Taylor Model Based Verified Integration for the Volterra Equations and the Lorenz System

Kyoko Makino[1] and Martin Berz[2]

[1]Department of Physics,
University of Illinois at Urbana-Champaign,
Urbane, IL 61801-3080, USA, makino@uiuc.edu
[2]Department of Physics and Astronomy, and
National Superconducting Cyclotron Laboratory
Michigan State University
East Lansing, MI 48824, USA, berz@msu.edu

One of the important fields in validated methods is solving initial value problems in ordinary differential equations (ODEs). The typical problem of overestimation in interval arithmetic is mostly caused by the lack of information of functional dependency. The dependency problem that is related to cancellation is one issue to be overcome. Besides, in the case of solving a system of multidimensional ODEs, there arises the so-called wrapping effect, which is caused by the inflation of the size of the geometric set enclosing the validated solution set at each time step. The wrapping effect is a particular form of the dependency problem based on the connection of current dynamical values on initial conditions, which often is more dramatic than the other sources of overestimation. The history of development of new schemes for verified integration of ODEs illustrates the struggle with those two challenging questions [13, 6, 14, 7, 15].

The Taylor model method [10, 9] combines interval method for validation and high order automatic differentiation for local functional behavior. The method models a function f in the domain $\vec{D}$ by a high order multivariate Taylor polynomial P and the remainder error interval I :

$$\forall \vec{x} \in \vec{D}, \quad f(\vec{x}) \in P(\vec{x} - \vec{x}_0) + I, \tag{1}$$

where $\vec{x}_0$ is the reference point of the Taylor expansion. The nth order Taylor polynomial P is expressed with floating point number coefficients, and it captures the bulk of functional dependency, hence the major source of interval overestimation is removed. The Taylor remainder and any numerical errors arisen in the domain $\vec{D}$ are kept in an interval, namely the remainder error interval I, and the size of I is proportional to $|\vec{D} - \vec{x}_0|^{n+1}$, which can be very small in practice by choosing the size of $\vec{D}$ sufficiently small. The standard binary operations and intrinsic functions on Taylor models were implemented in the code COSY Infinity [9, 2]. It is of particular significance that an antiderivation operation ∂^{-1} is treated as an intrinsic function in the Taylor model structure [9], and this formally removes the difference between the solution of ODEs and merely algebraic equations based on fixed point methods.

We applied the Taylor models to verified integrations of ODEs,

$$\frac{d\vec{x}\,(t;\vec{x}_{ini})}{dt} = \vec{f}\left(\vec{x}\,(t;\vec{x}_{ini})\,,t\right) \quad \text{with} \quad \vec{x}(t_{ini};\vec{x}_{ini}) = \vec{x}_{ini},$$

and the basic algorithm is discussed in [3, 9]. The Taylor approach is applied to expand not only in the independent variable t, but also in the initial value $\vec{x}_{ini}$, which is possible with our Taylor model implementation with high order multivariate Taylor polynomials, and several advantages have been observed.

- The direct availability of the antiderivation on Taylor models allows us to treat the Picard operator like any other function, avoiding the need to explicitly bound error terms of integration formulas.
- The inclusion requirement asserting existence of a solution reduces to a mere inclusion of the remainder intervals.
- The explicit dependency on initial variables can be carried through the whole integration process. This controls the dependency problem optimally, and, most importantly, there is no need to re-package the momentary solution set at each time step, and hence there is no wrapping effect. Thus, it allows for a much larger domain of initial condition and longer integration times.

We have shown how the Taylor models control the dependency problems efficiently for non "single use expression" (SUI) problems [11, 12], and the same efficiency applies to complicated ODEs like the near earth asteroid problem [4, 5]. When the ODEs have SUI expressions, i.e. the right hand side of the equations do not have a source of overestimation of arithmetic nature, the overestimation mostly comes from the pure wrapping effect. Such ODEs are suitable to study the difficulties unique to ODE initial value problems. In this paper, we study SUI ODEs, and by doing that, we want to show the essence of why and how the Taylor model based verified integrator is successful for the near earth asteroid problem.

We use the Volterra equations

$$\frac{dx_1}{dt} = 2x_1(1-x_2), \quad \frac{dx_2}{dt} = -x_2(1-x_1)$$

to illustrate how the method works. The Volterra equations have been historically used as a test case of validated initial value problems [1, 14]. For the purpose of illustration, we take a large interval box for the initial condition

$$x_{1ini} \in 1 + [-0.05, 0.05], \quad x_{2ini} \in 3 + [-0.05, 0.05].$$

We used our Taylor model based integrator VI coded in COSY Infinity [2] and AWA by Lohner [8, 7] to study the performance. AWA represents the conventional methods, since it is one of the most successful codes based on conventional methods and it is widely spread. Despite of the large size of the initial condition, the total error is easily kept around 10^{-10} for the whole one cycle with COSY-VI, while AWA cannot complete the cycle. Both codes take about the same CPU time. The extensive study on the problem addresses why the conventional approach [13, 6, 14, 7, 15] could not handle the problem.

The Lorenz system is another good example to illustrate how the Taylor model based verified integrator works.

$$\frac{dx_1}{dt} = 10(x_2 - x_1), \quad \frac{dx_2}{dt} = x_1(28 - x_3) - x_2, \quad \frac{dx_3}{dt} = x_1 x_2 - \frac{8}{3} x_3.$$

Similar to the Volterra equations, the right hand side is SUI. Since the system exhibits a chaotic motion, it is particularly challenging to validating methods. Even for a large initial condition box

$$x_{1ini} \in 15 + [-0.01, 0.01], x_{2ini} \in 15 + [-0.01, 0.01], x_{3ini} \in 36 + [-0.01, 0.01],$$

the Taylor model approach can integrate beyond the time 5 easily, while AWA breaks down around the time 1.5, indicating that the Taylor model method can be used for validation of various ODE initial value problems for a larger domain and longer times.

References

[1] W. F. Ames and E. Adams, “Monotonically convergent numerical two-sided bounds for a differential birth and death process”, In: K. Nickel (ed.), *Interval Mathematics*, Vol. 29 of *Lecture Notes in Computer Science*, Springer-Verlag, Berlin–New York, 1975, pp. 135–140,

[2] M. Berz and J. Hoefkens. *COSY INFINITY Version 8.1 – programming manual*, Technical Report MSUCL-1196, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, 2001; see also http://cosy.pa.msu.edu.

[3] M. Berz and K. Makino, “Verified integration of ODEs and flows with differential algebraic methods on Taylor models”, *Reliable Computing*, 1998, Vol. 4, pp. 361–369.

[4] M. Berz, K. Makino, and J. Hoefkens, “Verified integration of dynamics in the solar system”, *Nonlinear Analysis*, 2000.

[5] J. Hoefkens, *Rigorous Numerical Analysis with High-Order Taylor Models*, Ph.D. thesis, Michigan State University, East Lansing, Michigan, USA, 2001.

[6] F. Krückeberg, "Ordinary differential equations", In E. Hansen (ed.), *Topics in Interval Analysis*, Clarendon Press, Oxford, 1969, pp. 91–97.

[7] R. Lohner, *Einschliessung der Loesung gewoehnlicher Anfangs- und Randwertaufgaben und Anwendungen*, Ph.D. thesis, Universitaet Karlsruhe, Karlsruhe, Germany, 1988.

[8] R. Lohner, *AWA, the progam AWA (AnfangsWertAufgabe)*; see also http://www.uni-karlsruhe.de/ Rudolf.Lohner/english/index.html.

[9] K. Makino, *Rigorous Analysis of Nonlinear Motion in Particle Accelerators*, PhD thesis, Michigan State University, East Lansing, Michigan, USA, 1998; also available as Technical Report MSUCL-1093, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824.

[10] K. Makino and M. Berz, "Remainder differential algebras and their applications", In: M. Berz, C. Bischof, G. Corliss, and A. Griewank (eds.), *Computational Differentiation: Techniques, Applications, and Tools*, SIAM, Philadelphia, 1996, pp. 63–74.

[11] K. Makino and M. Berz, "Efficient control of the dependency problem based on Taylor model methods", *Reliable Computing*, 1999, Vol. 5, pp. 3–12.

[12] K. Makino and M. Berz, "Higher order verified inclusions of multidimensional systems by Taylor models" *Nonlinear Analysis*, 2000.

[13] R. E. Moore, *Interval Analysis*, Prentice-Hall, Englewood Cliffs, NJ, 1966.

[14] R. E. Moore, *Methods and Applications of Interval Analysis*, SIAM, 1979.

[15] N. Nedialkov, *Computing Rigorous Bounds on the Solution of an Initial Value Problem for an Ordinary Differential Equation*, Ph.D. thesis, University of Toronto, Toronto, Canada, 1999.