VERIFIED HIGH-ORDER INTEGRATION OF DAES AND HIGHER-ORDER ODES

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Abstract Within the framework of Taylor models, no fundamental difference exists between the antiderivation and the more standard elementary operations. Indeed, a Taylor model for the antiderivative of another Taylor model is straightforward to compute and trivially satisfies inclusion monotonicity.

This observation leads to the possibility of treating implicit ODEs and, more importantly, DAEs within a fully Differential Algebraic context, i.e. as implicit equations made of conventional functions as well as the antiderivation. To this end, the highest derivative of the solution function occurring in either the ODE or the constraint conditions of the DAE is represented by a Taylor model. All occurring lower derivatives are represented as antiderivatives of this Taylor model.

By rewriting this derivative-free system in a fixed point form, the solution can be obtained from a contracting Differential Algebraic operator in a finite number of steps. Using Schauder's Theorem, an additional verification step guarantees containment of the exact solution in the computed Taylor model. As a by-product, we obtain direct methods for the integration of higher order ODEs. The performance of the method is illustrated through examples.

Keywords: Intervals, Taylor models, Differential Algebra, Antiderivation, Ordinary Differential Equations, Differential Algebraic Equations

1. Introduction

While sophisticated general-purpose methods for the verified integration of explicit ODEs have been developed (Lohner, 1987; Berz and Makino, 1998; Nedialkov et al., 1999), none of these can readily be used for the verified integration of implicit ODEs or Differential Algebraic Equations. Here we will present a new method for the verified integration of implicit ODEs that can be extended to general high index DAEs.

By using a structural analysis (Pantelides, 1988; Pryce, 2000), it is often possible to transform a given DAE into an equivalent system of implicit ODEs. If the derived system is described by a Taylor model, representing each derivate by an independent variable, verified inversion of functional dependencies (Berz and Hoefkens, 2001; Hoefkens and Berz, 2001) can be utilized to solve for the highest derivatives. The resulting Taylor model forms an enclosure of the right hand side of an explicit ODE that is equivalent to the original DAE. While this explicit system is suitable for integration with Taylor model solvers (Berz and Makino, 1998), the approach is limited to relatively small systems, since the intermediate inversion requires a substantial increase in the dimensionality of the problem. An implementation of this inversion-based DAE integration has recently been presented (Hoefkens et al., 2001).

Here, we will derive a method for the verified integration of implicit ODEs that is based on the observation that solutions can be obtained as fixed points of a certain operator containing the antiderivation. We will show that this differential algebraic operator is particularly well suited for practical applications, since it is guaranteed to converge to the exact solution in at most n steps (where $n \in \mathbb{N}$ is the order of the Taylor model). The underlying mathematical concepts are reviewed in Section 2 and the main algorithm is presented, together with an example, in Section 3.

Since the method can also determine the index (Ascher and Petzold, 1998) and a scheme for transforming DAEs into implicit ODEs, it can be used to compute Taylor model enclosures of the solutions of DAEs. Additionally, due to the high order of the Taylor model methods ($n = 20$ is not uncommon), the scheme can be applied to high-index problems that are even hard to integrate with existing non-verified DAE solvers.

2. Mathematical Structures

In this section we review the mathematical concepts that form the basis of the Taylor model method and the new integration scheme to be introduced in Section 3. Since our main focus is the presentation of said algorithm, and since most of the material has been presented elsewhere, we will be quite terse and provide appropriate references wherever necessary.

2.1. Differential Algebraic Methods

The differential algebra ${}_nD_v$ (Berz, 1999) plays an important role in the remainder of this paper. After giving a brief introduction, we will state an important fixed point theorem for operators defined on ${}_nD_v$. In Section 3, this theorem will enable us to obtain solutions of implicit ODE systems by mere iteration of a relatively simple operator.

Definition 1 *Let $U \subset \mathbb{R}^v$ be open and assume that $0 \in U$. For $f, g \in \mathcal{C}^{n+1}(U, \mathbb{R}^w)$ we say that f* equals g up to order n *if $f(0) = g(0)$ and all partial derivatives of orders up to n agree at the origin. If f equals g up to order n, we denote that by $f =_n g$.*

The relation "$=_n$" is an equivalence relation on $\mathcal{C}^{n+1}(U, \mathbb{R}^w)$, and the set of equivalence classes is called ${}_nD_v$; the class containing $f \in \mathcal{C}^{n+1}(U, \mathbb{R}^w)$ is denoted by $[f]_n$, and the individual equivalence classes are called DA vectors.

Proposition 1 *Let f be as in the previous definition. If we denote the n-th order Taylor expansion of f at the origin by T_f, then T_f is a representative of the class $[f]_n$ — i.e. $T_f \in [f]_n$.*

Since n-th order Taylor polynomials can be chosen as representatives for the DA vectors, the structure and its elementary operations are the foundation of the implementation of the Taylor polynomial data type in the high order code COSY Infinity (Berz et al., 1996). It should be noted that ${}_nD_v$ becomes an algebra if the elementary operations (and even intrinsic functions like $\exp$ and $\sin$) are defined appropriately. Moreover, after properly extending the derivative operation ∂ from the set $\mathcal{C}^{n+1}(U, \mathbb{R}^w)$ to ${}_nD_v$, the latter forms a differential algebra. The relevance of this structure for computational applications stems from results that are based on the following definition.

Definition 2 *For $[f]_n \in {}_nD_v$, the* depth *$\lambda([f]_n)$ is defined to be the order of the first, at the origin non-vanishing derivative of f if $[f]_n \neq 0$ and $n + 1$ otherwise.*

Let $\mathcal{O}$ be an operator defined on $M \subset {}_nD_v$. $\mathcal{O}$ is contracting *on M, if for any $[f]_n \neq [g]_n$ in M, we have*

$$\lambda(\mathcal{O}([f]_n) - \mathcal{O}([g]_n)) > \lambda([f]_n - [g]_n).$$

If one compares the depth λ with a norm on Banach spaces, this definition resembles the corresponding definition of contracting operators. Moreover, a theorem that is equivalent to the Banach Fixed Point Theorem can be established. But, unlike in the usual case, the fixed point theorem on ${}_nD_v$ guarantees convergence of the sequence of iterates in at most $n + 1$ steps.

Theorem 1 (DA Fixed Point Theorem) *Let $\mathcal{O}$ be a contracting operator and self-map on $M \subset {}_nD_v$. Then $\mathcal{O}$ has a unique fixed point $a \in M$. Moreover, for any $a_0 \in M$ the sequence $a_k = \mathcal{O}(a_{k-1})$ converges in at most $n + 1$ steps to a.*

A detailed proof of this theorem has been given in (Berz, 1999). Since the DA Fixed Point Theorem assures the convergence to the exact n-th order result in at most $n+1$ iterations, contracting operators are particularly well suited for practical applications. For the remainder of this article, the most important examples of contracting operators are the antiderivation, purely nonlinear functions defined on the set of origin-preserving DA vectors, and sums of contracting operators.

2.2. Taylor Models

Taylor models are a combination of multivariate high order Taylor polynomials with floating point coefficients and remainder intervals for verification. They have recently been used for a variety of applications, including verified bounding of highly complex functions, solution of ODEs with substantial reduction of the wrapping effect (Makino and Berz, 2000), and high-dimensional verified quadrature (Makino and Berz, 1996; Berz, 2000).

Definition 3 *Let $\boldsymbol{D} \subset \mathbb{R}^v$ be a box with $x_0 \in \boldsymbol{D}$. Let $P : \boldsymbol{D} \to \mathbb{R}^w$ be a polynomial of order n ($n, v, w \in \mathbb{N}$) and $R \subset \mathbb{R}^w$ be an open non-empty set. Then the quadruple $(P, x_0, \boldsymbol{D}, R)$ is called a* Taylor model of order n with expansion point x_0 over $\boldsymbol{D}$.

In general we view Taylor models as subsets of function spaces by virtue of the following definition.

Definition 4 *Given a Taylor model $T = (P, x_0, \boldsymbol{D}, R)$. Then T is the set of functions $f \in \mathcal{C}^{n+1}(\boldsymbol{D}, \mathbb{R}^w)$ that satisfy $f(x) - P(x) \in R$ for all $x \in \boldsymbol{D}$ and the n-th order Taylor expansion of f around $x_0 \in \boldsymbol{D}$ equals P. Moreover, if $f \in \mathcal{C}^{n+1}(\boldsymbol{D}, \mathbb{R}^w)$ is contained in T, T is called a Taylor model for f.*

It has been shown (Makino and Berz, 1996; Makino and Berz, 1999) that the Taylor model approach allows the verified modeling of complicated multidimensional functions to high orders, and that compared to naive interval methods, Taylor models

- increase the sharpness of the remainder term with the $(n+1)$-st order of the domain size;
- avoid the dependency problem to high order;
- offer a cure for the dimensionality curse.

There is an obvious connection between Taylor models and the differential algebra ${}_nD_v$ through the prominent role of n-th order multivariate Taylor polynomials. This connection has been exploited by basing the implementation of Taylor models in the code COSY Infinity on the highly optimized implementation of the differential algebra ${}_nD_v$.

Antiderivation of Taylor Models. For a polynomial P, we denote by P_n all terms of P of orders up to (and including) n and by $\boldsymbol{B}(P, \boldsymbol{D})$ a bound of the range of P over the domain box $\boldsymbol{D}$. Then, the antiderivation of Taylor models is given by the following definition (Berz and Makino, 1998; Makino et al., 2000).

Definition 5 *For a n-th order Taylor model $T = (P, x_0, \boldsymbol{D}, R)$ and $k = 1, \ldots, v$, let*

$$Q_k = \int_0^{x_k} P_{n-1}\left(x_1, \ldots, x_{k-1}, \xi_k, x_{k+1}, \ldots, x_v\right) d\xi_k.$$

The antiderivative ∂_k^{-1} of T is defined by

$$\partial_k^{-1}(T) = \left(Q_k, x_0, \boldsymbol{D}, \left(\boldsymbol{B}(P_n - P_{n-1}, \boldsymbol{D}) + R\right) \cdot \boldsymbol{B}(x_k, \boldsymbol{D})\right).$$

Since Q_k is of order n, the definition assures that for a n-th order Taylor model T, the antiderivative $\partial_k^{-1}(T)$ is again a n-th order Taylor model. Moreover, since all terms of T of exact order n are bound into the remainder, the antiderivation is inclusion monotone and lets the following diagram commute.

$$\begin{array}{ccc} f & \hookrightarrow & T_f \\ \Big\downarrow {\scriptstyle \int_0^{x_k}} & & \Big\downarrow {\scriptstyle \partial_k^{-1}} \\ \int_0^{x_k} f(\xi) d\xi_k & \hookrightarrow & \partial_k^{-1}(T_f) \end{array}$$

It is noteworthy that the antiderivation does not fundamentally differ from other intrinsic functions on Taylor models. Moreover, since it is DA-contracting and smoothness-preserving, it has desirable properties for computational applications. Finally, it should also be noted that the antiderivation of Taylor models is compatible with the corresponding operation on the differential algebra ${}_nD_v$.

3. Verified Integration of Implicit ODEs

In this section we present the main result of this article: a Taylor model based algorithm for the verified integration of the general ODE initial value problem

$$F(x, x', t) = 0 \text{ and } x(0) = x_0.$$

Without loss of generality, we will assume that the problem is stated as an implicit first order system with a sufficiently smooth F.

Using Taylor model methods for the verified integration of initial value problems allows the propagation of initial conditions by not only expanding the solution in time, but also in the transverse variables (Berz and Makino, 1998). By representing the initial conditions as additional DA variables, their dependence can be propagated through the integration process, and this allows Taylor model based integrators to reduce the wrapping effect to high order (Makino and Berz, 2000). Moreover, in the context of this algorithm, expanding the consistent initial conditions in the transversal variables further reduces the wrapping effect and allows the system to be rewritten in a derivative-free, origin preserving form suitable for verified integration.

Later, it will be shown that the new method also allows the direct integration of higher order problems, often resulting in a substantial reduction of the problem's dimensionality. After presenting the algorithm, an example will demonstrate its performance, and in 3.2 the individual aspects of the method will be discussed in more detail.

A single n-th order integration step of the basic algorithm consists of the following sub-steps:

1 Using a suitable numerical method (e.g. Newton), determine a consistent initial condition $x'(0) = x'_0$ such that $F(x_0, x'_0, 0) = 0$.

2 Utilizing the antiderivation, rewrite the original problem in a derivative-free form:

$$\Phi(\xi, t) = F\left(x_0 + \int_0^t \xi(\tau) d\tau, \xi, t\right) = 0.$$

3 Substitute $\zeta = \xi - x'_0$ to obtain a new function $\Psi(\zeta, t) = \Phi(\zeta + x'_0, t)$.

4 Using the DA framework of ${}_nD_v$, extract the constant and linear parts from the previous equation: $\Psi(\zeta, t) =_1 C + L_\zeta(\zeta) + L_t(t)$.

5 If L_ζ is invertible, transform the original problem to an equivalent fixed point form

$$\zeta = \mathcal{O}(\zeta) = -L_\zeta^{-1} \left(\Psi(\zeta, t) - L_\zeta(\zeta)\right).$$

On the other hand, if L_ζ is singular, no solution exists for the given consistent initial condition.

6 Iteration with a starting value of $\zeta^{(0)} = 0$ yields the n-th order solution polynomial $P(t) =_n \zeta(t)$ in at most n steps.

7 Verify the result by constructing a Taylor model T, with the reference polynomial P, such that $\mathcal{O}(T) \subset T$.

8 Recover the time expansion of the dependent variable $x(t)$ by adding the constant parts and using the antiderivation:

$$x(t) = x_0 + \int_0^t \left(\zeta(\tau) + x'_0\right) d\tau.$$

From this outline, it is apparent that, by replacing all lower order derivatives of a particular function by its corresponding antiderivatives, the method can easily be modified to allow direct integration of higher order ODEs. In that case, the general second order problem

$$G(x, x', x'', t) = 0 \;\; x(0) = x_0, \;\; x'(0) = x'_0$$

could be written as

$$\Phi(\xi, t) = G\left(x_0 + \int_0^t \left(x'_0 + \int_0^\tau \xi(\sigma)d\sigma\right) d\tau, x'_0 + \int_0^t \xi(\tau)d\tau, \xi, t\right) = 0.$$

And once the function Φ has been determined, the algorithm continues with minor adjustments at the third step. Similar arguments can be made for more general higher order ODEs.

3.1. Example

Earlier, we indicated that the presented method can also be used for the direct integration of higher order problems. To illustrate this, and to show how the method works in practice, consider the implicit second order ODE initial value problem

$$\begin{aligned} e^{x''} + x'' + x &= 0 \\ x(0) = x_0 &= 1 \\ x'(0) = x'_0 &= 0. \end{aligned}$$

While the demonstration of this example uses explicit algebraic transformations for illustrative purposes, it is important to keep in mind that the actual implementation uses the DA framework and does not rely on such explicit manipulations.

1 Compute a consistent initial value for $x''_0 = x''(0)$ such that $e^{x''_0} + x''_0 + x_0 = 0$. A simple Newton method, with a starting value of 0, finds the unique solution $x''_0 = -1.278464542761074$ in just a few steps.

2 Rewrite the original ODE in a derivative-free form by substituting $\xi = x''$:

$$\Phi(\xi, t) = e^{\xi(t)} + \xi(t) + \left(x_0 + \int_0^t \left(x'_0 + \int_0^\tau \xi(\sigma)d\sigma\right) d\tau\right) = 0.$$

3 Define the new dependent variable ζ as the relative distance of ξ to its consistent initial value and substitute $\zeta = \xi - x''_0$ in Φ to obtain the new function Ψ:

$$\Psi(\zeta, t) = \zeta + x''_0 + e^{x''_0} e^{\zeta} + 1 + \frac{x''_0}{2} t^2 + \int_0^t \int_0^\tau \zeta(\sigma) d\sigma d\tau = 0.$$

4 The linear part $L_\zeta(\zeta)$ of Ψ is $1 + e^{x_0''}$; 1 is the constant coefficient and $e^{x_0''}$ results from the linear part of the exponential function e^ζ.

5 With L_ζ from the previous step, the solution ζ is a fixed point of the contracting operator $\mathcal{O}$:

$$\zeta = \mathcal{O}(\zeta) = \frac{1}{1+e^{x_0''}}\left(e^{x_0''}(\zeta - e^\zeta) - x_0'' - 1 - \frac{x_0''}{2}t^2 - \int_0^t \int_0^\tau \zeta(\sigma)d\sigma d\tau\right).$$

6 Start with an initial value of $\zeta^{(0)} = 0$, to obtain the n-th order expansion P of ζ in exactly n steps: $\zeta^{(k+1)} = \mathcal{O}\left(\zeta^{(k)}\right)$.

7 The result is verified by constructing a Taylor model T with the computed reference polynomial P such that $\mathcal{O}(T) \subset T$ (reference point $t_0 = 0$ and time domain $[0, 0.5]$). With the Taylor model $T = \left(P, (-10^{-14}, 10^{-14})\right)$ (reference point and domain omitted), it is

$$\mathcal{O}(T) = \left(P, (-0.659807722506 \cdot 10^{-14}, 0.659857319143 \cdot 10^{-14})\right).$$

Since P is a fixed point of $\mathcal{O}$, the inclusion $\mathcal{O}(T) \subset T$ can be checked by simply comparing the remainder bounds of T and $\mathcal{O}(T)$; the inclusion requirement is obviously satisfied for the constructed T.

8 Lastly, a Taylor model for x is obtained by using the antiderivation of Taylor models:

$$x(t) \in S = x_0 + \int_0^t (x_0' + \int_0^\tau (x_0'' + \zeta(\sigma))d\sigma)d\tau.$$

The following listing shows the actual result of order 25 computed by COSY Infinity

```
RDA VARIABLE:   NO=  25, NV=     1
    I  COEFFICIENT            ORDER
    1   1.000000000000000       0
    2  -.6392322713805370       2
    3  0.4166666666666668E-01   4
    4  -.1993921404777223E-02   6
    5  0.6314945441169959E-04   8
    6  0.2635524930464548E-05  10
    7  -.4411105791086625E-06  12
    8  -.1533094467519992E-07  14
    9  0.8104707776528831E-08  16
   10  -.3384116382961162E-09  18
   11  -.1389729003787960E-09  20
   12  0.1981078695604361E-10  22
   13  0.1549987273495670E-11  24
   ----------------------------------
```

```
VAR    REFERENCE POINT        DOMAIN INTERVAL
  1  0.000000000000000     [0.00000, 0.50000]
               REMAINDER BOUND INTERVAL
  R     [-.2500253775762034E-014,0.2500000000000003E-014]
*******************************************************
```

This example has shown how the new method can integrate implicit ODE initial value problems to high accuracy. It should be noted that the magnitude of the final enclosure of the solution is in the order of 10^{-14} for a relatively large time step of $\Delta t = 0.5$.

Extensions of this basic algorithm include the automated integration of DAE problems with index analysis, multiple time steps and automated step size control, and propagation of initial conditions to obtain flows of differential equations.

3.2. Remarks

We will now comment on the individual steps of the basic algorithm and focus on how they can be performed automatically, without the need for manual user interventions.

Step 1. In the integration of explicit ODEs, the initial derivative is computed automatically as part of the main algorithm. Here, the consistent initial condition x'_0 has to be obtained during a pre-analysis step (which is quite similar to the computation of consistent initial conditions in the case of DAE integration).

Since the consistent initial condition may not be unique, verified methods have to be used for an exhaustive global search. To simplify this, the user should be able to supply initial search regions for x'_0. As an illustration of the non-uniqueness of the solutions, consider the problem

$$\left(x'\left(t\right)\right)^2 + \left(\sin\left(t\right)\right)^2 = 1 \text{ and } x(0) = 0.$$

Obviously, $x'_0 = -1$ and $x'_0 = +1$ are both consistent initial conditions and lead to the two distinct solutions $x_1(t) = -\sin(t)$ and $x_2(t) = +\sin(t)$.

Finally, it should be noted, that we have to find both a floating point number x'_0 (such that $F(x_0, x'_0, 0) = 0$ is satisfied to machine precision) and a guaranteed interval enclosure $\boldsymbol{x'_0}$ of the real root. We will revisit this issue in the discussion of steps 6, 7 and 8.

Step 2. With a suitable user interface and a dynamically typed runtime environment (e.g. COSY Infinity), the substitution of the variables with antiderivatives can be done automatically, and there is no need for the user to rewrite the equations by hand.

Step 3. By shifting to coordinates that are relative to the consistent initial condition x'_0, the solution space is restricted to the set $M = \{a \in {}_nD_v : \lambda(a) \geq 1\}$ of origin-preserving DA vectors. In step 6, this allows the definition of a DA-contracting operator, and the application of the DA Fixed Point Theorem. Again, this coordinate shift can be performed automatically within the semi-algebraic DA framework of COSY Infinity.

Step 4. Like in the previous two steps, the semi-symbolic nature of the DA framework allows the linear part L_ζ to be extracted accurately and automatically. And while the one-dimensional example resulted in L_ζ being represented by a single number, the method will also work in several variables with matrix expressions for L_ζ. We note that within a framework of retention of the dependence of final conditions on initial conditions, as in the Taylor model based integrators (Berz and Makino, 1998), the linearizations are computed automatically and are readily available.

Step 5. With a consistent initial condition, an implicit ODE system is described by a nonlinear equation involving the dependent variable x, its derivative x' and the independent variable t. If we view x and x' as mutually independent and assume regularity of the linear part in x', the Implicit Function Theorem guarantees solvability for x' as a function of x and t. Since the usual statements about existence and uniqueness for ODEs apply to the resulting explicit system, regularity of the linear part guarantees the existence of a unique solution for the implicit system.

Step 6. With an origin-preserving polynomial Q_1 and a purely nonlinear polynomial Q_2, the operator $\mathcal{O}$ can be written as

$$\mathcal{O}(\zeta) = Q_1\left(Q_2\left(\zeta\right), \partial_t^{-1}(\zeta), t\right).$$

Therefore, $\mathcal{O}$ is a well defined operator and self-map on $M = \{\zeta : \lambda(\zeta) \geq 1\} \subset {}_nD_1$, and because of its special form, $\mathcal{O}$ is DA-contracting. Hence the DA Fixed Point Theorem guarantees that the iteration converges in at most $n+1$ steps (since the iteration starts with the correct constant part $\zeta^{(0)} = 0$, the process even converges in n steps).

The iteration finds a floating point polynomial which is a fixed point of the (floating point) operator $\mathcal{O}$. While this polynomial might differ from the mathematically exact n-th order expansion of the solution, it is sufficient to find a fixed point of $\mathcal{O}$ only to machine precision, since deviations from the exact result will be accounted for in the remainder bound.

Step 7. It has been shown (Makino, 1998) that for explicit ODEs and the Picard operator $\mathcal{P}$, inclusion is guaranteed if the solution Taylor model T satisfies

$\mathcal{P}(T) \subset T$. Although $\mathcal{O}$ differs from $\mathcal{P}$, similar arguments can be made for it and further details on this will be published in the near future. Additionally, it should be noted that this step requires a verified version of $\mathcal{O}$, using Taylor model arithmetic and interval enclosures of x_0' and L_ζ.

While all previous steps are guaranteed to work whenever at least one consistent x_0' can be found for which the linear part is regular, this stage of the algorithm can fail if no suitable Taylor model can be constructed. However, decreasing the size of the time domain will generally lead to an eventual inclusion. Further details on the construction of the so-called Schauder candidate sets are given in (Makino, 1998).

Step 8. This final step computes an enclosure of the solution to the original problem from the computed Taylor model containing the derivative of the actual solution, and it relies on the antiderivation being inclusion-preserving. However, in order to maintain verification, the interval enclosure $\boldsymbol{x_0'}$ of the consistent initial condition has to be added to the Taylor model from step 7.

Integration of DAEs. Structural analysis of Differential Algebraic Equations (Pryce, 2000) allows the automated transformation of DAEs to solvable implicit ODEs. In conjunction with the presented algorithm, it can therefore be used to compute verified solutions of DAEs. However, the regularity of L_ζ already offers a sufficient criterion for the solvability of the derived ODEs: while the linear map L_ζ will generally be singular, by repeatedly differentiating the individual equations of the DAE, we eventually obtain a regular linear map L_ζ. Additionally, the minimum number of differentiations needed determines the index of the DAE.

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