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Verified Integration of ODEs and Flows Using Differential Algebraic Methods on High-Order Taylor Models

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Abstract. A method is developed that allows the verified integration of ODEs based on local modeling with high-order Taylor polynomials with remainder bound. The use of such Taylor models of order n allows convenient automated verified inclusion of functional dependencies with an accuracy that scales with the $(n + 1)$-st order of the domain and substantially reduces blow-up.

Utilizing Schauder's fixed point theorem on certain suitable compact and convex sets of functions, we show how explicit nth order integrators can be developed that provide verified nth order inclusions of a solution of the ODE. The method can be used not only for the computation of solutions through a single initial condition, but also to establish the functional dependency between initial and final conditions, the so-called flow of the ODE. The latter can be used efficiently for a substantial reduction of the wrapping effect.

Examples of the application of the method to conventional initial value problems as well as flows are given. The orders of the integration range up to twelve, and the verified inclusions of up to thirteen digits of accuracy have been demanded and obtained.

1. Introduction

In [3], [5], [6], an automated method was developed that provides guaranteed inclusions of functional dependencies with an accuracy that scales with a high order of the domain interval. Different from a mere verified bounding of the remainder term of Taylor's formula, a Taylor polynomial with real floating point coefficients and a guaranteed bound of the expansion are carried through all occurring arithmetic operations in parallel. The resulting inclusion can be seen to scale with the $(n+1)$-st order of the domain over which the functional dependency is evaluated, and thus provides a mechanism to obtain very tight inclusions even over extended ranges of domains. This is particularly useful for problems of higher dimensionality, as the computational expense scales with number of required domain interval raised to the dimension of the problem.

Besides providing bounds of order $(n + 1)$, the method also allows substantial control of the dependency problem, as the bulk effect of the functional dependency is always carried in the real Taylor polynomial part, where cancellations of terms do not have adverse effects on the inclusion interval. As it turns out, even highly complicated functional dependencies with severe cancellation can be treated with very limited blow up of the inclusion interval.

The methods have been previously applied to some six dimensional optimization problems [2], [3], where global bounds of highly complicated functions of about 10^6 floating point operations exhibiting substantial cancellation problems had to be found to an accuracy of better than 10^{-8}. Contrary to conventional interval optimization strategies, which suffered from severe blow up and the dimensionality, verified bounds for the functions could be established to the required tolerance.

In this paper, we apply the methods for the development of verified integration algorithms for ODEs and flows of ODEs. In Section 2, we study derivations and anti-derivations on the set of Taylor models, and thus provide a framework for the verified study of differential algebraic problems. Schauder's fixed point theorem on a class of bounded Lipschitz functions is used to obtain inclusions for solutions of ODEs with Taylor models, resulting in nth order integration schemes. We conclude the paper with several examples.

2. Taylor Models for Derivations and Antiderivations

In the spirit of the idea of embedding the elementary operations of addition, multiplication, and differentiation and their inverses that are defined on the class of C^∞ functions onto the structure of Taylor Models, we now come to the mapping of the derivation operation ∂ as well as its inverse ∂^{-1}. Similar to the case of the Differential Algebra on the set of Truncated Power Series, and following one of the main thrusts of the theory of Differential Algebras, we will use these for the solution of the initial value problem

$$\frac{d}{dt}\vec{r} = \vec{F}(\vec{r}, t), \tag{2.1}$$

where $\vec{F}$ is continuous and bounded. We are interested in both the case of a specific initial condition $\vec{r}_0$, as well as the case in which the initial condition $\vec{r}_0$ is a variable, in which case our interest is in the flow of the differential equation

$$\vec{r}(t) = \mathcal{M}(\vec{r}_0, t) \tag{2.2}$$

describing the functional dependency of final coordinates on initial coordinates and t.

2.1. The Operation ∂^{-1} on Taylor Models

Given an n-th order Taylor model (P_n, I_n) of a function f consisting of the floating point Taylor polynomial P_n and the remainder interval I_n, we can determine a Taylor model for the indefinite integral $\partial_i^{-1} f = \int f \, dx_i'$ with respect to variable i. The Taylor polynomial part is obviously just given by $\int_0^{x_i} P_{n-1} \, dx_i'$, and a remainder bound can be obtained as $(B(P_n - P_{n-1}) + I_n) \cdot B(x_i)$, where $B(x_i)$ is an interval bound for the variable x_i obtained from the range of definition of x_i, and $B(P_n - P_{n-1})$ is a bound for the part of P_n that is of precise order n. We thus define the operator ∂_i^{-1} on the space of Taylor models as

$$\begin{aligned}\partial_i^{-1}(P_n, I_n) &= (P_{n,\partial^{-1}}, I_{n,\partial^{-1}}) \\ &= \left(\int_0^{x_i} P_{n-1}\,\mathrm{d}x_i',\ \left(B(P_n - P_{n-1}) + I_n\right)\cdot B(x_i)\right). \end{aligned} \tag{2.3}$$

With this definition, a bound for a definite integral with respect to the variable x_i from x_{il} to x_{iu} both in the domain of validity of the Taylor model (P_n, I_n) enclosing a function can be obtained as

$$\int_{x_{il}}^{x_{iu}} f\,\mathrm{d}x_i \in \left(P_{n,\partial^{-1}}(x_{iu}) - P_{n,\partial^{-1}}(x_{il}),\ I_{n,\partial^{-1}}\right).$$

In the following, we will use the operation ∂^{-1} to obtain automated solutions of ODEs.

3. Verified Integration with Taylor Models

Our goal is now to establish a Taylor model for $\mathcal{M}(\vec{r}_0, t)$, and thus in particular a rigorous bound for the remainder term of the flow of the differential equation over a domain $[\vec{r}_{01}, \vec{r}_{02}] \times [t_0, t_2]$. This need precludes us from the direct use of conventional numerical integrators, as they do not provide rigorous bounds for the integration error but only estimates thereof. Rather, we have to start from scratch from the foundations of the theory of differential equations.

3.1. Schauder's Fixed Point Theorem

As is common for the application of functional analysis tools to the study of differential equations, we re-write the differential equation as an integral equation

$$\vec{r}(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}(\vec{r}(t'), t')\,\mathrm{d}t', \tag{3.1}$$

noting that the initial value problem has a (unique) solution if and only if the corresponding integral equation has a (unique) solution. Now we introduce the operator

$$A : \vec{C}^0[t_0, t_1] \to \vec{C}^0[t_0, t_1] \tag{3.2}$$

on the space of continuous functions from $[t_0, t_1]$ to R^n via

$$A(\vec{f})(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}(\vec{f}(t'), t')\,\mathrm{d}t'; \tag{3.3}$$

so a general function $\vec{f}$ in $\vec{C}^0[t_0, t_1]$ is transformed into a new function in $\vec{C}^0[t_0, t_1]$ via the insertion into $\vec{F}$ and subsequent integration. Having introduced the operator

A, the problem of finding a solution to the differential equation is reduced to a fixed-point problem

$$\vec{r} = A(\vec{r}). \tag{3.4}$$

It is common fare in the theory of differential equations to establish that Schauder's fixed point theorem asserts the existence of a solution of an ODE over the $[t_0, t_1]$ in case $\vec{F}$ is continous on $[t_0, t_1] \times R^n$ and bounded there. If $\vec{F}$ is even Lipschitz with respect to the first argument $\vec{f}$, then Banach's fixed point theorem asserts a locally unique solution.

We will now apply Schauder's fixed point theorem in a different way to rigorously obtain a Taylor Model for the flow describing the functional dependency on initial conditions.

THEOREM (Schauder). *Let A be a continous operator on the Banach Space X. Let $M \subset X$ be compact and convex, and let $A(M) \subset M$. Then A has a fixed point in M, i.e. there is an $\vec{r} \in M$ such that $A(\vec{r}) = \vec{r}$.*

One should be reminded that the fixed point is not necessarily unique (for example, the identity map on M has every element of M as fixed points); furthermore compactness and convexity of M are essential, as simple counter-examples show.

3.2. Strategy to Satisfy the Requirements of Schauder's Theorem

In our specific case, $X = \vec{C}^0[t_0, t_1]$, the space of continuous vector functions on the interval, equipped with the usual maximum norm, and A is the integral operator in (3.3). From continuity of $\vec{F}$, it follows easily that A is continous on X. The process of our application of Schauder's theorem now has three major steps:

1. Determine a sufficiently large family Y of subsets of X from which to draw candidates for the set M. To satisfy the requirements of Schauder's theorem, the sets in Y have to be **compact** and **convex**; and to fit within our computational framework, it should be possible to contain each one of them in suitable **Taylor models.**
2. Using the differential algebraic structure on Taylor models, construct an initial set $M_0 \in Y$ that satisfies the **inclusion** property $A(M_0) \subset M_0$. Once this set has been determined, all requirements of the fixed point theorem are satisfied, and the existence of a solution in M_0 has been established. Since the sets in Y were chosen in such a way that they can be contained in Taylor models, a Taylor model inclusion of a solution of the ODE has been found.
3. Finally, the set M_0 is iteratively reduced in size in order to obtain a bound that is as sharp as possible. For this purpose, for $i = 1, 2, 3, \ldots$ we construct the sequence $M_i = A(M_{i-1})$. We have the chain $M_1 \supset M_2 \supset \cdots$, and we may continue to iterate until no significant further reduction in size is possible.

3.3. Schauder Candidate Sets

For the first step, it is necessary to establish a family of sets Y from which to draw candidates for M_0. We define Y in the following way. Let $(\vec{P}+\vec{I})$ be a Taylor model depending on time as well as the initial condition $\vec{r}_0$. Then we define the associated set $M_{\vec{P}+\vec{I}}$ as follows:

$$\begin{aligned} M_{\vec{P}+\vec{I}} &\subset \vec{C}^0[t_0,t_1], \quad \text{and for} \quad \vec{r} \in M_{\vec{P}+\vec{I}}: \\ \vec{r}(t_0) &= \vec{r}_0; \\ \vec{r}(t) &\in \vec{P}+\vec{I} \ \ \forall t \in [t_0,t_1] \ \ \forall \vec{r}_0; \\ |\vec{r}(t') - \vec{r}(t'')| &\leq k|t'-t''| \ \ \forall t',t'' \in [t_0,t_1] \ \ \forall \vec{r}_0. \end{aligned}$$

In the last condition, k is a bound for $\vec{F}$, the existence of which will be shown below. The last condition means that all $\vec{r} \in M_{\vec{P}+\vec{I}}$ are uniformly Lipschitz with constant k. Define the family of candidate sets Y as

$$Y = \bigcup_{\vec{P}+\vec{I}} M_{\vec{P}+\vec{I}}.$$

3.4. Convexity, Compactness, and Invariance of Schauder Candidate Sets

Let $M \subset Y$ be a Schauder candidate set. Then M is convex, because

$$\begin{aligned} \vec{x}_1, \vec{x}_2 &\in M \Rightarrow \\ \alpha\vec{x}_1 + (1-\alpha)\vec{x}_2 &\in M \ \ \forall \alpha \in [0,1], \end{aligned}$$

as any such linear combination of two k-Lipschitz functions is k-Lipschitz, is in the same Taylor models as $\vec{x}_1$ and $\vec{x}_2$, and assumes the value $\vec{r}_0$ at t_0.

Furthermore, M is compact, i.e. any sequence in M has a clusterpoint in M. To see this, let $(\vec{x}_n)$ be a sequence of functions in M. Then all $\vec{x}_n$ are k-Lipschitz and hence uniformly equicontinuous; since they are in the same Taylor model, they are uniformly bounded. Thus according to the Ascoli-Arzela Theorem, $(\vec{x}_n)$ has a uniformly convergent subsequence. Let $\vec{x}^*$ be the limit of this subsequence. Since the $\vec{x}_n$ are continous, so is $\vec{x}^*$, and we obviously have $\vec{x}^*(t_0) = \vec{r}_0$. Since the elements of the subsequence converging to $\vec{x}^*$ are k-uniformly Lipschitz, so is $\vec{x}^*$ itself, as a simple indirect proof reveals. Similarly, since the subsequence converging to $\vec{x}^*$ is in $\vec{P}+\vec{I}$, so is $\vec{x}^*$.

Finally, the operator A maps any set in Y into another set in Y. Indeed, the image functions of A go through $\vec{r}_0$ and are continuous because they are integrals, and they are k-Lipschitz because $\vec{F}$ is bounded by k. Finally, since A is continuous, all images of functions inside a Taylor model are bounded and hence themselves in a Taylor model.

Hence the entire problem is reduced to finding a Taylor model $\vec{P}+\vec{I}$ such that

$$A(\vec{P}+\vec{I}) \subset \vec{P}+\vec{I}, \tag{3.5}$$

which asserts both the necessary inclusion condition as well as the boundedness of the function $\vec{F}$. This requirement can now be checked computationally using the differential algebraic operations on the set of Taylor models.

3.5. Satisfying the Schauder Inclusion Requirement

For practical purposes it is of course in addition desirable to have $\vec{I}$ small. For this purpose it turns out to be important to determine a starting candidate that is on the one hand sufficiently small in width, but on the other hand shaped in such a way as to contain the true solution. This thought leads to attempt sets M^* of the form

$$M^* = M_{\mathcal{M}_n(\vec{r},t)+\vec{I}^*}, \tag{3.6}$$

where $\mathcal{M}_n(\vec{r},t)$ is the n-th order Taylor expansion in time and initial conditions of the solution. If n is high enough, we may expect that the true solution of the ODE and hence the fixed point problem is sufficiently close to the n-th order expansion, and hence that it may be possible to choose $\vec{I}^*$ rather small.

This approach requires the knowledge of the solution $\mathcal{M}_n(\vec{r},t)$, and contrary to the usual situation in which we are only interested in $\mathcal{M}_n(\vec{r},t)$ at the final value of t, here the explicit dependence on t is required. This quantity can be obtained by iterating (3.3) within the DA of Truncated Taylor Series. To this end, one chooses an initial function

$$\mathcal{M}_n^{(0)}(\vec{r},t) = \mathcal{I}, \tag{3.7}$$

where $\mathcal{I}$ is the identity function, and then iteratively sets

$$\mathcal{M}_n^{(k+1)} =_n A(\mathcal{M}_n^{(k)}). \tag{3.8}$$

This process converges to the exact result $\mathcal{M}_n$ in $n+1$ steps.

Next, we try to find $\vec{I}^*$ such that in fact $A(\mathcal{M}_n(\vec{r},t)+\vec{I}^*) \subset \mathcal{M}_n(\vec{r},t)+\vec{I}^*$, the inclusion property necessary for Schauder's theorem.

The suitable choice of $\vec{I}$ requires a little experimenting, it is however greatly simplified by the observation that it is necessary that computationally,

$$\vec{I}^* \supset \vec{I}_0 = A\big(\mathcal{M}_n(\vec{r},t)+[0,0]\big) - \mathcal{M}_n(\vec{r},t). \tag{3.9}$$

We may expect that I_0 is a good benchmark for the size of intervals that is to be expected; and so we iteratively try the sequence

$$\vec{I}^{(k)} = 2^k \cdot \vec{I}_0, \tag{3.10}$$

until a computational inclusion can be found, which means that we have established

$$A\left(\mathcal{M}_n(\vec{r},t)+\vec{I}^{(k)}\right)\subset\mathcal{M}_n(\vec{r},t)+\vec{I}^{(k)}. \tag{3.11}$$

Once this computational inclusion has been determined, a solution of the ODE is with certainty contained in the Taylor model $\mathcal{M}_n(\vec{r},t)+\vec{I}^{(k)}$, satisfying our demand.

3.6. Iterative Refinement of the Inclusion

For practical purposes it is useful to note that the sharpness of this solution can be further improved. Denoting $\vec{I}_1=\vec{I}^{(k)}$, we iteratively define a sequence of Taylor models

$$\mathcal{M}_n(\vec{r},t)+\vec{I}_k=A\left(\mathcal{M}_n(\vec{r},t)+\vec{I}_{k-1}\right). \tag{3.12}$$

If the utilized interval arithmetic satisfies inclusion monotonicity, we then must have $\vec{I}_k\subset\vec{I}_{k-1}$ for all $k=2,3,\ldots$ To see this, we observe that by definition of $\vec{I}_1$, this is the case for $k=2$, and then we infer inductively

$$\begin{aligned}
\mathcal{M}_n(\vec{r},t)+\vec{I}_k &\subset \mathcal{M}_n(\vec{r},t)+\vec{I}_{k-1} \Rightarrow\\
A\left(\mathcal{M}_n(\vec{r},t)+\vec{I}_k\right) &\subset A\left(\mathcal{M}_n(\vec{r},t)+\vec{I}_{k-1}\right) \Rightarrow\\
\mathcal{M}_n(\vec{r},t)+\vec{I}_{k+1} &\subset \mathcal{M}_n(\vec{r},t)+\vec{I}_k.
\end{aligned}$$

But furthermore, the fixed point function $\vec{r}$ must actually be contained in each of the elements of the sequence of Taylor models $\mathcal{M}_n(\vec{r},t)+\vec{I}_k$. In fact, again by definition it is contained in $\mathcal{M}_n(\vec{r},t)+\vec{I}_1$, and by induction we see

$$\begin{aligned}
\vec{r} &\in \mathcal{M}_n(\vec{r},t)+\vec{I}_k \Rightarrow\\
A(\vec{r}) &\in A\left(\mathcal{M}_n(\vec{r},t)+\vec{I}_k\right) \Rightarrow\\
\vec{r} &\in \mathcal{M}_n(\vec{r},t)+\vec{I}_{k+1}.
\end{aligned}$$

So this provides a mechanism to iteratively refine the inclusion until no further worthwhile decrease in size can be obtained.

4. Examples

In this section, we will provide two examples for the practical use and performance of the method

4.1. Integrating the Circle

The purpose of the first example is a test of the integration algorithm; it is the motion on a circle defined by the differential equations and initial conditions

$$\begin{aligned}
\dot{x} &= -y, & \dot{y} &= x,\\
x(0) &= 1, & y(0) &= 0.
\end{aligned}$$

The integration from 0 to 2π was performed using tenth order Taylor models with a fixed step size of $\pi/36$. The resulting interval inclusions based on double precision interval arithmetic are

$$+1.000000000000001\text{E}+00 + [-.43837892\text{E}-13,\ +0.43837892\text{E}-13];$$
$$-0.630435635804016\text{E}-14 + [-.43587934\text{E}-13,\ +0.43587934\text{E}-13].$$

4.2. The Flow of a Dipole Magnet

In this example, we analyze the motion of a charged particle in a magnet with constant magnetic field, a problem typical for beam physics. Different from the previous example, not only one ray is integrated, but the flow of the differential equation over a region of initial conditions is determined, which allows the study of the consequences of the wrapping effect. The motion is described by four coupled differential equations

$$\begin{aligned} \frac{dx}{ds} &= a \cdot \frac{1 + x/R}{\sqrt{1 - a^2 - b^2}}, \\ \frac{da}{ds} &= \frac{\sqrt{1 - a^2 - b^2}}{R} - \frac{1 + x/R}{R}, \\ \frac{dy}{ds} &= b \cdot \frac{1 + x/R}{\sqrt{1 - a^2 - b^2}}, \\ \frac{db}{ds} &= 0, \end{aligned}$$

where the independent variable is the arclength, R is the deflection radius of the magnet, which for the purpose of the example was chosen to be 1 m. The integration was carried out over a deflection angle of 36 degrees with a fixed step size of 4 degrees. The initial conditions are within the domain intervals

$$[-.02, .02] \times [-.02, .02] \times [-.02, .02] \times [-.02, .02],$$

and the Taylor polynomial describing the dependence of the four final coordinate values on the four initial coordinate values was determined. The order in time and initial conditions was chosen to be 12, and the step size was estimated so as to ascertain an overall accuracy below 10^{-9}; since no automatic step size control was utilized, the estimate proved conservative and the actual resulting error was somewhat lower:

$$[-0.4496880372277553\text{E}-09,\ +0.3888593417126594\text{E}-09];$$
$$[-0.1301070602141642\text{E}-09,\ +0.1337099965985420\text{E}-09];$$
$$[-0.3417079805637740\text{E}-10,\ +0.3417079805637740\text{E}-10];$$
$$[-0.0000000000000000\text{E}+00,\ +0.0000000000000000\text{E}+00].$$

In the light of the significantly larger magnitude of the box of initial conditions, these tight bounds illustrate the far-reaching control of the wrapping effect; indeed, the original box of initial conditions is mapped to a distorted box the boundaries of which are high-order Taylor polynomials; the inaccuracy of this new "wrapping" is given by the new remainder bounds above.

The resulting Taylor polynomials describing the dependence of final on initial coordinates were compared with those obtained by our particle optics code COSY INFINITY [1], [4], and agreement was found. A further check was possible based on the fact that the motion in a constant magnetic field follows a spiral orbit. A program was used that traces rays by geometric means based on this fact, and its results were compared for a large collection of rays with the results of the flow calculated by the verified integrator. For all rays studied, the difference between the final coordinates determined geometrically and those predicted by the twelfth order Taylor polynomial were within the calculated remainder bounds.

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