

# 1 Numerical integration of high-order variational equations of ODEs

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## 13 Abstract

14 This paper discusses the numerical integration of high-order variational equations of  
15 ODEs. It is proved that, given a numerical method (say, any Runge-Kutta or Taylor method),  
16 to use automatic differentiation on this method (that is, using jet transport up to order  $p$  with  
17 a time step  $h$  for the numerical integration) produces exactly the same results as integrating  
18 the variational equations up to of order  $p$  with the same method and time step  $h$  as before.  
19 This allows to design step-size control strategies based on error estimates of the orbit and of  
20 the jets. Finally, the paper discusses how to use jet transport to obtain power expansions of  
21 Poincaré maps (either with spatial or temporal Poincaré sections) and invariant manifolds.  
22 Some examples are provided.

23 **Keywords:** Jet transport | Variational equations | Poincaré map | Parametrization method.

## 24 1 Introduction

25 It is well-known that invariant objects (equilibrium points, periodic orbits, invariant tori and  
26 their stable/unstable manifolds) play a key role in the understanding of the global properties  
27 of a dynamical system. They can be seen as the skeleton of the dynamics and, therefore, their  
28 knowledge provides insight on the properties of the system. To have a complete and reliable  
29 picture of the dynamics, it is common to combine theoretical results with numerical methods to  
30 analyze these manifolds.

31 To study dynamical systems defined as the flow of an Ordinary Differential Equation (ODE)  
32 it is common to use suitable Poincaré sections. They reduce the dimensions (phase space and  
33 invariant objects) by one and usually simplify the use of numerical methods. One of the difficul-  
34 ties of using Poincaré maps is that it has to be computed by means of a numerical integration of  
35 the flow. When the derivatives of the Poincaré map are needed it is usual to resort to variational  
36 equations, whose numerical integration provides the derivatives of the flow with respect to initial

1 conditions and/or parameters: let us denote by  $\Phi(t; t_0, x_0)$  the flow of the Initial Value Problem  
2 (IVP)

$$\dot{x} = f(t, x), \quad x(t_0) = x_0. \quad (1)$$

3 Then, if we denote the matrix  $D_{x_0}\Phi(t; t_0, x_0)$  as  $V(t)$ , it follows that  $V$  satisfies the linear  
4 differential equation  $\dot{V} = D_x f(t, x(t))V$ , where  $x(t)$  is the solution of (1). These equations are  
5 usually written together in the form

$$\begin{aligned} \dot{x} &= f(t, x), & x(t_0) &= x_0, \\ \dot{V} &= D_x f(t, x)V, & V(t_0) &= I, \end{aligned}$$

6 where  $I$  denotes the identity matrix. Similarly, one can look at the differential equations satisfied  
7 by higher order derivatives of the flow  $\Phi$ . However, they are usually complicated expressions  
8 involving high order derivatives of  $f$ .

9 There are several situations in which high order derivatives of a Poincaré map are needed.  
10 One of them is the computation of high order approximation to invariant manifolds by means of  
11 the parametrization method [HCL<sup>+</sup>16]. The main idea of the parametrization method is to look  
12 for a suitable parametrization of the required manifold. For instance, under generic conditions,  
13 the stable and unstable manifolds of a fixed point can be represented as a high-order Taylor  
14 expansion w.r.t. a parameter along the manifold. Then, it can be seen that the coefficients  
15 of this Taylor expansion satisfy a set of linear equations. These equations involve high order  
16 derivatives of the map.

17 This paper focuses on the effective computation of high-order derivatives of stroboscopic  
18 and spatial Poincaré maps. We discuss, as a particular example, the computation of high-order  
19 approximations of stable/unstable manifolds of fixed points, which correspond to periodic orbits  
20 of the ODE flow. We are also interested on the efficiency, to allow the use of extended precision  
21 arithmetic when required. A similar process has already been applied for invariant manifolds of  
22 tori of stroboscopic maps [GJNO22]. The computation of invariant manifolds is a classical topic  
23 in dynamical systems, and the standard methods to compute them are based on computing first  
24 a linear approximation to the manifold and then to globalize it [Sim90, KOD<sup>+</sup>05]. What we  
25 propose here is to compute first a high order approximation of the manifold and then to globalize  
26 it. The advantage of using a high order approximation is that we can start the globalization  
27 further away from the fixed point, and this: i) reduces the total computation time; and ii)  
28 increases the accuracy of the computed manifold. This is shown in Section 6.2 with the help on  
29 an example.

30 One of the main tools used here is automatic differentiation (AD) [Gri00], which is an  
31 alternative way of computing derivatives at a given point. It is based on replacing the arithmetic  
32 of real numbers of a given algorithm by a (truncated) formal power series arithmetic so that the  
33 same algorithm will produce not only the result of the algorithm but also its derivatives.

34 In this paper we use these ideas to compute the derivatives of a Poincaré map. As the  
35 numerical integration of the flow is written as a sequence of formulas, we can replace the floating  
36 point arithmetic by a truncated power series arithmetic with floating point coefficients. We  
37 prove that regardless of the numerical integrator –e.g. Runge-Kutta, Taylor, etc– the process  
38 can be implemented. Note that these ideas can be viewed as an extension of the phase space to  
39 propagate the derivatives of the flow in addition to the trajectory. We are going to refer to this  
40 technique as “jet transport” ([AFJ<sup>+</sup>08, JPN10]) since the set of derivatives of a function on a  
41 point is sometimes called the jet of derivatives of the function at this point.

1 A natural question is the accuracy of the derivatives of the flow obtained by using automatic  
2 differentiation on a time stepper for ODEs. As usual, by accuracy we mean the difference  
3 between these values and the exact solution of the variational flow. The error introduced by the  
4 time stepper on the orbit is a well studied topic and its knowledge is used, for instance, to derive  
5 algorithms of step size control according to a prescribed threshold. If, for instance, the time  
6 stepper (with step  $h$ ) has an error  $O(h^p)$ , do the derivatives of the flow w.r.t. initial conditions  
7 obtained by jet transport also have an error  $O(h^p)$ ? Does this error depend on the order of  
8 the derivative? How to derive a suitable step size control for a time stepper that includes jet  
9 transport? These questions are also addressed in this paper. The answer comes from the fact  
10 (proved in Section 3) that the error in the derivatives obtained using jet transport is exactly  
11 the same as the error obtained when applying the time stepper (without jet transport) to the  
12 corresponding variational equations. Therefore, we can estimate the error in the coefficients of  
13 the jet using the same error formulas used to estimate the error of the orbit, since the coefficients  
14 of the jet coincide (exactly) with the values obtained applying the time stepper to the variational  
15 equations. In particular, if the error of the time stepper on the orbit is  $O(h^p)$ , the error on the  
16 derivatives of the flow obtained using jet transport is also  $O(h^p)$ . This implies that we can use  
17 the existing step size control strategies for general ODEs when using jet transport, handling the  
18 coefficients of the jets as the components of the solution of the variational equations.

19 There is a vast literature on the applications of the numerical integration of high-order vari-  
20 ational equations. This contribution is also devoted to its combination with the parametrization  
21 method for the computation of the high-order approximation of invariant manifolds. It is worth  
22 noting that these techniques have been used to tackle problems that range from those that arise  
23 from the theory of dynamical systems to applications to astrodynamics and orbital mechanics.  
24 The following gives an overview to the reader of the state of the art of the topic.

25 Jet transport techniques can be used to study problems in computational dynamical systems.  
26 This allows to deal with high-order derivatives of solutions of ODE that can be used, e.g., in  
27 the following contexts:

- 28 • The non-integrability of Hamiltonian systems can be established by studying its high-order  
29 variational equations via the so-called Morales-Ramis and Morales-Ramis-Simó theories.  
30 See [MS09] and references therein, where these are applied and exemplified.
- 31 • Jet transport has been extensively used to cope with the problem of propagation of un-  
32 certainties, namely in the loss of accuracy for long term integrations due to the change of  
33 shape of the propagated set of initial conditions, [AFJ<sup>+</sup>08, AFJ<sup>+</sup>09, JPN10, ADLBZB10].  
34 Jet transport allows to propagate not only an initial condition but a region whose shape  
35 is determined by some polynomial, see [PPMG13, PPGM18, VADLL13]. In [WDLA<sup>+</sup>15],  
36 the authors present an automatic method of to split the propagated domains to increase  
37 accuracy. The method relies on detecting when the flow expansion with respect to ini-  
38 tial conditions is no longer accurate enough, and to split the region into two subregions.  
39 Each subregion is further propagated using the same polynomial representation before the  
40 splitting, but centered on different point (on each subregion).
- 41 • These same ideas can be used to refine techniques for detecting invariant structures. These  
42 techniques, that include e.g. Fast Lyapunov Indicators (FLI for short), usually rely on  
43 linear approximations of the dynamics. By means of jet transport one can use high-order  
44 approximations to get a better insight of the dynamics, see [PPMG14, PPMG15].

1 From the perspective of applications to orbital mechanics problems, jet transport techniques  
2 are a tool that allows to refine and extend the results using reference solutions.

- 3 • The computation of collision probability can also be addressed using jet transport tech-  
4 niques, see, for instance, [MADLBZ15]. In this work, the authors look first for close  
5 approaches (regular integrations with standard double arithmetic), and then once closest  
6 approaches are detected, collision probabilities are computed via propagation of uncertain-  
7 ties using jet transport.
- 8 • Affine optimal control problems, that is, problems that can be set as the equations of mo-  
9 tion being affine in the controls, have been dealt with and jet transport as well. Integration  
10 of high-order variational equations can be used to find expansions of the solutions of the  
11 optimal control problem around a reference trajectory. Examples of such systems are low  
12 thrust transfers, see [LABZB14].
- 13 • High-order numerical and analytical extended Kalman Filters are implemented using jet  
14 transport techniques to easily go to high-orders in the derivatives, to reduce computa-  
15 tional effort and to improve accuracy. This is applied to orbit determination problems,  
16 see [VADLL14].
- 17 • Two-point boundary value problems are dealt with jet transport techniques. A reference  
18 solution is found via classical iterative methods. An expansion around this reference solu-  
19 tion is computed transporting the Jet to high-orders to find close new solutions, obtained  
20 via evaluation of the obtained Taylor expansions, see [LAL08].
- 21 • Validation of a-posteriori theorems. In [CCGd22] the computation of high-order derivatives  
22 of a stroboscopic Poincaré map with extended arithmetic precision was used to validate the  
23 existence a KAM torus close to its breakdown in a quasi-conformally symplectic system.  
24 The norm computation of these derivatives were needed to verify the inequalities of an  
25 a-posteriori theorem in [CCd13].
- 26 • Jet transport has been used in computer assisted proofs, such as [KS17] and implemented  
27 in computational libraries and packages, such as [CAP].

28 This paper starts in Section 2 fixing the notation of basic notions in automatic differentiation.  
29 After that, Section 3 presents the main contribution of the paper showing that the use of jet  
30 transport is equivalent to integrate high-order variational flows. Section 4 applies the previous  
31 results to the computation of high-order derivatives of Poincaré maps which is later applied in  
32 Section 5 to the parametrization method. Finally, Section 6 shows some illustrative examples  
33 using all this new methodology.

## 34 **2 Automatic differentiation and jet transport**

35 Automatic differentiation is a technique used to obtain high-order derivatives of the output  
36 of a given algorithm with respect to the input, see [GC91, Gri00, Nau12]. In this section,  
37 we summarize the main ideas involved in this tool. An essential ingredient for the successful  
38 implementation of automatic differentiation is the manipulation of (formal) power series.

## 1 2.1 Formal power series in one variable

2 A formal power series in one variable  $s$  is an expression of the form

$$\sum_{k \geq 0} a_k s^k, \tag{2}$$

3 where the coefficients  $a_k$  belong to a field. If  $f$  is a  $C^\infty$  function defined on a neighborhood of  
4 0, we can choose as  $a_k$  its  $k$ -th *normalized derivative*,

$$a_k = \frac{1}{k!} f^{(k)}(0),$$

5 and then (2) can be seen as a formal series that encodes the *jet* of derivatives of  $f$  at 0. The  
6 manipulation of formal power series goes back to L. Euler. A modern reference for the topic is,  
7 for instance, the book by D. Knuth [Knu98]. To discuss the arithmetic of formal power series,  
8 let us define

$$A = \sum_{k \geq 0} a_k s^k, \quad B = \sum_{k \geq 0} b_k s^k, \quad C = \sum_{k \geq 0} c_k s^k.$$

9 The basic operations of power series,  $A \pm B$  and  $AB$  are defined in a natural way. If  $b_0 \neq 0$ ,  
10 the quotient  $C = A/B$  is obtained by writing  $BC = A$  and taking the coefficients of degree  $k$  at  
11 both sides,

$$b_0 c_k + b_1 c_{k-1} + \cdots + b_k c_0 = a_k,$$

12 which implies

$$c_k = \frac{1}{b_0} (a_k - b_1 c_{k-1} - \cdots - b_k c_0),$$

13 and this allows to compute the coefficients  $c_k$  recursively, starting from  $c_0 = a_0/b_0$ .

14 Let us see how to perform other operations. For instance, let us focus on  $C = A^\alpha$  for  $\alpha \in \mathbb{R}$ .  
15 We assume  $\alpha \neq 0, 1$  (these two cases are trivial) and  $a_0 \neq 0$ . Taking formal derivatives w.r.t.  $s$   
16 we obtain  $C' = \alpha A^{\alpha-1} A'$  which implies  $C' A = \alpha C A'$ . Now we equate the coefficients of degree  
17  $k - 1$  at both sides to obtain

$$\sum_{j=0}^k j c_j a_{k-j} = \alpha \sum_{j=0}^k (k-j) a_{k-j} c_j,$$

18 and, therefore

$$c_k = \frac{1}{k a_0} \sum_{j=0}^{k-1} [\alpha k - (\alpha + 1)j] a_{k-j} c_j,$$

19 which allows to compute the coefficients  $c_k$  ( $k \geq 1$ ) recursively starting from  $c_0 = a_0^\alpha$ . We note  
20 that this formula includes the inversion ( $\alpha = -1$ ) and the square root ( $\alpha = \frac{1}{2}$ ).

21 The same idea can be used to compute  $C = h(A)$  when  $h$  is any function that satisfies a  
22 simple differential equation. This includes  $\log$ ,  $\exp$  and the trigonometric functions.

23 *Remark 1.* As a formal series  $A$  codifies the derivatives of a  $C^\infty$  function  $f$  at, say, 0. The formal  
24 series  $h(A)$  codifies the derivatives of the composition  $h \circ f$  at 0. In other words, the operations  
25 with formal series can be seen as the “transport” of derivatives through these operations.

## 1 2.2 Formal power series in several variables

2 In a similar way, we can consider power series of  $n$  variables,

$$A = \sum_{m \geq 0} \sum_{|k|=m} a_k s^k, \quad (3)$$

3 where  $k \in \mathbb{N}^n$ ,  $|k| = k_1 + \dots + k_n$  and  $s^k = s_1^{k_1} \dots s_n^{k_n}$ . As before, if  $f$  is a  $C^\infty$  multivariate  
4 function defined on a neighborhood of 0, we can take

$$a_k = \frac{\partial^k f}{k_1! \dots k_n!}(0),$$

5 then (3) encodes the jet of partial derivatives of  $f$  at 0. The arithmetic of multivariate power  
6 series is very similar to the case of one variable. As an example, let us show how to compute  
7  $C = A^\alpha$  for  $\alpha \in \mathbb{R}$ . As before, we assume  $\alpha \neq 0, 1$ . We replace  $s_j$  by  $s_j z$  ( $z$  is an extra one-  
8 dimensional variable that, at the end, it will be selected equal to 1 to recover the initial form)  
9 and we obtain,

$$A = \sum_{m \geq 0} A_m z^m, \quad \text{where} \quad A_m = \sum_{|k|=m} a_k s^k.$$

10 Using the same notation for  $C$ , we can use the procedure derived in Section 2.1 to obtain,

$$C_m = \frac{1}{mA_0} \sum_{j=0}^{m-1} [\alpha m - (\alpha + 1)j] A_{m-j} C_j,$$

11 where now  $A_j$  and  $C_j$  denote homogeneous polynomials of degree  $j$ . As the only required  
12 operations are sums and products of homogeneous polynomials (note that  $A_0$  appears in a  
13 denominator but it is always a number), the formula can be carried out easily. In the same  
14 way, similar formulas can be obtained for other operations. As in the one dimensional case,  
15 operations with multivariate formal series can be seen as the “transport” of partial derivatives  
16 through these operations.

## 17 2.3 Truncated power series

18 The computer implementation of these techniques is done using truncated power series. For  
19 instance, assume we are working with truncated series up to order, say,  $M$ . Then, the equality  
20  $C = A^\alpha$  means that  $C$  is a truncated power series whose coefficients coincide with the ones of  
21  $A^\alpha$ . Note that this does not mean that they coincide as functions of their variables (in fact they  
22 do not, since  $A^\alpha$  contains terms of order higher than  $M$  that we are neglecting). We expect that  
23 this notation will not confuse the reader.

24 Note that the efficiency of the operations depends on the efficiency of the product of homo-  
25 geneous polynomials. Moreover, note that the complexity of these operations is very low: for  
26 instance, the cost of  $A^\alpha$  is similar to the cost of a product of two truncated power series of order  
27  $M$ . It is not difficult to see that this is the complexity of all the standard operations.

## 28 2.4 Jet transport

29 The automatic differentiation can be used on an algorithm for the numerical integrations of  
30 ODEs to compute the derivative of the final point of the orbit with respect to the the initial

1 data and/or parameters. More concretely, given an ODE, an initial condition  $(t_0, x_0)$  and a  
2 numerical method for ODEs, let us denote by  $\Phi(t_0, x_0; h)$  the algorithm of numerical integration  
3 that, from the initial data  $(t_0, x_0)$  approximates the point of the orbit at time  $t_0+h$ . Jet transport  
4 is the result of using automatic differentiation on this algorithm, that is, to replace the usual  
5 floating point arithmetic by an arithmetic of power series, truncated at degree  $m$ . Then, running  
6 this algorithm on the data  $(t_0, x_0 + s)$ , where we assume  $x_0 \in \mathbb{R}^n$  and  $s = (s_1, \dots, s_n)$  we obtain  
7 something like  $x_1 + A_1(s) + A_2(s) + \dots + A_m(s)$ , where  $x_1$  is the (approximation to the) new  
8 point on the orbit,  $A_1(s)$  is an  $n$ -dimensional vector of polynomials of degree 1 in  $s$  which are the  
9 first order terms of the Taylor series of  $\Phi(t_0, x_0; h)$  at  $x_0$ ,  $A_2(s)$  contains the second order terms,  
10 and so on. In this way we compute a numerical approximation to high-order variations of  
11 the flow by computing high-order derivatives of the numerical integration algorithm. A natural  
12 question is about the difference between this result and the exact integration of the corresponding  
13 variational equations. In particular, if the error is higher for high-order derivatives. This will  
14 be useful to design a step size control that takes into account that the numerical integration has  
15 been overloaded with jet transport. This is the goal of the next section.

### 16 3 Variational flow and jet transport

17 Consider a generic Initial Value Problem (IVP),

$$\dot{x} = f(t, x), \quad x(t_0) = x_0, \quad (4)$$

18 where  $f$  is smooth and  $x$  belongs to a suitable domain of  $\mathbb{R}^n$ . We want to compare the results  
19 of using jet transport on a numerical integrator for this equation and the results obtained by  
20 integrating the corresponding variational equations with the same numerical integrator. In this  
21 comparison, we restrict ourselves to Runge-Kutta methods (explicit or implicit), Taylor method  
22 and multistep methods. The main result is given by the next theorem.

23 **Theorem 3.1.** *Given a step size  $h$ , the use of jet transport of order  $m$  on a Runge-Kutta*  
24 *method, Taylor method or multistep method produces exactly the same results as the integration*  
25 *of variational equations up to order  $m$  with the same method.*

26 *Proof.* First, we will show in the following subsections (Propositions 3.2 and 3.3) that the use of  
27 jet transport of order 1 on a Runge-Kutta or Taylor method for (4) produces exactly the same  
28 results as the ones obtained by using this numerical integrator on the first order variational  
29 equations,

$$\begin{aligned} \dot{x} &= f(t, x), & x(t_0) &= x_0, \\ \dot{v} &= D_x f(t, x)v, & v(t_0) &= v_0, \end{aligned} \quad (5)$$

30 where  $v(t) \in \mathbb{R}^n$  and  $v_0 \neq 0$  is an arbitrary direction. Then, the proof of the theorem is easily  
31 completed proceeding recurrently on  $m$ : note that the variational flow of (5) contains the second  
32 variational flow of (4) so we can use the previous proposition to show that the result is true up  
33 to second order variational equations, and so on. The proof for the multistep method is very  
34 similar to the proof for the Runge-Kutta case and we omit the details.  $\square$

35 To describe the numerical methods in this section we use the notation

$$\dot{y} = F(t, y), \quad y(t_0) = y_0, \quad (6)$$

1 to refer either to IVP (4) or (5). To simplify the presentation, we assume that  $F$  is smooth  
 2 enough on a suitable domain. We will focus on a single (time) step of the methods, using a  
 3 given time step  $h$ . Once it is shown that the jet transport results and the results of integrating  
 4 the variational flow are equal, it is clear that if we apply the same step size control strategy to  
 5 both methods we also obtain the same step sizes for the integration.

### 6 3.1 Runge-Kutta methods

7 A generic  $\sigma$ -stage Runge-Kutta method for the IVP (6) is defined by the formulas (see, for  
 8 instance, [But87, HNW00]),

$$\begin{aligned} \kappa_i &= F(t_0 + c_i h, y_0 + h(a_{i,1}\kappa_1 + \cdots + a_{i,\sigma}\kappa_\sigma)), \quad i = 1, \dots, \sigma, \\ y_1 &= y_0 + h(b_1\kappa_1 + \cdots + b_\sigma\kappa_\sigma), \end{aligned} \quad (7)$$

9 where  $a_{ij}$ ,  $b_j$  and  $c_j$  are suitable real coefficients and  $h$  is the time step. It is well known that, if  
 10  $h$  is small enough, these equations have a unique solution ([HNW00]). When  $a_{ij} = 0$  for  $i \leq j$   
 11 the method is explicit, which means that the vectors  $\kappa_j$  can be obtained explicitly.

12 The goal of this section is to show that to use jet transport of order 1 on the  $\sigma$ -stage Runge-  
 13 Kutta method (7) to approximate the solution and the variational flow of (4) is exactly the  
 14 same as to apply the Runge-Kutta method (7) to the IVP (5). To this end, let us introduce the  
 15 following notation. Let us denote the values  $\kappa_j$  that corresponds to the IVP (5) as  $\kappa_j = (\bar{\kappa}_j, \hat{\kappa}_j)$   
 16 where  $\bar{\kappa}_j$  refers to the coordinates  $x$ , and  $\hat{\kappa}_j$  refers to the coordinates  $v$ .

17 **Proposition 3.2.** *Assume that we are using jet transport of order 1 on the scheme (7) when*  
 18 *applied to the IVP (4). Then, the  $\kappa_j$  values obtained are exactly  $\bar{\kappa}_j + \hat{\kappa}_j s$ .*

19 *Proof.* If we use jet transport of order 1 on a Runge-Kutta method applied to the IVP (4) we  
 20 obtain the equations

$$\bar{\kappa}'_i + \hat{\kappa}'_i s = f(t_0 + c_i h, x_0 + v_0 s + h \sum_{j=1}^{\sigma} a_{i,j} (\bar{\kappa}'_j + \hat{\kappa}'_j s)).$$

21 This equation is equivalent to

$$\bar{\kappa}'_i + \hat{\kappa}'_i s = f(t_0 + c_i h, x_0 + h \sum_{j=1}^{\sigma} a_{i,j} \bar{\kappa}'_j) + D_x f(t_0 + c_i h, x_0 + h \sum_{j=1}^{\sigma} a_{i,j} \bar{\kappa}'_j) (v_0 + h \sum_{j=1}^{\sigma} a_{i,j} \hat{\kappa}'_j) s,$$

22 which implies

$$\begin{aligned} \bar{\kappa}'_i &= f(t_0 + c_i h, x_0 + h \sum_{j=1}^{\sigma} a_{i,j} \bar{\kappa}'_j), \\ \hat{\kappa}'_i &= D_x f(t_0 + c_i h, x_0 + h \sum_{j=1}^{\sigma} a_{i,j} \bar{\kappa}'_j) (v_0 + h \sum_{j=1}^{\sigma} a_{i,j} \hat{\kappa}'_j). \end{aligned}$$

23 These are the equations (7) for  $\kappa_j = (\bar{\kappa}_j, \hat{\kappa}_j)$  corresponding to the IVP (5). As the solution is  
 24 unique ([HNW00]), we have that  $\bar{\kappa}_j = \bar{\kappa}'_j$ ,  $\hat{\kappa}_j = \hat{\kappa}'_j$ .  $\square$

25 This implies that a single step of a RK method (either explicit or implicit) with jet transport  
 26 of order 1 on (4) produces the same result as a single step of the RK on (5).

1 **3.2 Taylor method**

2 One of the oldest methods for the numerical integration of an IVP like (6) is based on the  
 3 computation of the Taylor series of the solution.

$$y_1 = y_0 + y_0^{[1]}h + y_0^{[2]}h^2 + \dots + y_0^{[p]}h^p,$$

4 where  $y_0^{[i]}$  denotes the normalized derivative of the solution of (6) at  $t_0$ ,

$$y_0^{[i]} = \frac{1}{i!} \frac{d^i y}{dt^i}(t_0).$$

5 The computation of the values  $y_0^{[i]}$  by taking derivatives to both sides of the ODE can be a difficult  
 6 process and, moreover, it produces very complex expressions for these derivatives so that the  
 7 resulting method is not very efficient, specially if high orders are required. On the other hand,  
 8 automatic differentiation can be used to compute these normalized derivatives very efficiently,  
 9 up to high orders, giving rise to very efficient implementations of Taylor method ([JZ05]). As  
 10 before, we can use jet transport on the Taylor method to approximate the variational flow. This  
 11 has been implemented in the new version of the package `taylor`, [GJZ22].

12 **Proposition 3.3.** *A step of Taylor method with first order jet transport on the IVP (4) produces*  
 13 *exactly the same results as a step of Taylor method on the IVP (5).*

14 *Proof.* The  $i$ -th normalized derivative of the orbit of (5) is

$$x_0^{[i]} = \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[f(t, x(t))](t_0, x_0), \quad v_0^{[i]} = \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[D_x f(t, x(t))](t_0, x_0)v_0,$$

15 which can be used to perform a Taylor step on (5).

16 To apply jet transport of order 1 to (4), we replace  $x_0$  by  $x_0 + v_0s$  and we propagate first  
 17 derivatives with respect to  $s$ ,

$$\begin{aligned} & \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[f(t, x(t))](t_0, x_0 + v_0s) \\ &= \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[f(t, x(t))](t_0, x_0) + D_x \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[f(t, x(t))](t_0, x_0)v_0s + O(s^2) \\ &= \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[f(t, x(t))](t_0, x_0) + \frac{1}{i!} \frac{d^{i-1}}{dt^{i-1}}[D_x f(t, x(t))](t_0, x_0)v_0s + O(s^2) \\ &= x_0^{[i]} + v_0^{[i]}s + O(s^2). \end{aligned}$$

18 That is, the Taylor coefficients obtained from jet transport of order 1 are exactly the same as the  
 19 Taylor coefficients coming from the variational equations. Hence, given an order and a nonzero  
 20 time step  $h$ , the output of a step of Taylor integration using jet transport of order 1 on (4) gives  
 21 exactly the same results as using Taylor method on (5). □

22 *Remark 2.* Theorem 3.1 is also true for methods (either explicit or implicit) in which the new  
 23 point on the orbit is found as a linear combination of evaluations of the vector field at given  
 24 points. We do not include the details since the proofs are very similar to the ones for the  
 25 Runge-Kutta case.

### 1 3.3 Step size control

2 As the use of jet transport is equivalent to the integration of the normalized variational equa-  
3 tions<sup>1</sup>, we can use the standard step size control of the numerical integration. This means that  
4 we can use the coefficients of the  $A_j$  (see Section 2.4) as if they were the values obtained of  
5 the numerical integration of the normalized variational equations. Therefore, applying the step-  
6 size control using these coefficients gives the same result as applying the step size control on an  
7 integration of the (normalized) variational flow.

8 In some cases, for instance when we are computing very high-order derivatives, we do not  
9 require the same level of accuracy for all of them (sometimes, high-order derivatives require less  
10 accuracy than the low order ones). Then, we could use a weighted norm in the step size control.

## 11 4 Power expansion of Poincaré maps

12 Assume that we have a flow defined by a smooth ordinary differential equation defined on an  
13 open subset of  $\mathbb{R}^n$ , and that we are using a suitable Poincaré section to study its flow. To  
14 simplify the discussion, we will consider two separate cases. One when the section is based on a  
15 known time of integration (temporal section) and a second one based on an unknown time but  
16 determined by the crossing on a certain region (spatial section).

17 In what follows,  $\Phi(t; t_0, x^{(0)})$  denotes the solution at time  $t$  of the initial value problem  
18 corresponding to the initial data  $(t_0, x^{(0)})$ .

### 19 4.1 Temporal Poincaré sections

20 This is a common situation when we have a periodically time-dependent ODE with a period,  
21 say,  $T > 0$ . Then, it is usual to define a Poincaré map  $P$  as the time  $T$  flow of the ODE, that  
22 is,  $P(x) = \Phi(T; 0, x)$ . Periodic orbits of period  $T$  appear as fixed points of  $P$ ,  $P(x^*) = x^*$ .  
23 The linear stability of the periodic orbit follows from the monodromy matrix  $D_x P(x^*)$ , but to  
24 study nonlinear aspects of the dynamics higher order terms are needed. A typical example is  
25 the analysis of bifurcations ([Kuz04]).

26 The power expansion (up to order  $m$ ) of  $P$  at a given point  $x^{(0)} \in \mathbb{R}^n$  can be obtained  
27 by evaluating  $P$  on  $x^{(0)} + s$ , using a jet arithmetic of order  $m$  for the  $n$ -dimensional vector of  
28 symbols  $s$ .

### 29 4.2 Spatial Poincaré sections

30 To simplify the discussion, we focus on an autonomous ODE in  $\mathbb{R}^n$ . This is in fact the usual  
31 situation in which spatial sections are used. Let us assume (also for simplicity) that the Poincaré  
32 section  $\Sigma$  is defined by a plane in general position. Let  $x^{(0)}$  be a point on the plane  $\Sigma$ , and  
33 let us denote by  $\vec{n}$  the normal vector to this plane. We assume that, after some integration  
34 time  $T(x^{(0)})$ , depending on the initial point, the trajectory comes back to the section, i.e.  
35  $\Phi(T(x^{(0)}); 0, x^{(0)}) \in \Sigma$ . To produce the expansion, we have to define coordinates on the plane.  
36 Without loss of generality, let us choose  $x^{(0)}$  as the origin of coordinates, and let us choose  
37 suitable linearly independent unitary vectors  $v_1, \dots, v_{n-1}$  such that  $x^{(0)} + v_1 s_1 + \dots + v_{n-1} s_{n-1}$   
38 is a parametric representation of  $\Sigma$ .

---

<sup>1</sup>By normalized variational equations we refer to the variational equations divided by the corresponding fac-  
torials so that they are the normalized derivative of the flow.

1 Now we start the integration of the ODE at the point  $x^{(0)} + v_1 s_1 + \dots + v_{n-1} s_{n-1}$  using a  
2 jet arithmetic of order, say,  $m$ , with the symbols  $s = (s_1, \dots, s_{n-1})$ . Note that if we stop the  
3 integration at time  $T(x^{(0)})$  what we obtain is the power expansion of the flow at time  $T(x^{(0)})$   
4 w.r.t. the  $n - 1$  variables that are the coordinates on  $\Sigma$ , but this is not the power expansion  
5 of the Poincaré map  $P: \Sigma \rightarrow \Sigma$  because this expansion does not lay inside  $\Sigma$ . To produce the  
6 power expansion of the Poincaré map up to a given order  $m$ , we stress that the time needed for  
7 an orbit to return to the section  $\Sigma$  depends on the initial point. This means that the return  
8 time also depends on  $s$ , that is, we have to write the return time as a formal series on  $s$ ,

$$T(x^{(0)} + v_1 s_1 + \dots + v_{n-1} s_{n-1}) = T(x^{(0)}) + \sum_{|k|=1}^m \tau_k s^k, \quad (8)$$

9 whose coefficients  $\tau_k$  are real numbers that have to be determined from the condition

$$\Phi(T(x^{(0)} + v_1 s_1 + \dots + v_{n-1} s_{n-1}); 0, x^{(0)} + v_1 s_1 + \dots + v_{n-1} s_{n-1}) \in \Sigma. \quad (9)$$

10 As usual, this condition must hold up to order  $m$  in  $s$ . In other words, we expect that the  
11 distance between the evaluation of the power expansion of the Poincaré map and  $\Sigma$  behaves like  
12  $O_{m+1}(\|s\|)$ . As we will see, the coefficients  $\tau_k$  in (8) can be computed recurrently, degree by  
13 degree. To shorten the following formulas, we denote  $T_0 = T(x^{(0)})$  and

$$\bar{s} = v_1 s_1 + \dots + v_{n-1} s_{n-1}.$$

14 Let us denote  $x^{(1)} = \Phi(T_0; 0, x^{(0)}) \in \Sigma$  and we recall that the ODE is  $\dot{x} = f(x)$ . Let us start by  
15 the degree  $m = 1$ . The flow at time  $t = T_0 + \sum_{|k|=1} \tau_k s^k$  can be written as

$$\begin{aligned} \Phi(T_0 + \sum_{|k|=1} \tau_k s^k; 0, x^{(0)} + \bar{s}) &= \Phi(T_0; 0, x^{(0)} + \bar{s}) + D_t \Phi(T_0; 0, x^{(0)} + \bar{s}) \sum_{|k|=1} \tau_k s^k \\ &= \Phi(T_0; 0, x^{(0)}) + \sum_{|k|=1} a_k s^k + D_t \Phi(T_0; 0, x^{(0)}) \sum_{|k|=1} \tau_k s^k \\ &= x^{(1)} + \sum_{|k|=1} a_k s^k + f(x^{(1)}) \sum_{|k|=1} \tau_k s^k, \end{aligned}$$

16 where the values  $a_k$  come from the first order expansion of  $\Phi(T_0; 0, x^{(0)} + \bar{s})$  w.r.t.  $s$ ,

$$\Phi(T_0; 0, x^{(0)} + \bar{s}) = x^{(1)} + \sum_{|k|=1} a_k s^k.$$

17 Hence, to impose condition (9) at first order (at order 0 is already satisfied) we have to ask that

$$\sum_{|k|=1} \langle a_k + \tau_k f(x^{(1)}), \vec{n} \rangle = 0,$$

18 where  $\langle \cdot, \cdot \rangle$  denotes the standard scalar product. This condition implies that

$$\tau_k = -\frac{\langle a_k, \vec{n} \rangle}{\langle f(x^{(1)}), \vec{n} \rangle}.$$

19 From a geometric point of view, this is equivalent to project the directional derivatives w.r.t.  
20 each component of  $s$  on the Poincaré section, following the flow (see Figure 1).

1 The computation of the higher order terms is more involved. In particular, it requires to  
 2 perform integration steps with step sizes that also depend on  $\bar{s}$ . This introduces a limitation: if,  
 3 for instance, we have to perform the step size  $h = \sum_{|k|=1} \tau_k s^k$  and the numerical integration has  
 4 a local truncation error of  $O(h^p)$ , then the resulting power expansion in  $s$  will have an error of  
 5 the order of  $O(|s|^p)$  and this means that we cannot trust the resulting expansion in  $s$  for orders  
 6 equal and higher than  $p$ . Therefore, we have to limit the degree of these expansions by the order  
 7 of the local truncation error of the numerical integration algorithm. We note that this is not a  
 8 limitation for Taylor methods, since the order can be easily increased to the desired value.

9 Now let us focus in the computation of high-order derivatives, assuming that the order of  
 10 the local error is large enough for the derivatives we want to obtain. We proceed in a recurrent  
 11 way. Assume now that we have computed the values  $\tau_k$  for  $|k| \leq m$ , and we want to compute  
 12 them for  $|k| = m + 1$ :

$$\begin{aligned} & \Phi \left( T(x^{(0)}) + \sum_{|k|=1}^m \tau_k s^k + \sum_{|k|=m+1} \tau_k s^k; 0, x^{(0)} + \bar{s} \right) \\ &= \Phi \left( T(x^{(0)}) + \sum_{|k|=1}^m \tau_k s^k; 0, x^{(0)} + \bar{s} \right) + D_t \Phi \left( T(x^{(0)}) + \sum_{|k|=1}^m \tau_k s^k; 0, x^{(0)} + \bar{s} \right) \sum_{|k|=m+1} \tau_k s^k \\ &= x^{(1)} + \sum_{|k|=1}^{m+1} a_k s^k + f(x^{(1)}) \sum_{|k|=m+1} \tau_k s^k. \end{aligned}$$

13 To obtain the last equality note that, as  $D_t \Phi$  is multiplying  $\sum_{|k|=m+1} \tau_k s^k$  which is already of  
 14 order  $m + 1$ , we have to use the terms of degree 0 of  $D_t \Phi$ , that is,  $D_t \Phi(T(x^{(0)}); 0, x^{(0)})$  which  
 15 is  $f(x^{(1)})$ . Therefore, for  $|k| = m + 1$ , imposing condition (9) leads to the same expression as  
 16 before,

$$\tau_k = -\frac{\langle a_k, \vec{n} \rangle}{\langle f(x^{(1)}), \vec{n} \rangle}.$$

17 Let us summarize how to apply these formulas. We first integrate for a time  $T(x^{(0)})$  such that  
 18 the orbit starting at the initial condition  $x^{(0)}$  lands on the Poincaré section  $\Sigma$ . This integration  
 19 can be done with jet transport so that we obtain  $\Phi(T(x^{(0)}); 0, x^{(0)} + \bar{s})$ . Then, to compute the  
 20 return time (8) such that the power expansion of the flow lays inside  $\Sigma$  up to degree  $m$ , we  
 21 proceed degree by degree in (8): for degree 1, we use first the formulas above to compute the  
 22 numbers  $\tau_k$ , and then we perform a step of numerical integration with step

$$h = \sum_{|k|=1} \tau_k s^k, \quad (10)$$

23 starting at  $\Phi(T(x^{(0)}); 0, x^{(0)} + \bar{s})$  to obtain  $\Phi(T(x^{(0)}) + \sum_{|k|=1} \tau_k s^k; 0, x^{(0)} + \bar{s})$  which is a power  
 24 expansion with its first order terms inside  $\Sigma$ . Next, using the second order terms w.r.t  $s$  in  
 25  $\Phi(T(x^{(0)}) + \sum_{|k|=1} \tau_k s^k; 0, x^{(0)} + \bar{s})$  (the coefficients of these terms are the values  $a_k$  above) we  
 26 compute the values  $\tau_k$  for  $|k| = 2$  and we perform another numerical integration step,

$$h = \sum_{|k|=2} \tau_k s^k, \quad (11)$$

27 starting at  $\Phi(T(x^{(0)}) + \sum_{|k|=1} \tau_k s^k; 0, x^{(0)} + \bar{s})$  to obtain  $\Phi(T(x^{(0)}) + \sum_{|k|=1}^2 \tau_k s^k; 0, x^{(0)} + \bar{s})$  with  
 28 its second order terms inside  $\Sigma$ . This process is continued up to the desired order. Figure 1

1 illustrates these ideas. Another approach is to consider a Newton approach to find the  $\tau_k$  in (8)  
 2 imposing the condition on (9), see [Sim90].

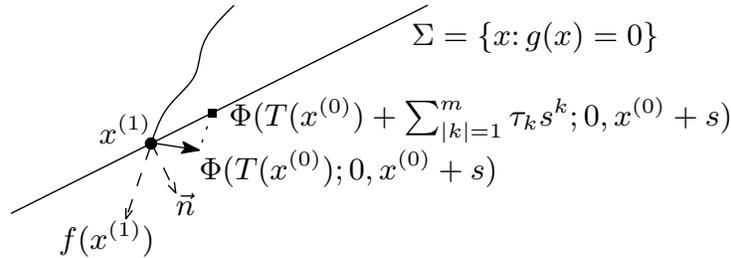


Figure 1: Projection of a directional derivative of the flow on the Poincaré section.

3 It is important to note that, in this procedure, the truncation error of the time stepper can  
 4 affect to the jets. For instance, if we use a time stepper with a local truncation error of the form  
 5  $O(h^{p+1})$ , after a step of the form (10) or (11), the error of the numerical integration contains  
 6 terms of order  $p + 1$  in  $s$  and, therefore, it is impossible to obtain derivatives of the spatial  
 7 Poincaré map of order higher than  $p$ . So, if high order derivatives are wanted, it is better to use  
 8 a numerical integration method like the Taylor method, where it is very easy to obtain a high  
 9 order truncation error.

### 10 4.3 On normal forms

11 One of the applications of the power expansion of a Poincaré map is the computation of normal  
 12 forms. A normal form is a local (and high order) integrable approximation of the dynamics in  
 13 a neighborhood of an invariant object like a fixed point or an invariant curve, and it is useful to  
 14 have accurate information of the nearby dynamics [DJ22]. So, it is possible to use the machinery  
 15 in this paper to compute high order normal forms [GJJC<sup>+</sup>].

## 16 5 The parametrization method

17 The origin of the parametrization method goes back to the 80's when it was used by C. Simó  
 18 (see also [FR81]) for numerical computations. It is remarkable that this method is also excellent  
 19 to prove the existence of invariant manifolds, as shown by X. Cabré, E. Fontich and R. de la  
 20 Llave [CFdLL05]. Here, we are only interested in computing these invariant manifolds from an  
 21 algorithmic point of view. A complete description of the method can be found in the book  
 22 [HCL<sup>+</sup>16].

23 Let  $P$  be a Poincaré map. To discuss the parametrization method for invariant manifolds,  
 24 let us first focus on the case for which the manifold is unstable. The stable one can be computed  
 25 similarly replacing  $P$  by  $P^{-1}$ . In the case that  $P$  is given in terms of a flow map, its inverse is  
 26 obtained integrating the differential equation backwards in time (see [GJNO22] for more details).  
 27 The main idea of the method is to consider that the manifold can be parametrized by a map  
 28  $K$  which we denote as a formal power series. Then  $K$  is plugged into the invariance equation  
 29 involving  $K$ ,  $P$ , and internal dynamics of the manifold. Thus, each term of the formal series can  
 30 be solved order by order. You will note that, as far as the final series is converging, the map  $K$   
 31 will be unique up to a scaling factor. We assume:

- 32 • There exists a fixed point  $z_0$  by the map  $P$ , i.e.  $P(z_0) = z_0$ ,

- 1 • there exists a decomposition  $\mathbb{R}^n = \Lambda_u \oplus \Lambda_c \oplus \Lambda_s$ , where  $\dim(\Lambda_u) = d$  and  $\dim(\Lambda_s) = r$ .  
 2 Here  $\Lambda_u$  is the eigenspace corresponding to the  $d$  unstable eigenvalues  $\lambda_u = (\lambda_1, \dots, \lambda_d)$   
 3 of the matrix  $DP(z_0)$ . Similarly,  $\Lambda_s$  and  $\Lambda_c$  are the eigenspaces related to the unstable  
 4 eigenvalues and the elliptic eigenvalues. For the sake of simplicity, we assume that all these  
 5 eigenvalues are real. The complex eigenvalue case can be handled similarly.

6 Assume that the parametrization, with parameters  $u = (u_1, \dots, u_d)$ , is given by

$$K(u) = \sum_{m \geq 0} A_m, \quad \text{with} \quad A_m = \sum_{|k|=m} a_k u^k, \quad (12)$$

7 where  $k = (k_1, \dots, k_d) \in \mathbb{N}^d$ , is a multi-index,  $|k| = k_1 + \dots + k_d$ ,  $u^k = u_1^{k_1} \dots u_d^{k_d}$ , and  $a_k u^k$  are  
 8 the different monomials of degree  $|k| = m$ . The invariance equation characterizes the invariant  
 9 manifold –parametrized by the map  $K$ – under the dynamics. It is given by

$$P \circ K = K \circ U, \quad U = \text{diag}(\lambda_1, \dots, \lambda_d), \quad (13)$$

10 which we will solve it, order by order, recursively.

11 The zeroth order is set by the coordinates of the fixed point  $z_0$ , i.e.  $A_0 = z_0$ . The next  
 12 order has the form  $A_1 = \sum_{j=1}^d v_j u_j$ , where  $\{v_j\}_{1 \leq j \leq d}$  are the eigenvectors of the matrix  $DP(z_0)$   
 13 corresponding to the eigenvalues  $\{\lambda_j\}$ . This choice verifies the invariance equation at first  
 14 degree order but we have a freedom by scaling the parameters  $u$  leading to an equivalent result.  
 15 Although they are equivalent, a suitable rescaling of the parameters allows to improve the  
 16 numerical behavior of the series, see Section 5.1.

17 To compute the next degree orders, we proceed inductively order by order. Assume we have  
 18 computed the coefficients of  $A_m$  up to degree  $j$ . Then we can write the series at degree  $j+1$  by  
 19  $K_j(u) + A_{j+1}$ , where  $A_{j+1}$  must be determined and

$$K_j(u) = \sum_{m=0}^j A_m, \quad \text{with} \quad A_m = \sum_{|k|=m} a_k u^k.$$

By applying the invariance condition (13), an expression to  $A_{j+1}$  is deduced:

$$\begin{aligned} P(K_j(u) + A_{j+1}) &= P \circ K_j + DP(z_0)A_{j+1} + \mathcal{O}(u^{j+1}) \\ &= K_j \circ U + B_{j+1} + DP(z_0)A_{j+1} + \mathcal{O}(u^{j+1}). \end{aligned}$$

20 Here  $B_{j+1}$  is the Taylor term of order  $j+1$  of  $P(K_j(u))$  which is obtained following the jet  
 21 transport technique described in Section 4. To be more precise, it has the form

$$B_{j+1} = \sum_{|l|=j+1} b_l u^l. \quad (14)$$

22 Neglecting the term  $\mathcal{O}(u^{j+1})$  and imposing that the last equation has to be equal to  $K_{j+1} \circ U$ ,  
 23 we get

$$B_{j+1} + DP(z_0)A_{j+1} = A_{j+1} \circ U.$$

24 Then, for  $l$  such that  $|l| = j+1$  is given by solving the linear systems

$$(DP(z_0) - \lambda_u^l I_n) a_l = -b_l, \quad (15)$$

and then,

$$A_{j+1} = \sum_{|l|=j+1} a_l u^l,$$

1 is the homogeneous polynomial of degree  $j + 1$  we are looking for.

2 Note that from the computational point of view, the step consisting in getting (14) is, by far,  
 3 the most expensive step when the computation of  $P$  requires to integrate an ODE. Also note  
 4 that (15) is assumed to be a solvable linear system for each of the different values of  $l$ . Those  
 5 conditions for which the linear systems have a solution are called non-resonance conditions and,  
 6 in such cases, the manifold admits the locally convergent power series of the form in (12).

7 *Remark 3.* Some modifications are convenient when this method is applied in combination with  
 8 a multiple shooting method, where the map  $P$  is split as the composition of several maps.  
 9 An exhaustive explanation can be found in [GJNO22] in the context of the parametrization of  
 10 invariant manifolds of high-dimensional tori.

## 11 5.1 Scaling factor

12 The parametrization of the invariant manifold is not unique. In particular, if  $K(u)$  is a parametriza-  
 13 tion in (13), then  $K(cu)$  for  $c \neq 0$  is also a parametrization. An effect of  $c$  is to rescale the  
 14 coefficients  $a_k$  in (12) as  $c^k a_k$ . In some situations, to minimize the error propagation, we want  
 15 to avoid the norms of the coefficients to grow or decrease too fast with  $|k|$  [Ric80, FdIL92].

16 If the radius of convergence w.r.t.  $u$  in (12) is known,  $\rho$ , we can use the scaling  $c = \rho$ , which  
 17 scales the radius of convergence to 1 and, hence, gives a mild increasing or decreasing of the  
 18 size of the coefficients. If the radius of convergence is not known, it can be estimated using, for  
 19 instance, a root test. If this estimation of the radius  $\rho_k$  and the scaling is done at each degree  
 20  $k$  of the manifold computation, then the scaling factor at each degree  $k$  is  $\rho_k/\rho_{k-1}$  with  $\rho_1 = 1$ .

21 Note that, one may consider to perform the scaling after the end of the parametrization  
 22 up to a fixed degree, however, to undo and do scaling at each degree is computationally more  
 23 efficient and it helps the integration of the high-order variational flows since the magnitudes  
 24 involved are of similar order.

## 25 5.2 On the choice of the degree

26 A numerical implementation of the explained parametrization method in truncating the formal  
 27 power series (12) up to a certain degree. As the power expansion is computed degree by degree,  
 28 a criterion to select the final degree consists in estimating, for each degree, the validity region  
 29 of the parameter  $u$ . This is the set of values of  $u$  for which the truncated power expression is an  
 30 accurate representation of the manifold. Assume that we know the coefficients up to degree  $m$ ,  
 31 then an estimation of the validity region of the variable  $u$  with tolerance  $\epsilon$  consists in finding a  
 32 real positive number  $s$ , say  $s_m^{\max}$ , such that

$$\sum_{|k|=m} |a_k| s^m < \epsilon, \quad |s| \leq s_m^{\max}. \quad (16)$$

33 Equation (16) is a rough bound of valid parameters  $u$  but it is easily solvable. Indeed, so we  
 34 can take  $s_m^{\max} = (\epsilon / \sum_{|k|=m} |a_k|)^{1/m}$ .

35 To prevent the effect of symmetries (i.e., to deal with the situation when all the coefficients of  
 36 odd or even degree are zero) we can consider the minimum value of  $s^{\max}$  obtained from degrees

1  $m$  and  $m - 1$ . This computation can be done after the calculation of each degree to decide if  
2 this is enough. Hence, a suitable degree choice  $m$  is when, for instance, the gain between and  
3  $s_m^{\max}$  and  $s_{m-2}^{\max}$  has little significance, for example when  $s_m^{\max}/s_{m-2}^{\max}$  is below 1.01 or 1.001.

4 Note that there are, of course, other ways to estimate a validity region of  $u$  but they must  
5 be computationally easy enough to perform it at each new parametrization degree.

### 6 5.3 Globalization

7 The parametrization  $K$  is valid in a neighborhood of the fixed point. To extend the manifold  
8 outside this domain we can use a suitable mesh of points on the fundamental interval, and to  
9 iterate these points (forward for an unstable manifold, backward for a stable one) to extend  
10 the manifold outside this domain. To estimate the error propagation in these iterations we  
11 can accumulate, for each point in the fundamental interval, the products of the norms of the  
12 differential of the map along each orbit to have an estimate of the error growth factor. When  
13 this factor is larger than some prescribed threshold, the globalization should stop. These ideas  
14 can be easily extended to globalize higher dimensional manifolds.

## 15 6 Examples

16 In this section, we provide several examples in which we apply the parameterization method  
17 as explained in Section 5 to compute high order approximation of stable/unstable manifolds.  
18 Those examples are intended to illustrate different situations: In Section 6.1, we globalize the  
19 stable and unstable manifolds related to hyperbolic periodic orbits of the Hénon-Heiles system.  
20 To do so, a suitable spatial Poincaré section is used. In this example, we take advantage of the  
21 high-order approximation to the stable/unstable manifolds to globalize numerically them using  
22 fewer iterates of the map. The numerical integration in this example is done by means of a  
23 Taylor method. Its variable order allows to compute easily high order derivatives of the Poincaré  
24 map, see Section 4.2.

25 As example, in Section 6.2, we consider a pendulum with a fast periodic forcing. When the  
26 perturbation is activated, the system ceases to be integrable and the homoclinic connection of  
27 the hyperbolic equilibrium point splits, leading to chaotic behavior of the system. It is well  
28 known that, in this situation, the splitting angle is exponentially small with the size of the  
29 perturbation. This means that, if the angle is to be computed, extended precision is required.  
30 In this example we compare the efficiency between a linear approximation and a high order one  
31 when computing the splitting angle. The numerical integrations are done by means of a Taylor  
32 method.

33 In Section 6.3 we compute high-order approximations of the stable/unstable manifold of  
34 the dynamical equivalent of the triangular point  $L_4$  in the Bicircular Problem. This dynamical  
35 equivalent is a hyperbolic periodic orbit which is mildly unstable. Therefore, to globalize its  
36 stable/unstable manifolds starting from a linear approximation, a large number of iterates to  
37 move away from the periodic orbit is needed. Here we show that the the parameterization  
38 method produces a power expansion of the manifold which is valid in a quite large domain.  
39 In this example, the numerical integration is done by means of a Runge-Kutta-Fehlberg 7(8)  
40 method. As we are using a temporal (stroboscopic) Poincaré section, the order of the Runge-  
41 Kutta does not limit the order of the computed derivatives.

42 Finally, Section 6.4 deals with a system that models the behavior of an electron near an  
43 atomic core and excited by a laser field. Some trajectories, the recolliding orbits, are of especial

1 interest. These orbits get expelled from the ionic core and come back after some laser cycles.  
 2 Some of these recolliding trajectories are driven by a hyperbolic periodic orbit which has two  
 3 unstable directions: One strongly unstable and the other one mildly unstable. Our interest is in  
 4 computing the 2-dimensional unstable manifold. Notice that the fact that the two hyperbolic  
 5 eigenvalues are so different in size, brings numerical difficulties to the computation. Therefore, a  
 6 combination of a high order approximation to the manifold with extended precision arithmetic  
 7 is required.

## 8 6.1 The Hénon-Heiles system

9 The Hénon-Heiles (HH) system is a Hamiltonian model proposed by Michel Hénon and Carl  
 10 Heiles for the motion of massless star under the attraction of an effective potential due to other  
 11 stars in a galaxy. The dynamics of the system, of two degrees of freedom, is determined by the  
 12 Hamiltonian function

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{y^3}{3}.$$

13 The HH system stands out as a classical and simple example of chaotic conservative system. A  
 14 typical approach to study it, is to consider a certain Poincaré map (e.g.  $\{x = 0\}$ ). Then, the  
 15 dynamics can be described by means of a family of Area Preserving Maps (APM) parametrized  
 16 by the energy. When the energy is chosen to be very small, most of the phase space is populated  
 17 by invariant curves carrying quasi-periodic motion. In a typical converse KAM picture, these  
 18 invariant curves get destroyed (according to some arithmetic properties of their rotation number)  
 19 when the value of the energy is increased and the gaps left are occupied by chaotic motion. The  
 20 destruction of the invariant curve is related to the existence of hyperbolic periodic orbits and their  
 21 (stable and unstable) invariant manifolds. These manifolds intersect in a complicated tangle in  
 22 the phase space. The size of the chaotic motion depends on the angle of the intersection, the  
 23 so called splitting angle. In the case of the family of APM coming from the HH Hamiltonian,  
 24 these angles are quite large and can be computed easily by using a standard double precision  
 25 arithmetic.

26 As example, we have computed some periodic orbits and their stable and unstable manifolds.  
 27 We used a Taylor integrator [JZ05] with  $10^{-16}$  integration tolerance and modified to work with  
 28 jet arithmetic, [GJZ22]. The hyperbolic fixed points of the Poincaré map with section  $\{x = 0\}$   
 29 and fixed Hamiltonian level  $H = 0.125$  are reported in Table 1.

	$y$	$p_y$	$\lambda_u$
$q_1$	3.01400650333283e-01	2.99870268931536e-01	3.76068592161369
$q_2$	-1.85405087090801e-01	5.30699126253682e-15	3.76068592161372
$q_3$	3.01400650333287e-01	-2.99870268931531e-01	3.76068592161374

Table 1: Periodic orbits of HH and its unstable eigenvalue  $\lambda_u$ , being the stable one  $1/\lambda_u$ .

30 For each of the points  $q_\ell$  in Table 1, we compute a parametrization of the invariant manifold  
 31 associated to  $\lambda_u$  and also to  $\lambda_s = 1/\lambda_u$  (in this case using the inverse of the Poincaré map)  
 32 up to the degrees reported in Table 2. These degrees were determine following the strategy  
 33 described in Section 5.2. The Table 2 also shows the scalings based on estimating the radius  
 34 of convergence, see Section 5.1, and the validity region of the parametrization with a tolerance  
 35  $10^{-14}$  in (16), see Section 5.2. As we can inference from Figure 2 both quantities converge as  
 36 the degree increase.

	degree	scaling, $c$	validity region, $s^{\max}$	time (in sec.)
$W^s(q_1)$	66	7.825189525522893e-01	4.776699128424906e-01	10.471215
$W^u(q_1)$	44	2.301773423837667e-01	1.090485567028463e-01	13.105170
$W^s(q_2)$	88	5.097743807635171e-01	3.519317633442122e-01	54.432266
$W^u(q_2)$	88	5.097743807635167e-01	3.519317633442118e-01	54.484148
$W^s(q_3)$	44	2.301773423837770e-01	1.090485567028529e-01	13.105150
$W^u(q_3)$	66	7.825189525522871e-01	4.776699128424852e-01	10.537275

Table 2: Degree, scaling, validity region, and computational time of stable and unstable invariant manifolds for the periodic orbits  $q_\ell$  of HH with Hamiltonian level 0.125.

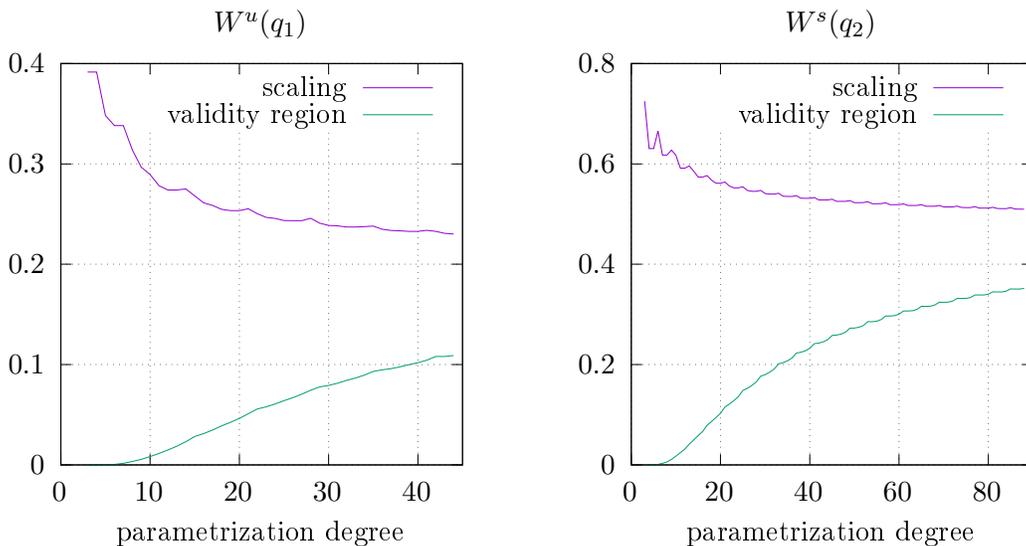


Figure 2: Evolution of the scaling and estimated validity region of the unstable manifold of  $q_1$  and the stable manifold of  $q_2$  in terms of the parametrization degree.

1 Figure 3 shows the image of the validity range by the Poincaré map done by evaluating the  
2 parametrized Taylor expansion for different values of  $s$ . The Figure 3 also shows the globalization  
3 of the invariant manifolds, following Section 5.3, until the iteration threshold of  $10^{12}$  with the  
4 Fröbenius norm. Each of the globalizations took around 40 seconds, and 7 or 8 iterations of the  
5 fundamental interval with  $10^4$  equispaced points in it.

## 6 6.2 Splitting of separatrices of a pendulum

7 Let us consider a model for a rapidly forced pendulum,

$$\begin{aligned} \dot{x} &= y, \\ \dot{y} &= -\sin x + \mu \sin \frac{t}{\varepsilon}. \end{aligned} \tag{17}$$

Here,  $0 < \varepsilon < 1$  and  $\mu$  are small parameters and  $x$  is an angular variable (defined mod  $2\pi$ ) so the phase space is topologically a cylinder. The unperturbed ( $\mu = 0$ ) equation has a simple behavior. It has two equilibrium points; an elliptic one at  $(0, 0)$  and another one at  $(\pm\pi, 0)$  which

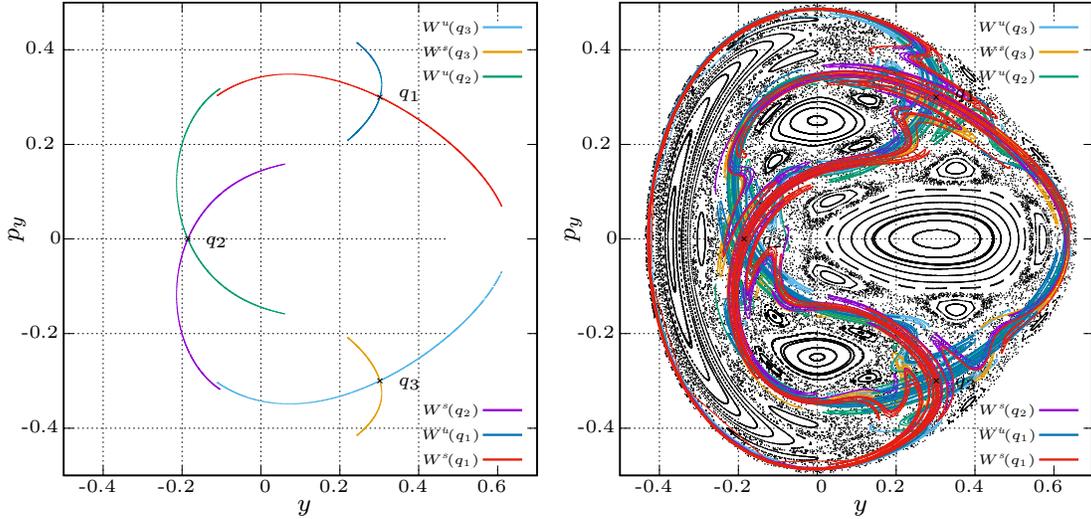


Figure 3: On the left the intervals  $[-s_{max}, s_{max}]$  and on the right globalization of the un/stable manifolds overlapping with background the Poincaré plot with Hamiltonian level 0.125.

is hyperbolic. The remaining trajectories are integral curves (the system is integrable, as it has one degree of freedom). These curves are classified in three types: librational (homotopically trivial), rotational (homotopically non-trivial), and separatrices which separate the libration and the rotational curves. The separatrices correspond to the (un)stable invariant manifold associated to the hyperbolic point. That means that the origin is a homoclinic point. As the system is integrable, the stable and unstable manifold coincide (see Figure 4, left). The two homoclinic orbits can explicitly be parameterized as  $\Gamma_{\pm} = \{(x_0(t), \pm y_0(t))\}$ , where

$$x_0(t) = 2 \arctan(\sinh t),$$

$$y_0(t) = \dot{x}_0(t) = \frac{2}{\cosh t}.$$

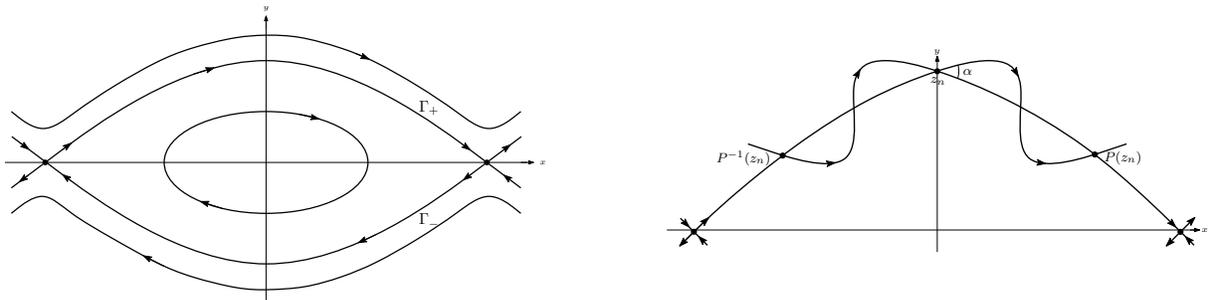


Figure 4: Sketch of the pendulum phase space; in the unperturbed case (left) the (un)stable manifolds coincide while in the perturbed one (right) intersect transversally.

- 1 The situation is different when  $\mu \neq 0$ . First, the system is no longer autonomous but
- 2 periodic time dependent: Henceforth, the phase space dimension increases by one. Moreover the
- 3 equilibrium point no longer exist. Using the Implicit Function Theorem, it can be proved that,

1 for sufficiently small values of  $\mu$ , the equilibria are replaced by periodic orbits of period  $T = 2\pi\varepsilon$   
 2 (these are usually called dynamical equivalents). A suitable tool to cope with periodically time  
 3 dependent systems is the stroboscopic map which is obtained by evaluating the flow at the  
 4 period:  $P(x, y) = \varphi(0, T; x, y)$  and  $\varphi$  stands for the flow of the ODE. Periodic orbits of period  
 5  $T$  are fixed points of  $P$ . Since in this example the system is Hamiltonian, the map will be  
 6 symplectic. Again, if  $\mu$  is small enough, the dynamical equivalent of the origin is a hyperbolic  
 7 fixed point of  $P$  and, therefore, there exist stable/unstable manifolds attached to the fixed point.  
 8 Another consequence of the perturbation is that the system is no longer integrable, therefore  
 9 the manifolds do not coincide, but they intersect infinitely many times, producing a homoclinic  
 10 tangle. Due to the symmetries of the system, these manifolds are forced to intersect at the  
 11 vertical axis (see Figure 4, right). The angle  $\alpha$  in the intersection of the manifolds provides  
 12 insight on the chaotic motion near the separatrices. In particular, if  $\alpha \neq 0$ , the invariant  
 13 manifolds intersect transversely and this leads to regions of chaotic motion. This angle can be  
 14 studied asymptotically as the next result shows:

15 **Theorem 6.1** ([DS92]). *For  $\varepsilon \rightarrow 0$  and  $\mu \rightarrow 0$ , the following asymptotic formula hold.*

$$\alpha = \frac{\pi}{2\varepsilon} \frac{\mu}{\cosh \frac{\pi}{2\varepsilon}} [1 + O(\mu, \varepsilon^2)]. \quad (18)$$

16 In this section we will discuss the numerical computation of this exponentially small in-  
 17 tersection angle, stressing the huge advantages provided by the use of high-order variational  
 18 flow, especially when high accuracy is needed. To this end, we have chosen the MPFR library  
 19 ([FHL<sup>+</sup>07]) that allows the user to select the number of digits and has proven to be efficient and  
 20 reliable. To use it from a C program we have “updated” it to C++ to use the operator overload  
 21 facility of this language to replace the standard double precision of the computer with MPFR.

22 Before starting with the computations, note that the symmetries of the Hamiltonian imply  
 23 that it is enough to compute the angle of intersection  $\alpha^*$  of the manifold with the vertical axis  
 24  $\{x = 0\}$ : the splitting angle is then  $\alpha = 2\alpha^*$  (note that  $\alpha^* = 0$  means that the manifold is  
 25 perpendicular to  $x = 0$ ). So, in what follows, we will compute  $\alpha^*$ . To this end we first compute  
 26 the hyperbolic point by a standard Newton method, then we produce an approximation of  
 27 the manifold and we globalize it till it intersects  $x = 0$ . The goal here is to compare the  
 28 performance of the method when the approximation of the manifold is linear against a high  
 29 order approximation. Independently of the approximation, a way to obtain the splitting angle  
 30 is as follows:

- 31 1. We select a fundamental domain  $J$  of the manifold, close enough to the fixed point so the  
 32 approximation of the manifold is valid with a fixed accuracy.
- 33 2. We compute  $m$  such that  $P^m(J)$  crosses the vertical axis  $\{x = 0\}$ . Notice that the  
 34 fundamental domain  $J$  can be chosen to be far away of the fixed point if the approximation  
 35 of the manifold is of high order and, therefore,  $m$  will be smaller in that case.
- 36 3. We compute the parameter  $s^* \in J$  for which  $P^m(K_u(s^*))$  is on the vertical axis  $\{x = 0\}$   
 37 at a point  $y = y_*$ .
- 38 4. We approximate, by means of numerical differentiation, the tangent vector of the manifold  
 39 at  $(0, y^*)$ .
- 40 5. Using the tangent vector, we compute  $\alpha^*$ .

1 One of the inconveniences one has to overcome with this computation is the accumulation  
2 of error. Indeed, close to the fixed point, the amplification of error can be estimated by means  
3 of the norm of the differential map  $DP^m(K_u(s^*))$ . As the unstable manifold is attracting at  
4 least near the fixed point, it is not difficult to produce a globalization of the manifold. However,  
5 in this case we are interested in computing the crossing point of the unstable manifold and the  
6 vertical axis. This is a little bit more complicated as the numerical error is also expanded along  
7 the stable direction (again, close to the fixed point) so that the error in the evaluation of  $P^m$   
8 is large at it does not allow an accurate computation of  $s^*$  (for instance, if  $\|DP^m(s^*)\| \approx 10^{20}$ ,  
9 then we will loose 20 decimal digits in this computation). Notice also that the amplification  
10 factor grows exponentially with the number of iterates and, therefore, it is advisable to keep it  
11 small.

12 We have tested the algorithm for the case  $\varepsilon = 1/32$  and  $\mu = 1/1024$ . As we have already  
13 discussed, extended accuracy is required for this computation. Hence, have chosen a Taylor  
14 method ([JZ05]) with MPFR arithmetic with mantissa of 65 decimal digits. To compute the  
15 hyperbolic fixed point of  $P$  near  $p_h = (-\pi, 0)$  we request  $P(x, y) - (x, y) = 0$ , using a Newton  
16 method with initial condition  $p_h$ . In Table 3 we display the coordinates of the fixed point, the  
17 unstable eigenvalue, and the related (normalized) eigenvector. We have computed the splitting  
18 for both the linear approximation of the manifold and an approximation of order 32. In  
19 Table 4 we display the results. The splitting angle computed for both cases is approximately  
20  $\alpha^* \approx 1.452038838722046 \times 10^{-23}$ . Notice that, the amplification factor in the case of the linear  
21 approximation is of order  $10^{32}$  and this implies that the linear approximation only allows to  
22 compute the splitting angle with accuracy of about  $10^{-33}$ . This restriction is not present when  
23 using the approximation of order 32 for the manifold.

24 To check the accuracy of each computation, we have ran again the program doubling the  
25 number of digits (that is, using a mantissa of 130 digits) and reduced the precision thresholds  
26 accordingly. Then, comparing the new splitting angle with the ones computed with the linear  
27 approximation and with the approximation of order 32 we see that the disagreement of the  
28 splitting angle for the linear approximation is of order  $10^{-33}$  while for the approximation of  
29 order 32 is of order  $10^{-64}$ . Errors of the same magnitudes are obtained when computing the  
30 crossing point at the vertical axis.

31 Regarding the computation time, there is no penalization in using high order approximation  
32 (of order 32). Using 65 digits, to compute the parameterization up to order 32 takes about 11  
33 seconds. The computation of the splitting using this high order parameterization, takes about 7  
34 seconds. The whole process to compute the splitting is, therefore, about 18 seconds. To compute  
35 the splitting using the linear approximation takes about 29 seconds.

36 The optimal degree to use depends on two factors: The computation time and the accuracy.  
37 Increasing the degree of the expansion increases the accuracy of the computation and also  
38 decreases the computing time of the splitting (once the manifold has already been obtained).  
39 However, the computing time devoted to compute the expansion increases remarkably as the  
40 order gets high. In Table 5 we display several runs of the program but using different orders  
41 and a mantissa of 65 digits. Order 1 corresponds to the linear approximation. The largest order  
42 (78) is the last order in which we obtain a significant increase on the radius of convergence  
43 (about 1%). The first column of Table 5 displays the order, the second column shows the time  
44 (in seconds) needed to compute the expansion of the manifold. In the third column shows the  
45 number of necessary iterates to cut the vertical axis in the computation of the splitting. This  
46 number is critical in both, accuracy and computing time. The fourth column displays the order  
47 of the amplification factor (**OAF**). The amplification factor is of order  $10^{OAF}$ . **OAF** provides

$x = -3.141592653589793238462643383279502884197169399375105820974945$
$y = -0.000030487804878048783487416419772730619101256927786545793950$
$\lambda = 1.216952205507613179976602185887735099160276249406737110608447$
$v_x = 0.707106781186587601240472487505335676116978201269367497887892$
$v_y = 0.707106781186507447561216234432918941136429806290507412844980$

Table 3: Hyperbolic fixed point  $(x, y)$ , its unstable eigenvalue  $\lambda$ , and its eigenvector  $v = (v_x, v_y)$ , with 60 digits.

<b>Linear approximation</b>	
Iterates	384
Amplif.	$2.0734198e+32$
Angle	$1.452038838722045922104153702944869222939807020304351191883856457e-23$
<b>High order approximation</b>	
Iterates	24
Amplif.	111.31778
Angle	$1.4520388383695661627181826237829704096625629214575036852867618694e-23$

Table 4: Number of iterates to cut the vertical axis, amplification factor and splitting angle. Top: Linear approximation. Bottom: Approximation of order 32.

1 an estimation of the digits lost due to the amplification factor. The fifth column displays the  
2 necessary time (in seconds) to compute the splitting (once the expansion is already obtained)  
3 and the sixth column displays the total time (in seconds).

4 The main takeaway of Table 5 is that we can avoid the propagation of errors due to the  
5 amplification factor if we go to order 78. Nevertheless, the computation time is exceeds the  
6 computation time using the linear approximation (149 seconds vs. 29 seconds). Going up to  
7 order 50 takes about 44 seconds to obtain the splitting losing just one digit. The best results  
8 (counting accuracy and computation time) are obtained for orders 16 and 20 (In both cases  
9 take about 13 seconds to compute the splitting losing 3 digits). Going up to order 32 provides  
10 better accuracy (losing 2 digits) for 18 seconds of computing time. Finally, going to order 8 and  
11 12 takes about 22 and 17 seconds respectively but more digits are lost (7 and 5). Most of the  
12 computing time for these two cases is spent in computing the splitting, as the expansions take  
13 less than a second. Notice the dramatic gain in accuracy from going to linear approximation  
14 (losing 32 digits) to order 8.

### 15 6.3 The unstable manifold of $L_4$ in the Bicircular Problem

16 In celestial mechanics, the (Earth-Moon) Bicircular Problem (BCP) is a common problem which  
17 comes from a restricted version of the Four Body Problem [Hua60, CRR64]. In suitable coordi-  
18 nates, this model is a perturbation of the well known Restricted Three Body Problem (RTBP),  
19 see [Sze67]. The Earth-Moon BCP assumes that the Sun and the Earth-Moon barycentre move  
20 along a circular orbit around the center of mass of the Sun-(Earth+Moon) system while Earth  
21 and Moon move as in the RTBP. While written in the standard units and (synodic) coordinates  
22 of the RTBP, the BCP is a periodic time dependent perturbation of the RTBP. The perturbation

Order	TM (s)	It	OAF	TS(s)	Total(s)
1		384	32	29	29
8	<1	84	7	21	<22
12	<1	59	5	16	<17
16	1	45	3	12	13
20	3	37	3	10	13
32	11	24	2	7	18
50	40	16	1	4	44
78	146	11	0	3	149

Table 5: Metrics for the computation of the splitting using different orders and a mantissa of 65 digits. The columns display the order, the time in seconds to compute the expansion of the manifold (**TM(s)**), the number of iterates to compute the splitting (**It**), the order of the amplification factor (**OAF**), the time in seconds to compute the splitting with the manifold already expanded (**TS(s)**) and the total time in seconds respectively.

1 preserves the Hamiltonian structure of the RTBP and its Hamiltonian function is

$$H_{BCP} = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) + yp_x - xp_y - \frac{1-\mu}{r_{PE}} - \frac{\mu}{r_{PM}} - \frac{m_S}{r_{PS}} - \frac{m_S}{a_S^2}(y \sin \theta - x \cos \theta). \quad (19)$$

2 where  $m_S$  is the mass of Sun,  $a_S$  the semi-major axis of Sun,  $r_{PE}^2 = (x - \mu)^2 + y^2 + z^2$ ,  
3  $r_{PM}^2 = (x - \mu + 1)^2 + y^2 + z^2$ ,  $r_{PS}^2 = (x - x_S)^2 + (y - y_S)^2 + z^2$ ,  $x_S = a_S \cos \theta$ ,  $y_S = -a_S \sin \theta$ ,  
4  $\theta = \omega_S t$  and  $\omega_S$  is the mean angular velocity of Sun in the synodic coordinates.

$\mu$	0.012150581623433623
$m_S$	328900.55
$a_S$	388.81114302335106
$\omega_S$	0.92519598551829646

Table 6: Values of the parameters for the BCP used in this work.

5 In the BCP the Lagrangian points are no longer equilibria, they are replaced by periodic  
6 orbits with the same period as the perturbation:  $T_S = 2\pi/\omega_S$ . In particular, the triangular  
7 point  $L_4$  is replaced by three periodic orbits of period  $T_S$ , see [SGJM95, CJ00, JCFJ18]. One  
8 of these orbits is slightly unstable, of linear type saddle×center×center. This unstable periodic  
9 orbit is seen as an hyperbolic fixed point of the stroboscopic map (the map obtained evaluating  
10 the flow at the period  $T_S$ ) has an unstable eigenvalue close to 1.098. Notice that this instability  
11 is remarkably mild, that is, an initial condition on the manifold near to the fixed point needs  
12 a large number of iterates to get far from it. Therefore, to grow numerically the manifold  
13 from the linear approximation is numerically expensive. We can, however, produce a high-order  
14 approximation of the manifolds and produce large pieces of the manifolds that can be mapped  
15 a few times to get even larger pieces of the manifold, see Figure 5.

16 Let us give some details on how Figure 5 is produced: First, we modify the well-known  
17 Runge-Kutta-Fehlberg 7(8) method [Feh68] to work with a jet arithmetic. Then we apply the  
18 parametrization method to obtain, order by order, a Taylor expansion of the manifolds. At each

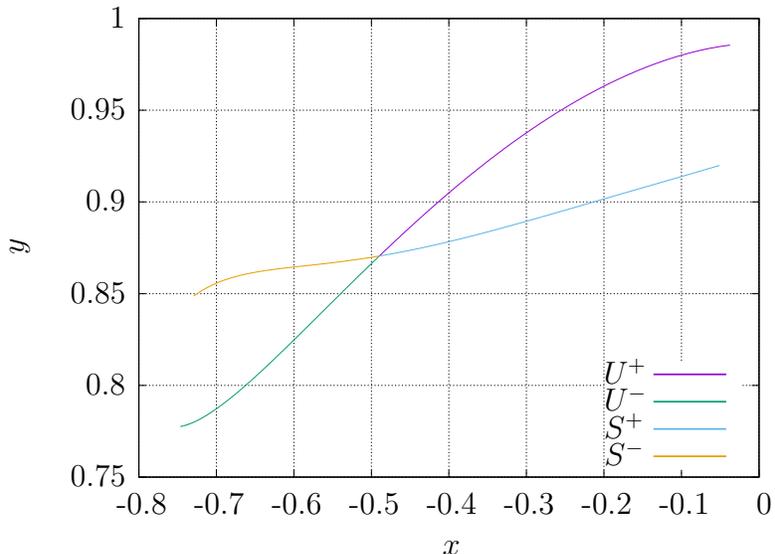


Figure 5: High-order approximations of the stable ( $S^+$ ,  $S^-$ ) and unstable ( $U^+$ ,  $U^-$ ) manifolds attached to the dynamical equivalent of  $L_4$  in the Earth-Moon BCP.

1 step, after we compute the coefficient of order  $k$ , we use the root criterion to estimate the radius  
2 of convergence. Obviously, this radius is increased at each step. When the gain of the radius of  
3 convergence is less than 1%, we stop the computation. We denote by  $U^+$  and  $U^-$  the two pieces  
4 of the unstable manifold, using the above-mentioned criterion, these manifolds are expanded up  
5 to order 54. On the other hand, the stable pieces, denoted by  $S^+$  and  $S^-$ , are expanded up to  
6 order 46. Then, all those Taylor expansions are evaluated to obtain the curves in Figure 5.

#### 7 6.4 A two-dimensional invariant manifold related to recolliding electrons

8 In this example, we consider the motion of an electron in an atom that is perturbed by a strong  
9 linearly polarized laser field. When the electron is “impacted” by the laser with sufficient energy,  
10 it gets expelled out from the atomic core. An interesting question is whether the electron is re-  
11 captured by the atom following the Coulomb’s laws. This phenomenon is known as recollision.  
12 Recollision physics is an emerging field, highly related to collision physics and optics, see [Cor93,  
13 Cor14] and it has been tackled from the dynamical systems perspective, see [MCU10, MKCU12,  
14 KCUM14, KMCU14, NCUW15, MKCU12] and references therein.

15 Most of these references, consider the case in which the electron is allowed to move in a  
16 line (i.e. the configuration space has dimension one). Here, we consider the two-dimensional  
17 configuration space case. It can be modeled as a Hamiltonian system with two degrees of freedom  
18 and periodic time dependence written as follows:

$$H = \frac{1}{2}(p_x^2 + p_y^2) - \frac{1}{\sqrt{x^2 + y^2 + 1}} + E_c x \cos(\omega t), \quad (20)$$

19 where  $\omega = 0.0584$  is the frequency of the laser,  $E_c = 0.1$  its amplitude. We notice that this  
20 Hamiltonian function has three terms: The kinetic energy, the potential energy and the laser  
21 interaction. In a neighborhood of the atom core, the laser acts as a periodic perturbation.

1 As usual, this problem is better faced by means of the stroboscopic map which, we recall, is  
 2 given by the flow of system (20) evaluated at the period  $2\pi/\omega$ .

3 The dynamical mechanism that guide most of the recolliding orbits is well understood when  
 4 the electrons move in a one dimensional space, that is, the dynamics restricted to the invariant  
 5 subspace  $\{y = 0, p_y = 0\}$  of system (20). The stable and unstable manifolds of some key  
 6 hyperbolic fixed point drive these trajectories to recollide many times, see [KCUM14]. Notice  
 7 that a fixed point of the stroboscopic map corresponds to a periodic orbit of period  $2\pi/\omega$ .

8 In the two dimensional configuration space, this fixed point does not drive recollisions outside  
 9 the invariant subspace  $\{y = 0, p_y = 0\}$ , see [DJCJC22]. The reason is that its normal behavior is  
 10 of type saddle $\times$ saddle. Therefore, the stable and unstable manifolds attached to the fixed point  
 11 are two-dimensional while the phase space is four-dimensional. This means that the invariant  
 12 manifold do not separate the phase space as in the one-dimensional case.

13 The hyperbolic fixed point studied in [KCUM14], is located near  $x = 30.5$ ,  $y = p_x = p_y = 0$ .  
 14 This orbit is easily refined by using a Newton method. The eigenvalues of the Jacobian matrix  
 of the stroboscopic map are displayed in Table 7.

$\lambda_1$	1.0598923797401292e+03
$\lambda_2$	2.1924563502992269e+00
$\lambda_3$	4.5610942259513210e-01
$\lambda_4$	9.4349201788190840e-04

Table 7: Eigenvalues related to the fixed point of the stroboscopic map.

15  
 16 There is a weak unstable direction and also a strong one. The weak direction is related to the  
 17  $1D$  manifold that appears in a model with one degree of freedom and that it is responsible for  
 18 the recollisions there [KCUM14]. The strongly unstable direction is consequence of adding the  
 19 direction which is transversal to the polarization laser. Henceforth, the dynamics near the fixed  
 20 point of the stroboscopic map is governed by the strongly unstable direction. The influence of  
 21 the strong unstable eigendirection makes most of the orbits close to the fixed point get expelled  
 22 away from the core and do not return back in a few laser cycles. However, it could be possible to  
 23 find thin strips close to the weak invariant subspace with a lot of recolliding trajectories. Still,  
 24 it is numerically challenging to compute these  $2D$  unstable and stable manifolds and, specially,  
 25 to globalize the weak  $1D$  manifold.

26 Let  $\Lambda_1$  and  $\Lambda_2$  be intervals containing the origin, let  $W : \Lambda_1 \times \Lambda_2 \rightarrow \mathbb{R}^4$  be a parametrization of  
 27 the  $2D$  unstable invariant manifold related to the fixed point, and let  $P$  be the stroboscopic map  
 28 associated to (20). The parametrization of the unstable manifold  $W$  must verify the following  
 29 invariance equation,

$$P(W(s_1, s_2)) = W(\lambda_1 s_1, \lambda_2 s_2).$$

30 Computing this  $2D$  manifold (using double precision) using the parametrization method up to  
 31 order 8 takes 0.5s. Using MPFR with a mantissa of 128 bits (39 decimal digits) it takes 1  
 32 minutes and 19 seconds. Computing up to order 16 requires 15 minutes and 26 seconds. To  
 33 compute it up to order 30 using a mantissa of 192 bits (around 57 decimal digits) takes 8 hours  
 34 and 50 minutes. Similarly to the  $1D$  case, we use these different approximations to estimate the  
 35 error on the coefficients of the expansion. Figure 6 plots the manifold. The computation stops  
 36 at order 17, when the gain in  $\min(s_1^{\max}, s_2^{\max})$  is less than 1.1.

37 Let us now discuss the globalization of the  $1D$  weak unstable manifold (the one related to the

1 eigenvalue  $\lambda \approx 2.1924563502992269$ ). To start the discussion, assume that we have an approxi-  
 2 mation to the weak unstable manifold and that  $p_0$  is a point provided by this approximation so  
 3 we assume it is very close to the true manifold, that is,  $p_0 + \delta$  is exactly on the manifold and  $\|\delta\|$  is  
 4 very small. When the map  $P$  is applied to the point  $p_0$ , the error  $\delta$  is multiplied, approximately,  
 5 by  $\lambda_1 \approx 1059$  at each iteration so that the distance to the weak manifold grows extremely fast.  
 6 Therefore, it is very convenient to combine a high degree expansion of the manifold (to start  
 7 the globalization as far as possible from the hyperbolic point) with extended precision. In this  
 8 situation, it is convenient to accumulate the product of the norms to have an estimate of the  
 9 growth of the error along the process.

10 In Table 8, we display an example of the error propagation when globalizing the weak  
 11 unstable manifold. We select a point on a power expansion of that manifold (computed up to  
 12 degree 30 with an arithmetic of 60 decimal digits) for the value of the parameter  $s = 1$ . The first  
 13 row shows an error estimate of that point (obtained as the size of the contribution of the terms  
 14 order 30 to the manifold) and the distance to the fixed point. Next rows refer to the iterations  
 15 of this initial point by the Poincaré map. The second column shows accumulated product of  
 16 the norms of the differential of the stroboscopic map at each point with the initial error, and  
 17 the third one the distance to the fixed point. It is clear that, at the beginning, we have a factor  
 18 growth around  $10^3$  due to the most unstable eigenvalue. From the table it can be read that, the  
 19 instability caused by the strongly unstable manifold decreases as the electron move away from  
 20 the fixed point. This simplifies the approximation of the manifold up to long distances.

iter	error	distance
0	7.996832e-46	1.001406e+00
1	8.466197e-43	2.199796e+00
2	8.928646e-40	4.848533e+00
3	9.240140e-37	1.081419e+01
4	8.411957e-34	2.553592e+01
5	2.083436e-32	1.745048e+01
6	1.966030e-29	1.976583e+01
7	1.310301e-27	7.533221e+01
8	1.615796e-27	1.267686e+02
9	1.771004e-27	1.773365e+02
10	1.873796e-27	2.275002e+02

Table 8: Estimated error for the first 10 iterations for a point in the weak unstable manifold. The third column displays the distance to the fixed point.

21 This experiment also shows that the propagation of error tends, in some cases, to soften at  
 22 some distance of the periodic orbit. This example shows the feasibility of the computation of  
 23 2D stable/unstable invariant manifolds and their globalization, despite of having very different  
 24 eigenvalues. The method is based on using a high-order approximation of a parametrization of  
 25 the 2D unstable manifold combined with extended precision arithmetic.

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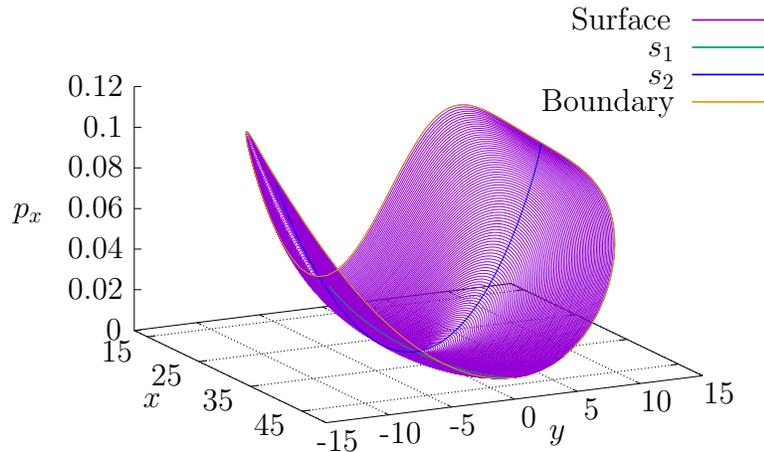


Figure 6: The 2D manifold from the expansion obtained in the parametrization method.

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