

# High-order Validated Representation of Poincaré Maps

JOHANNES GROTE, KYOKO MAKINO and MARTIN BERZ

Department of Physics and Astronomy

Michigan State University

East Lansing, MI 48824

USA

grotejoh@msu.edu, makino@msu.edu, berz@msu.edu <http://bt.pa.msu.edu/>

*Abstract:* For many questions in dynamical systems theory it is desirable to have Poincaré maps available as a tool to study long-term behavior of the dynamical system under consideration. In a validated setting, the Poincaré map should be defined over as large a domain as possible. Taylor model based validated integrators relate final coordinates to initial conditions via a high-order polynomial and a small remainder bound, which usually is many orders of magnitude smaller than the initial domain. It is shown how it is possible to obtain a Taylor model representation of the Poincaré map from the original Taylor model flow representation of the ODE. First a high-order polynomial approximation of the time necessary to reach the plane of the Poincaré map is determined as a function of the initial conditions. This is achieved by reducing the problem to a non-validated polynomial inversion. This approximate representation is inserted into the Taylor model of the time-dependent flow, leading to an approximate Poincaré map. A validated correction is performed that provides a rigorous enclosure of the Poincaré map.

*Key-Words:* Poincaré map, validated computation, differential algebra, Taylor model.

## 1 Introduction

Poincaré maps are a standard tool in general dynamical systems theory to study qualitative properties of a continuous dynamical system under consideration (e.g. the flow generated by an ordinary differential equation), most prominently the asymptotic stability of periodic or almost periodic orbits. The traditional notion of a Poincaré map is that it describes how on a plane  $S$  (the Poincaré section) transversed by a periodic orbit  $\mathcal{O}$  (the reference orbit) points which are sufficiently close to  $\mathcal{O} \cap S$  get mapped back onto  $S$  by the flow. The two key benefits in this approach are that long-term behaviour of the flow close to  $\mathcal{O}$  can be analyzed through the derivative of the Poincaré map at the intersection point of  $S$  and  $\mathcal{O}$ , which is available after just one revolution of  $\mathcal{O}$ , and that the dimensionality of the problem has been reduced by one since the Poincaré map is defined on  $S$  and neglects the 'trivial' direction of the flow perpendicular to the surface.

One is faced with the question which numerical

representations of a flow are particularly favorable in the sense that they easily allow the computation of corresponding Poincaré maps for a given reference orbit and Poincaré section. In this paper we present a method that yields both polynomial approximations of Poincaré maps of a certain type as well as their validation, i.e. a rigorous interval enclosure of the true map. The method assumes that a (validated) high-order polynomial approximation of the flow has been obtained previously using differential algebraic (DA) and Taylor model (TM) methods as described in [1, 4]. We focus on the case where the flow under consideration has been generated by an ODE.

The key question that will be discussed is how to project a domain box exactly to a given surface through the action of the flow.

## 2 Review: DA- and TM-Tools

The DA- and TM-tools which are necessary to appreciate the method are described in detail in [1, 4].

Here we review briefly the most important applications of DA/TM-methods as far as they relate to the problem discussed here: the DA-integration method employed to obtain high-order polynomial approximations of the flow  $\varphi(x_0, t)$ , the validation technique which finds rigorous interval enclosures for  $\varphi(x_0, t)$  and the functional inversion tools which are necessary in later steps of the algorithm.

## 2.1 DA-integration of ODEs

First we tackle the problem of obtaining a polynomial approximation of the solution of the initial value problem

$$\dot{x}(t) = f(x(t), t), \quad x(0) = X_0 + x_0 \quad (1)$$

where  $f : \mathbb{R}^{\nu+1} \supset U^{open} \rightarrow \mathbb{R}^{\nu}$  is defined for DA-vectors (see below), i.e.  $f$  is a composition of intrinsic functions which have been defined in DA-arithmetic. This also entails that  $f$  exhibits sufficient smoothness to guarantee existence and uniqueness of solutions for all initial conditions. The vector  $X_0 \in \mathbb{R}^{\nu}$  is constant and the midpoint of the domain box  $D = X_0 + [-d_1, d_1] \times \dots \times [-d_{\nu}, d_{\nu}] \subset \mathbb{R}^{\nu}$  for the small relative initial conditions  $x_0 \in D$ . Typical box widths  $d_i$  are of the order  $10^{-2}$  to  $10^{-8}$ . The desired polynomial approximation  $\varphi(x_0, t)$  of the flow of eq.(1) is an expansion in terms of the independent time coordinate  $t$  and the relative initial conditions  $x_0$ , and the representation of this approximation is a so-called DA-vector which stores the expansion coefficients up to a prespecified order  $n$  in a structured fashion.

To achieve the aforementioned goal, we recall that the standard procedure of a Picard iteration yields a polynomial approximation of the solution of (1) after repeated application of a Picard operator on the initial conditions. The iteration in general increases the order of the expansion by at least one in every step, and since a DA-vector can store coefficients up to order  $n$ , we see that the iteration converges after finitely many steps in the DA-case (for details see [4]).

The Picard-operator in the DA-computation is defined by

$$\mathcal{C}(\cdot) := (X_0 + x_0) + \partial_{\nu+1}^{-1} f(\cdot) \quad (2)$$

where  $f$  is computed in DA-arithmetic and  $\partial_{\nu+1}^{-1}$  is the *antiderivation operator*, essentially the integration with respect to the  $(\nu + 1)$ st variable  $t$ . It can now be shown that  $\mathcal{C}$  is a contracting operator (with a suitable definition of a contraction, see [4]) and fixed-point theorems exist which guarantee that repeated application of  $\mathcal{C}$  on the initial condition  $x(0) = X_0 + x_0$  will converge to the DA-vector representation of the solution  $\varphi(x_0, t)$  of (1) in  $n + 1$  steps, where  $n$  is the order of computation.

## 2.2 Taylor model validated integration of ODEs

Assuming we have obtained a DA-vector representation of the flow for one time step, we can use the method described in [4] to outfit this polynomial in time  $t$  and initial conditions  $x_0$  with a rigorous remainder interval which encloses the true flow in a validated fashion. We do not wish to go to great detail here, but the general idea is to make an educated estimate about the possible remainder bound, add it to the polynomial part of the flow representation and let the Picard operator (2) act on it using Taylor model arithmetic. It is clear that the polynomial part stays invariant under application of (2), and if the iterated remainder bound is enclosed in the original remainder bound we have proved that the latter was a validated enclosure of the flow. The last statement involves Schauder's fixed point theorem and some sophisticated consideration about its applicability in a Taylor model environment. Once this is established, repeated application of the Picard operator will make the remainder bounds converge to a smallest interval.

## 2.3 Functional inversion using DA-arithmetic

Next we review the actual functional inversion employed to obtain the inverse  $\mathcal{M}^{-1}$  of a function  $\mathcal{M}$ , or rather a DA-vector which stores the expansion coefficients of  $\mathcal{M}^{-1}$  up to order  $n$ . Assume we are given a smooth map  $\mathcal{M} : \mathbb{R}^{\nu} \rightarrow \mathbb{R}^{\nu}$  s.t.  $\mathcal{M}(0) = 0$  and its linearization  $M$  is invertible at

the origin. This assures the existence of a smooth inverse  $\mathcal{M}^{-1}$  in a neighborhood of the origin. If we write  $\mathcal{M} = M + \mathcal{N}$ , where  $\mathcal{N}$  is the nonlinear part, and insert this into the fundamental condition  $\mathcal{M} \circ \mathcal{M}^{-1} = \mathcal{I}$ , we easily obtain the relation

$$\mathcal{M}^{-1} = M^{-1} \circ (\mathcal{I} - \mathcal{N} \circ \mathcal{M}^{-1})$$

and see that the desired inverse  $\mathcal{M}^{-1}$  is a fixed point of the operator  $\mathcal{D}(\cdot) := M^{-1} \circ (\mathcal{I} - \mathcal{N} \circ \cdot)$ , which proves to be a contracting operator in the DA-picture (see [2]). Hence the existence of the fixed point  $\mathcal{M}^{-1}$  of  $\mathcal{C}$  is verified and  $\mathcal{M}^{-1}$  can be obtained through repeated iteration of  $\mathcal{C}$ , beginning with the identity  $\mathcal{I}$ . Also in this case the iteration converges to  $\mathcal{M}^{-1}$  in finitely many steps.

### 3 Computation of the Taylor Approximation

The first step we perform in order to find a Taylor model for the Poincaré map is to compute its Taylor polynomial part. This computation will be performed entirely in the DA-framework, i.e. without validation. It will prove possible to outfit the resulting polynomial with a rigorous error bound in a post-correction step.

#### 3.1 Preliminary remarks

##### 3.1.1 Reduction of the problem

We begin our discussion with the assumption that the ODE under consideration exhibits a periodic or almost periodic solution  $\varphi(X_0, t)$  which starts on a suitable Poincaré section  $S$  and returns after a period  $T$ , which has been determined approximately e.g. by a high-order Runge-Kutta-integration. Since tools for the validated integration of ODEs are available (as described in the previous section), the propagation of a domain box  $X_0 + D$ , where  $D := [-d_1, d_1] \times \dots \times [-d_\nu, d_\nu]$ , through one cycle is merely a technicality and we assume that it has been performed until the last time step.

The interesting question of how this transported box can be projected to  $S$  only becomes apparent in this last step. Since it is intuitively

clear that the time dependence of the TM-solution for the flow is necessary to perform this projection, we do not perform the usual insertion of the time-stepsize into the time dependence, but instead keep the full time expansion for this last time step at  $T$ .

##### 3.1.2 Treatable types of sections

We want to consider as large a class of surfaces as Poincaré sections as possible. A suitable assumption is that the Poincaré section  $S \subset \mathbb{R}^\nu$  is given implicitly in terms of a function  $\sigma : \mathbb{R}^\nu \rightarrow \mathbb{R}$  as  $S := \{x \in \mathbb{R}^\nu : \sigma(x) = 0\}$ . Since the function  $\sigma$  also needs to be expressed in terms of elementary functions available in the computer environment for DA/TM-arithmetic, it is necessarily smooth, and hence also the surface  $S$ . This contains most surfaces which are of practical interest, in particular the most common case where  $S$  is an affine plane of the form  $S := \{x \in \mathbb{R}^\nu : x_1 = c\}$  where the first component  $x_1$  of the vector  $x$  is set to the fixed value  $c \in \mathbb{R}$ ; here  $\sigma(x) = x_1 - c$ .

##### 3.1.3 Transversality of the flow

Another condition which needs to be met by  $S$  is that the flow is transversal to it for all possible initial conditions  $x_0 \in D$ . Without this assumption a Poincaré map cannot be defined meaningfully, however for our method this question can be neglected. In the 'pathological' case that the vectorfield is in the tangent space of the surface at any point, the functional inversion step described in the following will fail.

#### 3.2 Projection of the domain box to the section

The starting point of our discussion is that we have a Taylor model enclosure  $\varphi(x_0, t) + I_\varphi$  of the flow at the time  $T$ , i.e. the crossing time of the reference orbit. Furthermore  $\varphi(x_0, t) + I_\varphi$  still contains the dependence of the time-expansion around  $T$ .

Let  $t_l$  and  $t_u > t_l$  be times such that at  $t_l$  the transported domain box has not yet crossed  $S$  and that at  $t_u$  the entire transported box has crossed the section. These times should be roughly of the dimension of the stepsize at the final step

and the crossing condition can be checked using various range bounding tools as in [5]. Then the interval  $[t_l, t_u]$  contains a unique crossing time  $t_c(x_0) \forall x_0 \in D$  determined by the geometry of  $S$  and the flow (or the vectorfield of the ODE, respectively). From a purely analytic standpoint, the existence of such a crossing time near the reference orbit is only guaranteed locally, however in practice usually  $D$  is small and both the flow and  $S$  are somewhat well-behaved, and then  $t_c(x_0)$  exists globally on  $D$ .

The construction of the projection (and thus Poincaré map) enclosure  $\mathcal{P}(x_0) + I_{\mathcal{P}}$  can be reduced to the construction of a Taylor model for  $t_c(x_0) + I_{t_c}$  for the crossing time. If we succeed in doing this, then  $\mathcal{P}(x_0) + I_{\mathcal{P}}$  can be easily found simply by insertion of the crossing time into the flow

$$\mathcal{P}(x_0) + I_{\mathcal{P}} := \varphi(x_0 + [0, 0], t_c(x_0) + I_{t_c}) + I_{\varphi}$$

We note that from now on in this section all computations are performed in the nonvalidated DA-framework and proceed by constructing an artificial DA-valued function  $\psi(x_0, t)$  with components  $\psi_k(x_0, t)$  from the function  $x_0$  with components  $x_{0,k}$  via

$$\begin{aligned} \psi_k(x_0, t) &:= x_{0,k} \forall k \in \{1, \dots, \nu\} \\ \psi_{\nu+1}(x_0, t) &:= \sigma(\varphi(x_0, t)) \end{aligned}$$

where the indices  $k$  denote components of the respective vectors.

Note that only the polynomial part  $\varphi(x_0, t)$  of the Taylor model solution is used. To get an idea how the construction of  $\psi$  comes about, we remark that a functional inversion step is expected because of the implicit occurrence of the  $t_c(x_0)$  in the problem, and hence  $\psi$  needs to map between spaces of equal dimension. Furthermore  $t_c(x_0)$  depends on the variables  $x_0$  and is determined by the constraint condition

$$\sigma(\varphi(x_0, t_c(x_0))) = 0 \quad (3)$$

and  $\psi$  contains both the constraint condition (3) and the independent variables  $x_0$  as simple identities. Because of (3)  $t_c(x_0)$  satisfies

$$\psi(x_0, t_c(x_0)) = (x_0, 0)$$

and suppose  $\psi$  is invertible than we can evaluate

$$\psi^{-1}(x_0, 0) = \psi^{-1}(\psi(x_0, t_c(x_0))) = (x_0, t_c(x_0))^T$$

and immediately extract the DA-vector representation of  $t_c(x_0)$  bin terms of the  $x_0$  in the last component. In this case the invertibility of  $\psi$  at the point  $(x_0, t_c(x_0))$  is actually guaranteed (at least in an analytic sense) by the condition of transversality.

We can now employ the previously described DA inversion tools to manipulate  $\psi$  and obtain the inverse  $\psi^{-1}$ . Naturally, because of the identities in  $\psi$ , also  $\psi^{-1}$  will preserve these identities and hence only the component  $\psi_{\nu+1}^{-1}(x_0, 0)$  is nontrivial.

### 3.3 Summary of the algorithm for the Taylor approximation of the Poincaré map

We conclude the first part of the method by summarizing the algorithmic steps:

- (1) Perform a validated transport of the initial domain box  $X_0 + D$  for one cycle using polynomial expansion in time and initial conditions.
- (2) Keep the time-expansion in the last time step at  $T$ .
- (3) Find interval enclosure  $I_t := [t_l, t_u]$  for all crossing times  $t_c(x_0)$ ,  $x_0 \in D$
- (4) Check that  $0 \notin (\nabla\sigma(\varphi(D, I_t)), f(\varphi(D, I_t)))$  for transversality
- (5) Set up and invert the auxiliary function  $\psi$  using DA functional inversion to obtain a DA-vector representation of  $\psi^{-1}$ .
- (6) Obtain  $t_c(x_0) := \psi_{\nu+1}^{-1}(x_0, 0)$ .
- (7) Obtain the projection  $\mathcal{P}(x_0) := \varphi(x_0, t_c(x_0))$ .

## 4 Validation

### 4.1 Preliminary remarks

In the following we present a technique of finding a rigorous remainder bound for the truncation error of the polynomial approximation of the Poincaré

map, which we have obtained in the previous section.

We remark that methods have been developed that allow to find Taylor model enclosures of the inverse function directly from a Taylor model for a function (see [2]), which would directly lead to a Taylor model enclosure of the crossing time if applied to a Taylor model extension of  $\psi(x_0, t)$  in the previous section. However, these inversion techniques are much harder to implement than the method presented here.

Furthermore, for many applications the validation is actually not required and in those cases the nonvalidated method described above is satisfactory. The computation can be sped up by performing all TM-operations simply in the DA-framework and completely ignoring the remainder bounds.

As already noted, the validation of the Poincaré map automatically follows if we are able to find a validation for the crossing time  $t_c(x_0)$ . Recall that in the box  $D \times I_t$  the polynomial approximation of the crossing time models the solution manifold of points  $(x_0, t) \in D \times I_t$  which satisfy  $\sigma(\varphi(x_0, t)) = 0$ . The validation consists in finding a remainder bound which, if added to the polynomial  $t_c(x_0)$ , rigorously encloses the full part of the manifold which intersects  $D \times I_t$ .

For the purpose of validation we now also need a validated Taylor model representation of the constraint condition, i.e. in this case the parameterization of the section  $S$ . In other words, the function  $\sigma$  by the means of which the section is given implicitly needs to be enclosed in a Taylor model

$$\sigma(x_0) + I_\sigma := \sigma(x_{0,1} + [0, 0], \dots, x_{0,\nu} + [0, 0])$$

where the right hand side of the last equation is evaluated in Taylor model arithmetic.

#### 4.2 Heuristic enclosure of $t_c(x_0)$

We attempt to validate  $t_c(x_0)$  in a heuristic manner by simply making an educated guess about the form of this remainder bound, based on the fact that its magnitude can roughly be estimated by evaluating  $\sigma(D, t_c + [0, 0]) + I_\sigma$  using Taylor model range bounding techniques.

Pick random numbers  $\epsilon_u^{(1)}, \epsilon_l^{(1)} \geq 0$  and construct a remainder bound  $[-\epsilon_l^{(1)}, \epsilon_u^{(1)}]$  for  $t_c$ . The validation argument hinges on the fact that if we scan the complement  $C := (D \times I_t) \setminus \{t_c(x_0) + [-\epsilon_l^{(1)}, \epsilon_u^{(1)}] : x_0 \in D\}$  which lies 'above' and 'below'  $t_c(x_0) + [-\epsilon_l^{(1)}, \epsilon_u^{(1)}]$  and can verify that the constraint  $\sigma(\varphi(x, t)) = 0$  is violated there, then the feasible set of all times which satisfy the constraint must be contained in the Taylor model  $t_c(x_0) + [-\epsilon_l^{(1)}, \epsilon_u^{(1)}]$  and thus  $[-\epsilon_l^{(1)}, \epsilon_u^{(1)}]$  is indeed a rigorous enclosure. If this is not the case, choose  $\epsilon_u^{(2)} > \epsilon_u^{(1)}$  and  $\epsilon_l^{(2)} > \epsilon_l^{(1)}$  and repeat the construction. So the only condition that needs to be checked is

$$0 \notin \sigma(C) + I_\sigma,$$

compare also figure 1. This test can be performed by parameterizing the two disjoint parts  $C^\pm$  of  $C$  by the variables  $(x_1, \dots, x_\nu, t^\pm(y))$  where

$$\begin{aligned} t^+(y) &= (t_c + \epsilon_u^{(1)})(1 + y)/2 + t_u(1 - y)/2 \\ t^-(y) &= (t_c - \epsilon_l^{(1)})(1 + y)/2 + t_l(1 - y)/2 \end{aligned} \quad (4)$$

and then perform a range bounding of the two Taylor models

$$\begin{aligned} \sigma(x_{0,1} + [0, 0], \dots, x_{0,\nu} + [0, 0], t^+(y)) + I_\sigma \\ \sigma(x_{0,1} + [0, 0], \dots, x_{0,\nu} + [0, 0], t^-(y)) + I_\sigma \end{aligned}$$

over the set  $(x_{0,1}, \dots, x_{0,\nu}, y) \in D \times [-1, 1]$  for the scanning of  $C^\pm$  respectively. One might ask why we choose such a somewhat awkward parameterization for the  $C^\pm$  in terms of the variables  $x_1, \dots, x_\nu, y$ . This is a peculiarity of our computing environment. In principle it is arbitrary by which means we perform the range bounding in expression (4). However, we use the arbitrary order package COSY Infinity [3] for our computations, which fully supports both DA-arithmetic and interval arithmetic as well as the rigorous accounting for round-off and threshold errors. The range bounding necessary in (4) can easily be performed using Taylor model arithmetic (see [5]) in COSY, however fully rigorous error-handling in Taylor model arithmetic can for internal reasons only be guaranteed if all involved Taylor models

have the domain  $[-1, 1]$  for each of their expansion variables. Usually COSY will automatically rescale all Taylor models internally in such a way that they are defined on the domain  $[-1, 1]^{\nu+1}$ , but

for the parameterization (4) we can easily satisfy this requirement by hand calculation and prefer to do so.

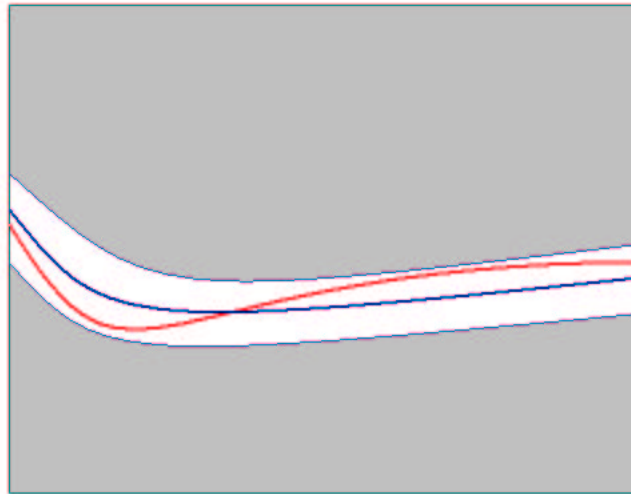


Figure 1: Domain box  $D \times I_t$ , solution manifold (grey line), Taylor model  $t_c(x_0) + [-\epsilon_l^{(1)}, \epsilon_u^{(1)}]$  (white), and complements  $C^\pm$  (grey region)

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