Contents

43 New Applications of Taylor Model Methods **359**
Kyoko Makino and Martin Berz
43.1 Taylor Model Arithmetic 359
43.2 Sharp Enclosure of Multivariate Functions and Global Optimization 360
43.3 Multidimensional Verified Quadratures 363
43.4 Verified Integration of ODEs 363

Index **367**

43

New Applications of Taylor Model Methods

Kyoko Makino and Martin Berz

ABSTRACT Taylor model methods unify many concepts of high-order computational differentiation with verification approaches covering the Taylor remainder term. Not only do they provide local multivariate derivatives, they also allow for highly efficient and sharp verification. We present several recent results obtained with Taylor model methods, including verified optimization, verified quadrature and verified propagation of extended domains of initial conditions through ODEs, approaches towards verified solution of DAEs and PDEs. In all cases, the methods allow the development of new numeric-analytic tools that efficiently capitalize on the availability of derivatives and sharp inclusions over extended ranges. Applications of the methods are given, including global optimization, very high-dimensional numeric quadrature, particle accelerators, and dynamics of near-earth asteroids.

43.1 Taylor Model Arithmetic

The remainder of any $(n+1)$ times continuously partially differentiable function f approximated by the nth order Taylor polynomial $P_{n,f}$ at the expansion point $\vec{x}_0$ can be bounded by an interval $I_{n,f}$ satisfying

$$\forall \vec{x} \in [\vec{a}, \vec{b}], \quad f(\vec{x}) \in P_{n,f}(\vec{x} - \vec{x}_0) + I_{n,f} \tag{43.1}$$

that scales with $|\vec{x} - \vec{x}_0|^{n+1}$. In practice, over reasonable box sizes, the remainder bound interval $I_{n,f}$ can be made very small. A pair $(P_{n,f}, I_{n,f})$ satisfying (43.1) is called a Taylor model of f and denoted by

$$T_{n,f} = (P_{n,f}, I_{n,f}).$$

Any computer representable function $f(\vec{x})$ can be modeled by Taylor models if the function f satisfies the above mentioned mathematical conditions in $[\vec{a}, \vec{b}]$. The expansion point $\vec{x}_0$ and the order n specify the Taylor polynomial part $P_{n,f}(\vec{x} - \vec{x}_0)$ uniquely with coefficients described by floating point numbers on a computer. The remainder interval part $I_{n,f}$ further depends on the domain $[\vec{a}, \vec{b}]$ and the details of the algorithm to compute it.

The dependency problem in interval arithmetic [1, 14, 18, 19, 20] is typically caused by cancellation effects. For example, if $I = [a, b]$, then

$I - I$, if not recognized to represent the same number, is computed as $[a, b] - [a, b] = [a, b] + [-b, -a] = [a - b, b - a]$, resulting in a width that is not zero, but twice as large as before. In Taylor models, the bulk of the functional dependency is kept in the Taylor polynomial part, and the cancellation of the dependency happens there, thus the dependency problem in interval computations is suppressed except for the small remainder bound interval part. Thus, not only do Taylor models provide local multivariate derivatives, they also allow for highly efficient and sharp verification. The benefit of the sharpness becomes dramatic for multi-dimensional problems, which otherwise require an unrealistically large number of subdivision of the interested multi-dimensional domain box.

The tools to calculate Taylor models for standard computer representable functions have been developed and implemented in the code COSY Infinity, starting from sums and products and covering intrinsic functions [3, 15, 16]. The arithmetic starts from preparing the variables of the function, $\vec{x}$, represented by Taylor models; the polynomial part is $\vec{x}_0 + (\vec{x} - \vec{x}_0)$, and there is no error involved. Then, Taylor model arithmetic is carried through binary operations and intrinsic functions which compose the function f sequentially. Because the resulting objects represent functions, it is very advantageous to use the antiderivation operation

$$\partial_i^{-1}(P_n, I_n) = \left(\int P_{n-1} dx_i \,,\ (B(P_n - P_{n-1}) + I_n) \cdot |b_i - a_i| \right), \qquad (43.2)$$

where B denotes the bounds of the argument, as a new intrinsic function in the spirit of the differential algebraic approach [15].

43.2 Sharp Enclosure of Multivariate Functions and Global Optimization

The straightforward Taylor model computation of a function $f(\vec{x})$ starting from the identity functions $i_i(\vec{x}) = x_i$ gives a resulting Taylor model of the function f, which carries the information on the derivatives as well as the sharp verification of the range enclosure of the function. This can be used directly for the exclusion procedure of domain decomposition approaches in verified global optimization methods.

To increase the accuracy of range enclosures, in general, the very first step should be a subdivision of the domain of interest. In naive interval arithmetic, the accuracy of the range enclosures increases linearly with the width of the argument; while in Taylor model arithmetic, the accuracy of the remainder intervals increases with $(n + 1)$st power, so the increase of the order of computation also could be the very first step.

Technically there are three questions for practical computation. First, the method requires an efficient mechanism to compute multivariate Taylor polynomials with floating point coefficients. The tools supplied in the

TABLE 43.1. Widths of the local bounds of Gritton's function around $x_0 = 1.5$ by non-verified rastering, the naive interval method, and the 10th order Taylor model method as well as the widths of the remainder intervals.

Subdomain Width	Widths of Local Bounds: Rastering	Interval	TM 10th	TM Remainder TM 10th
0.4000	0.2323	144507.	0.7775	2.998×10^{-6}
0.1000	1.854×10^{-2}	24555.	3.349×10^{-2}	6.360×10^{-13}
0.0250	5.478×10^{-3}	5788.	6.000×10^{-3}	1.472×10^{-19}

code COSY Infinity for more than ten years, have been used for various practical problems mostly in the field of beam physics [2, 3, 10]. The implementation of the Taylor model computation uses the existing multivariate Taylor polynomial computation tools [15]. The second problem is the rigorous estimation of the cumulative computational errors in the floating point arithmetic of the Taylor coefficients, which are all lumped into the remainder bound.

Finally, if the purpose of computation is to bound the range of a function, it is necessary to bound sufficiently sharply the range of the Taylor polynomial part. A variety of verified methods exist, and several methods are implemented in COSY Infinity, beginning with centered Horner methods. Because of the inherent dominance of lower order terms in the Taylor polynomial, it is possible to develop special-purpose tools that are sufficiently accurate while still being very fast. The key idea is to combine exact range solvers for the lower order parts of the polynomials with interval-based tools to enclose the higher order terms [15]. In most cases, however, already the majority of the benefit of the Taylor model approach can be achieved by very simple bounding techniques based on mere interval evaluation of the Taylor polynomial via Horner's scheme. In order not to distract the flow of the argument by discussing bounding techniques, we use this approach throughout the remainder of the chapter.

We show some challenging example problems for verified global optimization. The first example is Gritton's second problem from chemical engineering, addressed by Kearfott [13], which is known to suffer from a severe dependency problem. The function is an 18th order polynomial in one dimension, having 18 roots in the range $[-12, 8]$. The function varies roughly from -4×10^{13} to 6.03×10^{14}, and all the local maxima and minima have different magnitudes. As an illustration of its complicated structure, we note that there are four local extrema in the range $[1.4, 1.9]$ with function values varying only between around -0.1 and 0.1. Mere interval computation shows a severe blow up due to cancellation as summarized in Table 43.1. For intervals, to achieve the comparable result to the Taylor models in the 0.1 width subdomain, the domain would have to be cut to a practically hard to achieve size of 10^{-7}.

The pictures in Figure (1) show the absolute value of the function in

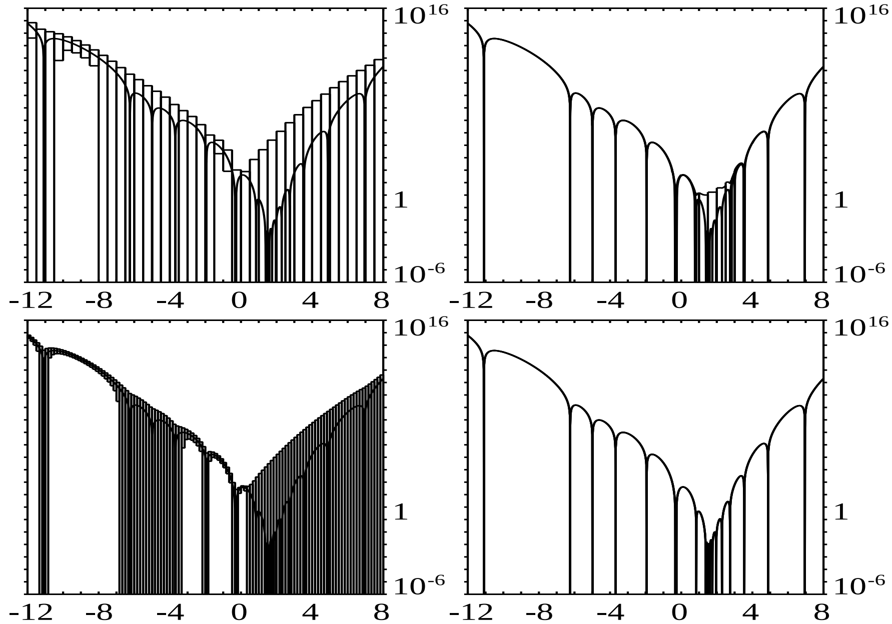

FIGURE 43.1. Gritton's function in $[-12, 8]$ evaluated by 40 (left top) and 120 (left bottom) subdivided intervals, and by 40 subdivided Taylor models with fourth order (right top) and eighth order (right bottom). The pictures show the absolute value of the function in logarithmic scale.

logarithmic scale. Any of the eighteen visible dips to the lower picture frame corresponds to a zero of the function. The left two pictures show enclosures by subdivided intervals; when the local bound interval contains zero, the lower end of the interval range box reaches the lower frame. In the pictures, the advantage of smaller subdivisions is hardly visible for $x > 0$. The right two pictures are obtained with 40 subdivided Taylor models. At order four (right top), there still remains a visible band width of the Taylor models in the range $0.5 \leq x \leq 3$, but at order eight (right bottom), the verified enclosure of the original function reaches printer resolution.

Another challenging example is the pseudo-Lyapunov function of weakly nonlinear dynamical systems [4]. The function is a six dimensional polynomial up to roughly 200th order which involves a large number of local minima and maxima, but the function value itself is almost zero. Hence, there is a large amount of cancellation, and the problem is a substantial challenge for interval methods. The study showed the Taylor model in sixth order already gives fairly tight enclosure of the function comparable to the rastering result in the domain box with the width 0.02 in each dimension. To achieve the similar sharpness in naive interval methods requires 10^{24} subdivided domains [15, 17].

TABLE 43.2. Bounds estimates of an eight dimensional integral, where the analytical answer is ≈ 99.4896438

Division	Step Rule	Trapezoidal	10th Taylor Models
1^8	[8E-15,164.73]	80.25	[99.105950,99.910689]
2^8	[53.06,137.03]	94.61	[99.489371,99.489920]
4^8	[77.25,119.51]	98.28	[99.489643,99.489644]

Points	Monte-Carlo Method
1	72.406666
100	95.614737
10000	99.865452
1000000	99.503242

43.3 Multidimensional Verified Quadratures

Using the handily available antiderivation operator (43.2), quadratures are computed with sharp verification straightforwardly, yet lead to a powerful method especially for the multi-dimensional case [8], where otherwise the Monte Carlo method often represents the only other viable approach.

Based on the following double definite integral

$$\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}} \frac{\sin y\sqrt{1-k^2\sin^2 x\sin^2 y}}{1-k^2\sin^2 y}\, dx\, dy = \frac{\pi}{2\sqrt{1-k^2}},$$

we construct an eight dimensional integral, having as integrand the summation of four terms [8], which is to have the value of $\pi^7/(32\sqrt{1-k^2})$, or approximately 99.4896438 for $k^2 = 0.1$. Even the evaluation with the simple trapezoidal rule without verification is quite expensive. The results are shown in Table 43.2 by the step rule with verification, the trapezoidal rule without verification, the tenth order Taylor model, and the non-verified Monte Carlo method with some numbers of subdivisions and sampling points. The tenth order Taylor model computation without any domain division already gives a remarkably good bound estimate.

43.4 Verified Integration of ODEs

ODE solvers in the Taylor model methods start from the integral form of the ODE to use the antiderivation operator (43.2), then bring it to a fixed point problem, where the nth order polynomial part P_n can be found in at most $(n+1)$ steps. The rest involves tasks to check the inclusion of intervals, which are trivially done [7]. Our Taylor model ODE solver carries the functional dependency of the solutions to the initial conditions in the frame work of Taylor models. Thus it can optimally eliminate the wrapping effect, which has been the most challenging issue in verified ODE solvers [5].

Here again, in the Taylor model approach, the fact that the bulk of the functional dependency is kept in the polynomial part is key. The suppression of the wrapping effect allows the method to deal with larger domains of initial conditions. When combined with methods for verified solutions of constraint conditions over extended domains using Taylor models, the ODE solver forms a natural basis of a verified DAE solver [11].

An important application of the method is the dynamics of near-earth asteroids, addressed by Moore [21] and described by the six dimensional ODEs

$$\begin{aligned}
\ddot{\mathbf{r}} = G\sum_i \frac{m_i(\mathbf{r}_i-\mathbf{r})}{r_i^3}\Bigg\{ & 1 - \frac{2(\beta+\gamma)}{c^2}G\sum_j \frac{m_j}{r_j} - \frac{2\beta-1}{c^2}G\sum_{j\neq i}\frac{m_j}{r_{ij}} \\
& + \frac{\gamma|\dot{\mathbf{r}}|^2}{c^2} + \frac{(1+\gamma)|\dot{\mathbf{r}}_i|^2}{c^2} - \frac{2(1+\gamma)}{c^2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}_i - \frac{3}{2c^2}\left[\frac{(\mathbf{r}-\mathbf{r}_i)\cdot\dot{\mathbf{r}}_i}{r_i}\right]^2 \\
& + \frac{1}{2c^2}(\mathbf{r}_i-\mathbf{r})\cdot\ddot{\mathbf{r}}_i\Bigg\} + \frac{3+4\gamma}{2c^2}G\sum_i\frac{m_i\ddot{\mathbf{r}}_i}{r_i} \\
& + \frac{1}{c^2}G\sum_i\frac{m_i}{r_i^3}\left\{[\mathbf{r}-\mathbf{r}_i]\cdot[(2+2\gamma)\dot{\mathbf{r}}-(1+2\gamma)\dot{\mathbf{r}}_i]\right\}(\dot{\mathbf{r}}-\dot{\mathbf{r}}_i),
\end{aligned}$$

where $\mathbf{r}_i$ is the solar-system barycentric position of body i, including the sun, the planets, the moon and the five major asteroids; $r_i = |\mathbf{r}_i - \mathbf{r}|$; β and γ are the parametrized post-Newtonian parameters [12, 22]. The problem is challenging since initial conditions for asteroids are usually not very well known. To perform verified integrations it is thus necessary to transport a large box over an extended period of time. Hence the system is very susceptible to wrapping effect problems, but poses no difficulty for the Taylor model based integrator. Refer to, for example, [9], which discusses the resulting Taylor models for the position of the asteroid 1997XF11 obtained via verified integration over a period of about 3.47 years, with relative overestimation of the size of the resulting domain of less than a magnitude of 10^{-5}, showing the far-reaching avoidance of the wrapping effect.

Acknowledgments: We thank many colleagues for various stimulating discussions. The work was supported in part by the US Department of Energy and an Alfred P. Sloan Fellowship.

[1] Götz Alefeld and Jürgen Herzberger. *Introduction to Interval Computations*. Academic Press, New York, 1983.

[2] Martin Berz. Forward algorithms for high orders and many variables with application to beam physics. In Andreas Griewank and George F. Corliss, editors, *Automatic Differentiation of Algorithms: Theory, Implementation, and Application*, pages 147–156. SIAM, Philadelphia, Penn., 1991.

[3] Martin Berz. COSY INFINITY Version 8 reference manual. Technical Report MSUCL–1088, National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, 1997. See `cosy.nscl.msu.edu`.

[4] Martin Berz. *Modern Map Methods in Particle Beam Physics*. Academic Press, San Diego, 1999.

[5] Martin Berz. Higher order verified methods and applications. In *Procedings of SCAN 2000*. Kluwer Academic Publishers, Dordrecht, Netherlands, 2001, submitted.

[6] Martin Berz, Christian Bischof, George Corliss, and Andreas Griewank, editors. *Computational Differentiation: Techniques, Applications, and Tools*. SIAM, Philadelphia, Penn., 1996.

[7] Martin Berz and Kyoko Makino. Verified integration of ODEs and flows with differential algebraic methods on Taylor models. *Reliable Computing*, 4:361–369, 1998.

[8] Martin Berz and Kyoko Makino. New methods for high-dimensional verified quadrature. *Reliable Computing*, 5:13–22, 1999.

[9] Martin Berz, Kyoko Makino, and Jens Hoefkens. Verified integration of dynamics in the solar system. *Nonlinear Analysis*, 2001, in print.

[10] Martin Berz, Kyoko Makino, Khodr Shamseddine, Georg H. Hoffstätter, and Weishi Wan. COSY INFINITY and its applications to nonlinear dynamics. In Berz et al. [6], pages 363–365.

[11] Jens Hoefkens, Martin Berz, and Kyoko Makino. Efficient high-order methods for ODEs and DAEs. In George Corliss, Christèle Faure, Andreas Griewank, Laurent Hascoët, and Uwe Naumann, editors, *Automatic Differentiation: From Simulation to Optimization*, Computer and Information Science, chapter 41, pages 343–348. Springer, New York, 2001.

[12] Jet Propulsion Laboratory. JPL Solar System Dynamics. See ssd.jpl.nasa.gov.

[13] R. Baker Kearfott and Alvard Arazyan. Taylor series models in deterministic global optimization. In George Corliss, Christèle Faure, Andreas Griewank, Laurent Hascoët, and Uwe Naumann, editors, *Automatic Differentiation: From Simulation to Optimization*, Computer and Information Science, chapter 44, pages 365–372. Springer, New York, 2001.

[14] Ulrich W. Kulisch and Willard L. Miranker. *Computer Arithmetic in Theory and Practice*. Academic Press, New York, 1981.

[15] Kyoko Makino. *Rigorous Analysis of Nonlinear Motion in Particle Accelerators*. PhD thesis, Michigan State University, East Lansing, Michigan, USA, 1998. Also MSUCL-1093 and bt.nscl.msu.edu/papers-cgi/display.pl?name=makinophd.

[16] Kyoko Makino and Martin Berz. Remainder differential algebras and their applications. In Berz et al. [6], pages 63–74.

[17] Kyoko Makino and Martin Berz. Efficient control of the dependency problem based on Taylor model methods. *Reliable Computing*, 5(1):3–12, 1999.

[18] Ramon E. Moore. *Interval Analysis*. Prentice Hall, Englewood Cliffs, N.J., 1966.

[19] Ramon E. Moore. *Methods and Applications of Interval Analysis*. SIAM, Philadelphia, Penn., 1979.

[20] Ramon E. Moore, editor. *Reliability in Computing: The Role of Interval Methods in Scientific Computing*. Academic Press, San Diego, 1988.

[21] Ramon E. Moore. Private communication, 1998.

[22] P. K. Seidelmann, editor. *Explanatory Supplement to the Astronomical Almanac*. University Science Books, Mill Valley, California, 1992.

Index

application
 near-earth asteroids, 364

COSY Infinity, 360

dependency problem, 359
differential algebraic equations, 359

floating point, 359

global optimization, 361
Gritton's second problem, 361

high order derivatives, 359

interval arithmetic, 359

near-earth asteroids, 364

ordinary differential equations, 359
ordinary differential equations, verified integration, 363

quadrature, multidimensional verified, 363

Taylor model, 359, 363
tools
 COSY Infinity, 360