $|\boldsymbol{\omega}_\perp|_{\infty(j)} \le \boldsymbol{\beta}_j$ hold, we successfully obtain the set W which includes the error $\boldsymbol{\omega}$. Note that we can redefine W using the left-hand sides of the above inequalities instead of $\boldsymbol{\alpha}_{j+1}$ and $\boldsymbol{\beta}_j$.
8. If failed, try again with

$$\begin{aligned}\boldsymbol{\alpha}_{j+1} &:= (1+\varepsilon)|[\boldsymbol{\eta}_{j+1}]|,\\ \boldsymbol{\beta}_j &:= (1+\varepsilon)\frac{h^2}{2}\left|\frac{d\boldsymbol{f}}{d\boldsymbol{u}}([\boldsymbol{u}])\boldsymbol{f}([\boldsymbol{u}])\right|_{\infty(j)},\end{aligned}$$

where ε is taken to be a small positive number.

6. Numerical examples

We will see the effectiveness of the application of Taylor models to the Nakao method through some simple example problems. All numerical experiments are carried out by a software package for validated computation INTLAB which is described by MATLAB. The specification of the used computer is as follows.

- CPU: Pentium4, 3 GHz
- FSB: 800 MHz
- L2-Cache: 512 KB
- RAM: 2 GB

We do not mention the cpu time because the main purpose of the experiments is investigation on improvement of the accuracy.

PROBLEM 1.

$$\begin{cases} \dfrac{d}{dt}u_1 = u_2, \\ \dfrac{d}{dt}u_2 = -u_1, \end{cases} \qquad 0 < t < T,$$

which is similar to (1) in the explanation of wrapping effect. The trajectory of the true solution is a circle with its origin at $\mathbf{0}$. The period of the solution for an initial point $\boldsymbol{u}_0 = (0, 4)^{\mathrm{T}}$ is around 6.3. We try to give validated computation to the solutions starting from the neighborhood of $\boldsymbol{u}_0$ until $T = 6.3$, and compare the following cases.

Case 1-1. The initial value is a point vector $\boldsymbol{u}_0$.

Case 1-2. The initial value is an interval vector

$$\boldsymbol{u}_0 + [\boldsymbol{\omega}_0],$$

where,

$$[\boldsymbol{\omega}_0] := \begin{pmatrix} [-0.05, 0.05] \\ [-0.05, 0.05] \end{pmatrix}.$$

PROBLEM 2.

$$\begin{cases} \dfrac{d}{dt}u_1 = u_2, \\ \dfrac{d}{dt}u_2 = u_1 - u_1^3, \end{cases} \qquad 0 < t < T.$$

This is a nonlinear problem whose solutions have also periodic trajectories around the origin. The period of the solution for the initial point $\boldsymbol{u}_0 = (0, 4)^{\mathrm{T}}$ is around 3.3. We try to give validated computation to the solutions starting from the neighborhood of $\boldsymbol{u}_0$ until $T = 3.3$, and compare the following cases.

Case 2-1. The initial value is a point vector $\boldsymbol{u}_0$.

Case 2-2. The initial value is an interval vector

$$\boldsymbol{u}_0 + [\boldsymbol{\omega}_0],$$

for the same $[\boldsymbol{\omega}_0]$ in Case 1-2.

RESULTS 1. The results of the method in the Section 4 are obtained as the following form

$$\boldsymbol{u}(t_j) = \tilde{\boldsymbol{u}}_j + Q_j[\boldsymbol{\omega}_0] + \boldsymbol{y}_j$$

on each time step t_j. The bounds of $\boldsymbol{y}_j$ are given by $\boldsymbol{\alpha}_j$ and the bounds of the interpolation error between (t_j, t_{j+1}) are given by $\boldsymbol{\beta}_j$. In the following figures, the solid line and the dashed line denote the first and the second elements, respectively, but the figures for $\boldsymbol{\alpha}_j$ show almost overlapping lines.

Case 1-1.

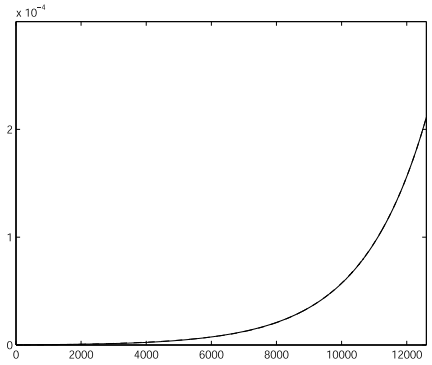

Fig. 2. $\boldsymbol{\alpha}_j$ to j for $h = 0.0005$

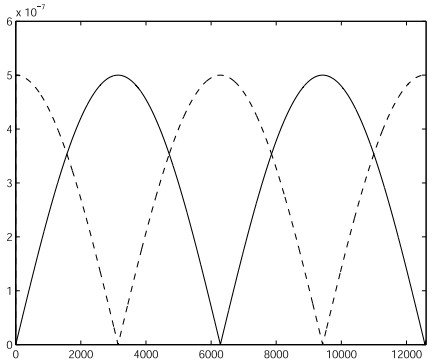

Fig. 3. $\boldsymbol{\beta}_j$ to j for $h = 0.0005$

We show the values of $\boldsymbol{\alpha}_j$ and $\boldsymbol{\beta}_j$ at $t = T$.

h	$\boldsymbol{\alpha}(T)$	$\boldsymbol{\beta}(T)$
0.005	$\begin{pmatrix} 0.02087808836177 \\ 0.02086847633695 \end{pmatrix}$	$\begin{pmatrix} 0.01360722840396 \\ 0.50514071358066 \end{pmatrix} \times 10^{-4}$
0.0005	$\begin{pmatrix} 0.21112084894261 \\ 0.21102494345241 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.00845965370046 \\ 0.49998213329746 \end{pmatrix} \times 10^{-6}$

Case 1-2.

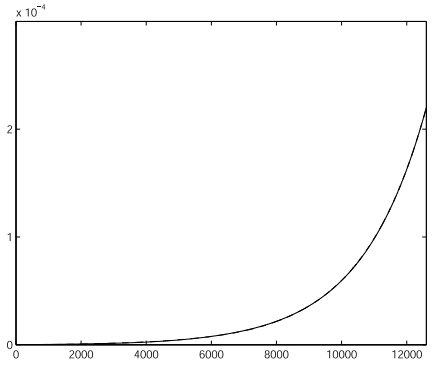

Fig. 4. $\boldsymbol{\alpha}_j$ to j for $h = 0.0005$

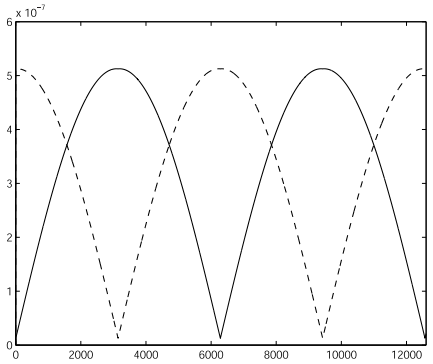

Fig. 5. $\boldsymbol{\beta}_j$ to j for $h = 0.0005$

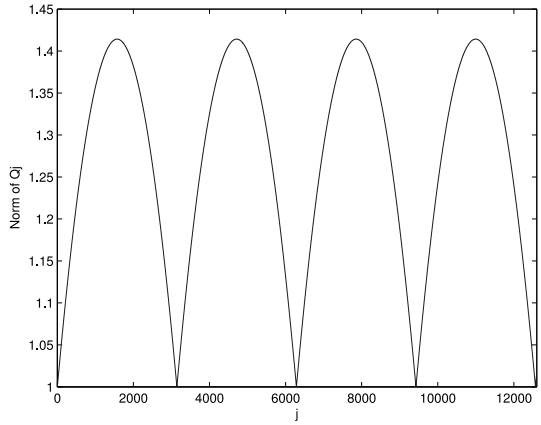

Fig. 6. $\|Q_j\|_\infty$ to j for $h = 0.0005$

The following table has the values of $\boldsymbol{\alpha}_j$, $\boldsymbol{\beta}_j$ and $|Q_j[\boldsymbol{\omega}_0]|$ at $t = T$.

h	$\boldsymbol{\alpha}(T)$	$\boldsymbol{\beta}(T)$	$\lvert Q_n[\boldsymbol{\omega}_0]\rvert$
0.005	$\begin{pmatrix} 0.02175018564017 \\ 0.02174076201021 \end{pmatrix}$	$\begin{pmatrix} 0.02650245326684 \\ 0.51803582619511 \end{pmatrix} \times 10^{-4}$	$\begin{pmatrix} 0.05083298171832 \\ 0.05083298171832 \end{pmatrix}$
0.0005	$\begin{pmatrix} 0.21995227632883 \\ 0.21985828405315 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.02116719629081 \\ 0.51268967474170 \end{pmatrix} \times 10^{-6}$	$\begin{pmatrix} 0.05083362039216 \\ 0.05083362039216 \end{pmatrix}$

We can see that the widths of the initial values give only small effect to the values of $\boldsymbol{\alpha}(T)$ and $\boldsymbol{\beta}(T)$ because of the treatment of the initial box since the problem is linear in these cases. For Case 1-1 with point initial values, it is shown that $\boldsymbol{\alpha}_j$ and $\boldsymbol{\beta}_j$ are of the second order w.r.t. h from the way of the construction of the approximate solutions. Almost the same orders are obtained even for Case 1-2 where the initial values are intervals. However, $\boldsymbol{\alpha}_j$ itself exponentially increase w.r.t. j. This comes from the fact that we do not adopt any devices against the wrapping effects caused by the discretization error and the round-off error. On the other hand, we find that the maximum norms of the matrices Q_j are bounded and vary periodically in these cases, which promises that the effect from the linear terms of the widths of the initial intervals will not increase so much.

Case 2. Since this problem causes much inflation of the error bounds, we have to stop our computation when any value of $\boldsymbol{\alpha}_j$ exceeds 1 even before $t = T$. The stopping times are as follows.

	Case 2-1	Case 2-2
0.005	$t = 2.915$	$t = 2.155$
0.0005	$t = T = 3.3$	$t = 2.1765$

Some graphs until the stopping times are shown in the figures. The solid line and the dashed line denote the first and the second elements, respectively.

Case 2-1.

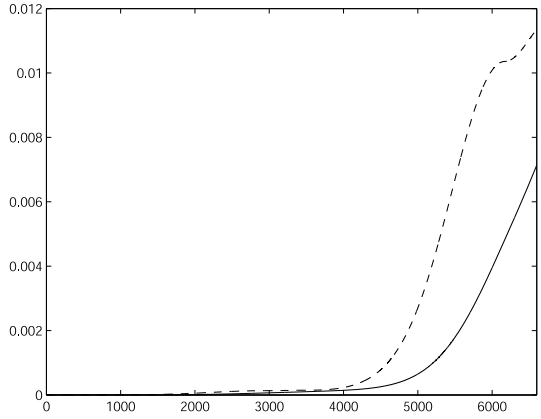

Fig. 7. $\boldsymbol{\alpha}_j$ to j for $h = 0.0005$

We show the values of $\boldsymbol{\alpha}_j$ and $\boldsymbol{\beta}_j$ at $t = 2$.

h	$\boldsymbol{\alpha}(2)$	$\boldsymbol{\beta}(2)$
0.005	$\begin{pmatrix} 0.01417716175586 \\ 0.02254760802745 \end{pmatrix}$	$\begin{pmatrix} 0.02777648130559 \\ 0.30704852198628 \end{pmatrix} \times 10^{-3}$
0.0005	$\begin{pmatrix} 0.14402413638156 \\ 0.23012604429191 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.02698694941277 \\ 0.30463225949696 \end{pmatrix} \times 10^{-5}$

Case 2-2.

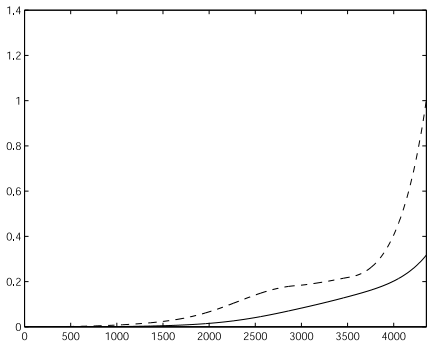

Fig. 8. $\boldsymbol{\alpha}_j$ to j for $h = 0.0005$

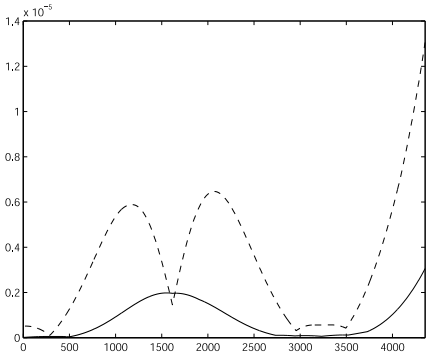

Fig. 9. $\boldsymbol{\beta}_j$ to j for $h = 0.0005$

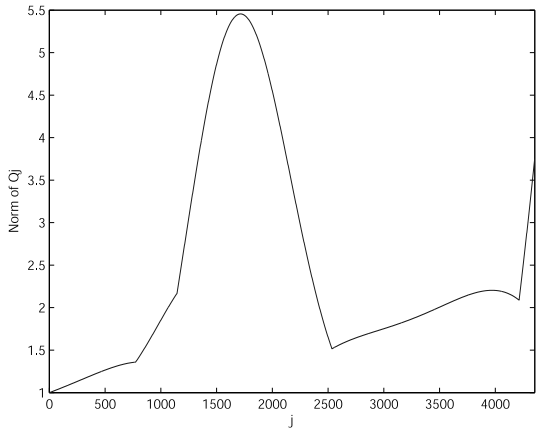

Fig. 10. $\|Q_j\|_\infty$ to j for $h = 0.0005$

The following table has the values of $\boldsymbol{\alpha}_j$, $\boldsymbol{\beta}_j$ and $|Q_j[\boldsymbol{\omega}_0]|$ at $t = 2$.

h	$\boldsymbol{\alpha}(2)$	$\boldsymbol{\beta}(2)$	$\lvert Q_j[\boldsymbol{\omega}_0]\rvert$
0.005	$\begin{pmatrix} 0.22364188349184 \\ 0.45014925033050 \end{pmatrix}$	$\begin{pmatrix} 0.10696355666516 \\ 0.58040655239817 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.11018163464376 \\ 0.04471169345112 \end{pmatrix}$
0.0005	$\begin{pmatrix} 0.20203434050070 \\ 0.40597690815457 \end{pmatrix}$	$\begin{pmatrix} 0.10238674358527 \\ 0.56710990306037 \end{pmatrix} \times 10^{-5}$	$\begin{pmatrix} 0.11012174142854 \\ 0.04439992681683 \end{pmatrix}$

Since the problem is nonlinear, there remains some influence of the widths of the initial interval vector in spite of the treatment of the initial box, and we find quite difference between Case 2-1 and Case 2-2. For the point initial values, we can see that the values of $\boldsymbol{\alpha}(2)$ are of the second order of h, however, the values for the initial box have almost no improvement. It might be said that this is because there are wrapping effect caused by higher order terms of the initial intervals. On the other hand, $\boldsymbol{\beta}(2)$ are of the second order of h in the both cases since the computation of $\boldsymbol{\beta}_j$ on each step is constructed from the estimation of the interpolation error which is less vulnarable to the wrapping effect from $[\boldsymbol{\omega}_0]$. The norms of the matrices Q_j are also less vulnarable to the wrapping effect, and almost the same behaviors are shown for different step sizes.

RESULTS 2. Let us show the results of the Nakao method with the application of Taylor models. An enclosure of the true solutions at each time t_j is given by

$$\boldsymbol{u}(t_j) = \tilde{\boldsymbol{u}}_j + Q_j \boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(P_j)\boldsymbol{x} + [\boldsymbol{z}_j], \quad \boldsymbol{x} \in [\boldsymbol{\omega}_0].$$

We show the results only for the Problem 2 because the Problem 1 gives similar results as Results 1, and discuss with the upper bounds $|\boldsymbol{z}_j|$ for $[\boldsymbol{z}_j]$ rather than $\boldsymbol{\alpha}_j$ which bound the values of $\boldsymbol{\eta}_j$.

Even applying Taylor models, there are cases where the validated computation should be stopped because of inflation of the error bounds, i.e., too large $\boldsymbol{\alpha}_j > 1$ before $t = T$. The following are the stopping times.

	Case 2-1	Case 2-2
0.005	$t = 2.955$	$t = 2.52$
0.0005	$t = T = 3.3$	$t = 2.7675$

Some graphs until the stopping times are shown in the figures. The solid line and the dashed line denote the first and the second elements, respectively.

Case 2-1.

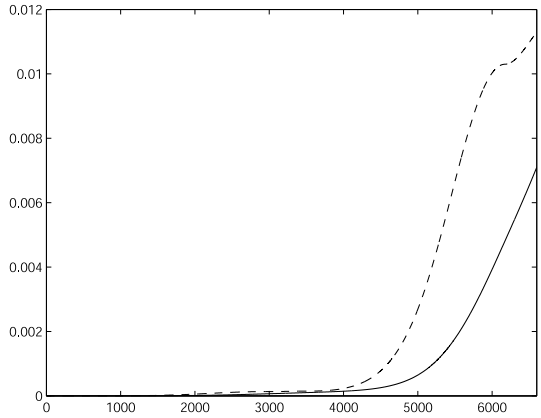

Fig. 11. $|\boldsymbol{z}_j|$ to j for $h = 0.0005$

Case 2-2.

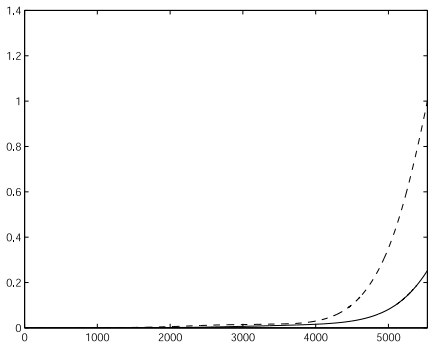

Fig. 12. $|\boldsymbol{z}_j|$ to j for $h = 0.0005$

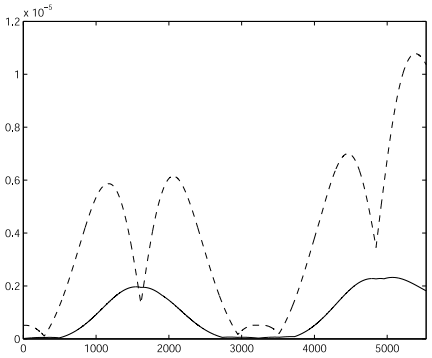

Fig. 13. $\boldsymbol{\beta}_j$ to j for $h = 0.0005$

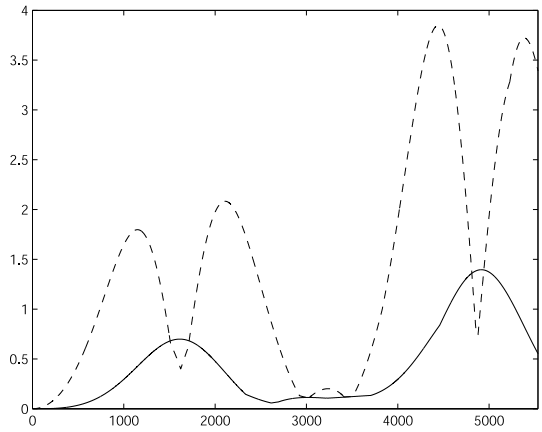

Fig. 14. $\|(\boldsymbol{P}_j)\|_\infty$ to j for $h = 0.0005$

The following tables have the values of $\boldsymbol{\alpha}_j$, $\boldsymbol{\beta}_j$, $|Q_j\boldsymbol{x}|$, $|\boldsymbol{z}_j|$, $|\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}|$ and the sums $|\boldsymbol{z}_j| + |\boldsymbol{x}'(\boldsymbol{P}_j)\boldsymbol{x}| + \boldsymbol{\alpha}_j$ at $t = 2$.

h	$\boldsymbol{\alpha}(2)$	$\boldsymbol{\beta}(2)$	$\lvert Q_j\boldsymbol{x}\rvert$
0.005	$\begin{pmatrix} 0.00275922551466 \\ 0.31676602563992 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.05433766291645 \\ 0.39349133500892 \end{pmatrix} \times 10^{-3}$	$\begin{pmatrix} 0.11018163464376 \\ 0.04471169345112 \end{pmatrix}$
0.0005	$\begin{pmatrix} 0.00005007829265 \\ 0.12423562878707 \end{pmatrix} \times 10^{-4}$	$\begin{pmatrix} 0.05064171208879 \\ 0.38038789024252 \end{pmatrix} \times 10^{-5}$	$\begin{pmatrix} 0.11012174142854 \\ 0.04439992681683 \end{pmatrix}$

h	$\lvert\boldsymbol{z}_j\rvert$	$\lvert\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}\rvert$	$\lvert\boldsymbol{x}^{\mathrm{T}}(\boldsymbol{P}_j)\boldsymbol{x}\rvert + \lvert\boldsymbol{z}_j\rvert + \boldsymbol{\alpha}(2)$
0.005	$\begin{pmatrix} 0.04095271013683 \\ 0.07580401510368 \end{pmatrix}$	$\begin{pmatrix} 0.0008805265627587402 \\ 0.00850026312623 \end{pmatrix}$	$\begin{pmatrix} 0.04183599592510 \\ 0.08462104425555 \end{pmatrix}$
0.0005	$\begin{pmatrix} 0.01580199938733 \\ 0.02989784248265 \end{pmatrix}$	$\begin{pmatrix} 0.00104800214199 \\ 0.00892109161928 \end{pmatrix}$	$\begin{pmatrix} 0.01685000653715 \\ 0.03883135766481 \end{pmatrix}$

By virtue of applying Taylor models, we find some improvement of the error bounds from comparison between the values of $\boldsymbol{\alpha}(2)$ in Results 1 and the sums $|\boldsymbol{z}_j| + |\boldsymbol{x}'(\boldsymbol{P}_j)\boldsymbol{x}| + \boldsymbol{\alpha}(2)$ in the above table beside the extension of the stopping times. This is an effectiveness of the expressions of the enclosures using the second degree polynomials w.r.t. $\boldsymbol{x}$.

On the other hand, the order of $|\boldsymbol{z}_j|$ w.r.t. h is less than an expected order $\mathcal{O}(h)$ from (21). This indicates that there may be some wrapping effect in the calculation of $\boldsymbol{z}_j$ and we should take some countermeasures e.g., QR factorization.

7. Concluding remarks

As is shown in the previous sections, Taylor models can be applied to the Nakao method for ODEs with initial conditions. Some useful tools may be developed from these applications for numerical verification methods to many kinds of problems, e.g., evolution equations.

However, the proposed methods have some defects.

- There is no countermeasure for the wrapping effect caused by discretization error and round-off error.
- The accuracy of this formulation for point initial conditions is up to the 2nd order w.r.t. h since we use the linear interpolation for $\tilde{\boldsymbol{u}}(t)$.

For the wrapping effect caused by discretization error and round-off error, the devices for zonotopes [3] may be useful as well as QR factorization. Then comparison with Lohner method can be done.

In order to get higher accuracy,

- Use higher order interpolation polynomials,
- Define the computational scheme for $\tilde{\boldsymbol{u}}_{j+1}$ using integration of the polynomial parts in the expression for $\boldsymbol{\omega}_{\perp}$,

which are our future works.

References

[1] P. Eijgenraam, The Solution of Initial Value Problems Using Interval Arithmetic. Math. Centre Tracts 144, Mathematisch Centrum, Amsterdam, 1981.

[2] J. Hoefkens, M. Berz and K. Makino, Verified high-order integration of DAEs and higher-order ODEs. Scientific Computing, Validated Numerics, Interval Methods, W. Kramer and J.W. Gudenberg (eds.), Kluwer Academic/Plenum Publishers, New York, 2001.

[3] W. Kühn, Rigorously computed orbits of dynamical systems without the wrapping effect. Computing, **61** (1998), 47–67.

[4] R.J. Lohner, Enclosing the solutions of ordinary initial and boundary value problems. Computerarithmetic, E. Kaucher, U. Kulisch and Ch. Ullrich (eds.), Teubner, Stuttgart, 1987, 225–286.

[5] R.J. Lohner, On the ubiquity of the wrapping effect in the computation of error bounds. Perspectives on Enclosure Methods, U. Kulish, R. Lohner and A. Facius (eds.), Springer, Wien, 2001.

[6] K. Makino, Rigorous analysis of nonlinear motion in particle accelerators. Ph.D. thesis, Michigan State Univ., East Lansing, Michigan, USA, 1998.

[7] K. Makino and M. Berz, Remainder differential algebras and their applications. Computational Differentiation: Techniques, Application, and Tools, M. Berz, C. Bishof, G. Corliss and A. Griewank (eds.), SIAM, Philadelphia, 1996, 63–74.

[8] K. Makino and M. Berz, Efficient control of the dependency problem based on Taylor model methods. Reliab. Comput., **5** (1999), 3–12.

[9] K. Makino and M. Berz, Taylor models and other validated functional inclusion methods. Int. J. Pure Appl. Math., **4** (2003), 379–456.

[10] K. Makino and M. Berz, COSY Infinity Version 9. Nuclear Instruments and Methods, A558, 2005, 346–350.

[11] K. Makino and M. Berz, Suppression of the wrapping effect by Taylor model-based verified integrators: long-term stabillization by preconditioning. International Journal of Differential Equations and Applications, **10** (2005), 353–384.

[12] K. Makino and M. Berz, Suppression of the wrapping effect by Taylor model-based verified integrators: long-term stabillization by shrink wrapping. International Journal of Differential Equations and Applications, **10** (2005), 385–403.

[13] R.E. Moore, Interval Analysis. Prentice Hall, Englewood Cliffs, N.J., 1966.
[14] M.T. Nakao, Numerical verification methods for solutions of ordinary and partial differential equations. Numer. Funct. Anal. Optim., **22** (2001), 321–356.
[15] A. Neumaier, The wrapping effect, ellipsoidal arithmetic, stability and confidence regions. Computing Suppl., **9** (1993), 175–190.
[16] N. Revol, K. Makino and M. Berz, Taylor models and floating point arithmetic: proof that arithmetic operations are bounded in COSY. J. Logic Algebr. Progr., **64** (2005), 135–154.
[17] R. Rihm, Interval methods for initial value problems in ODEs. Topics in Validated Computation, J. Herzberger (ed.), Elsevier (North-Holland), Amsterdam, 1994.