C^1 -Lohner algorithm

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Abstract

We present a modification of the Lohner algorithm for the computation of rigorous bounds for solutions of ordinary differential equations together with partial derivatives with respect to initial conditions. The modified algorithm requires essentially the same computational effort as the original one. We applied the algorithm to show an existence of several periodic orbits for Rössler equations and the 14-dimensional Galerkin projection of the Kuramoto-Sivashinsky PDE.

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1 Introduction

In recent years we witness a growing number of computer assisted proofs in the dynamics of ODE's, where the computer is used to check rigorously assumptions of abstract theorems from the dynamical systems theory (see for example [AZ, GZ, HZHT, MM, T, RNS]). For all these proofs rigorous bounds for an appropriate Poincaré map were obtained with a computer assistance.

The goal of this paper is to present a modification of the Lohner algorithm [Lo, Lo1], which for a given autonomous ordinary differential equation

$$\frac{dx}{dt} = f(x), \quad x \in \mathbb{R}^n, \quad f \in C^{\infty}$$
 (1)

and a section Θ , computes rigorously the Poincaré map $P(x_0)$ and $\frac{\partial P}{\partial x}(x_0)$, where $x_0 \in \Theta$.

For this end we need to solve a system of ODE's consisting of equation (1) and the variational equation corresponding to it

$$\frac{dV}{dt}(t,x_0) = \frac{\partial f}{\partial x}(x(t)) \cdot V(t,x_0), \quad V \in \mathbb{R}^{n \times n}$$
(2)

with an initial condition $V(0, x_0) = \text{Id}$, where by Id we denote the identity matrix.

Once we have rigorous bounds for a trajectory of equations (1) and (2) we need to consider its intersection with Θ to obtain P and its derivatives.

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By $\varphi(t, x_0)$ we will denote a solution at the time t of (1) with an initial condition $x(0) = x_0$. It is obvious from equations (1-2) that $V(t, x_0) = \frac{\partial \varphi}{\partial x}(t, x_0)$.

By a C^0 -algorithm we refer to a procedure which gives rigorous estimates for $\varphi(t,x)$ (or the Poincaré map P(x)). By a C^1 -algorithm we mean a rigorous procedure for the computation of $\varphi(t,x)$ and $\frac{\partial \varphi(t,x)}{\partial x}$ (or P(x) and $\frac{\partial P}{\partial x}$). Examples of C^0 -algorithms: algorithms based on the logarithmic norms

Examples of C^0 -algorithms: algorithms based on the logarithmic norms (used in [MM, GZ]), the Lohner algorithm [Lo] or the Hermite-Oberschkoff method proposed by Nedialkov and Jackson (see [NJ] for much more complete list).

One can perform a C^1 -computation just by a direct application a C^0 -algorithm to the problem consisting of equations (1) and (2). This approach totally ignores the structure of the system (1-2) and usually leads to a very poor performance and long computation times (see section 6 for more comments). In this paper we present a modification of the Lohner algorithm, which allows to perform the C^1 -computations essentially in the same time as the one required for the C^0 -algorithm.

The reader should be aware that the basic problem with rigorous computations of solutions of equation (1) is our inability to obtain good rigorous bounds on the difference between two nearby solutions (we will refer to it as the Lipschitz part of error). A part of this inability is due to the very nature of the interval computations – a phenomenon called the wrapping effect, which is discussed in virtually every paper in the field of rigorous computations for ODE's (see [NJ] and references given there). This is the reason for the apparent complexity of the Lohner-type algorithms – the original Lohner algorithm, the Hermite-Obreschkoff method [NJ] or the algorithm presented here, because an essential part of these algorithms is devoted to controlling the Lipschitz part of error to avoid or rather to suppress the wrapping effect. This complexity results in the slowness of these algorithms compared to the ones based on logarithmic norms or the direct interval evaluation, when we consider the time needed to compute one initial condition. But the bounds for the Lipschitz part of error obtained using this approach are so poor, that it turns out that the Lohner-type algorithms are much faster in the task of computing the image of Poincaré map of a cube with a desired accuracy.

There also exists another way to control effectively the Lipschitz part of error. We call it a division method. It was used in [MM, T, T1]. To explain the main idea let us consider the computation of P([x]), where [x] is a box in \mathbb{R}^n and P is a Poincaré map. As we compute $\varphi(t, [x])$ along the trajectory the obtained image (denoted here by $\langle \varphi(t, [x]) \rangle$) becomes soon considerably bigger than the true image $\varphi(t, [x])$ and usually starts to grow exponentially at much faster rate than the intrinsic growth rate from the ODE under consideration. To deal with this problem we divide at some moment t the current value of $\langle \varphi(t, [x]) \rangle$ into smaller pieces and we continue evolve them separately. The division procedure can be applied many times until we reach the Poincaré section. It turns out that the small pieces will move away one from another at the rate given by the ODE and since they are smaller their growth rate due to the numerics will be

usually smaller than that for the undivided set, hence resulting in much better bounds. In the result we allow the intrinsic dynamics of ODE to take part in the control of the Lipschitz part of error, but this happens at the cost of managing the division process and the computation of a larger number of initial value problems.

One can expect that the optimal algorithm will be a combination of both the Lohner-type approach and the division method, but how to link them in the most efficient way will probably depend on the particular ODE under consideration.

Sections 2 and 3 contain a detailed description of the proposed C^1 -Lohner algorithm. In section 6 we discuss briefly the relative cost of the C^0 -Lohner and the C^1 -Lohner algorithms, we also address there the issue of a direct computation of solutions of equations (1-2) using the C^0 -Lohner algorithm. Section 5 we describe how we extract P(x) and $\frac{\partial P}{\partial x}$ from rigorous estimates for $\varphi(t,x)$ and $\frac{\partial \varphi(t,x)}{\partial x}$.

In section 7 we report on two applications of the proposed algorithm to obtain proofs of an existence of single periodic orbits for the Rössler equation and the 14-dimensional Galerkin projection of the Kuramoto-Sivashinsky equations. The algorithm described here was also successfully applied to the Henon-Heiles hamiltonian (see [AZ2]) and to the planar restricted circular three body problem (see [WZ]) to obtain an infinite number of geometrically distinct homoand heteroclinic orbits to some periodic orbits.

The Appendix contains the formulas we used to generate the Taylor expansion for the applications described in section 7.

2 C^1 -Lohner algorithm

The goal of this section is to present the C^1 -Lohner algorithm for ODEs. In fact we give a description of three algorithms: the original Lohner algorithm (C^0 -computation) and two C^1 -algorithms called C^1_1 - and C^1_2 -algorithm.

We want to solve the system consisting of equations (1) and (2) with the following initial conditions

$$x(0) \in [x_0] \subset \mathbb{R}^n, \quad V(0, [x_0]) = Id \tag{3}$$

2.1 Notation

In the sequel, by arabic letters we denote single valued objects like vectors, real numbers, matrices. Quite often in this paper we will use square brackets, for example [r], to denote sets. Usually this will be some set constructed in the algorithm. Sets will be also denoted by single letters, for example S, when it is clear from the context that it represents a set. In situations when we want to stress (for example in the detailed description of algorithm) that we have a set in a formula involving both single-valued objects and sets together we will rather use square bracket, hence we prefer to write S instead of S to represent a set. From this point of view S and S are different symbols in the alphabet

used to name variables and formally speaking there is no relation between the set represented by [S] and the object represented by S. Quite often in the description of the algorithm we will have a situation that both variables [S]and S are used simultaneously, then usually $S \in [S]$, but this is always stated explicitly.

For a set [S] by $[S]_I$ we denote the interval hull of [S], i.e. the smallest product of intervals containing [S]. The symbol $\operatorname{hull}(x_1,\ldots,x_k)$ will denote the interval hull of intervals x_1, \ldots, x_k . For any interval set $[S] = [S]_I$ by m([S]) we will denote a center point of $[S]_I$. For any interval [a,b] we define a diameter by diam([a,b]) = b-a. For an interval vector or an interval matrix $[S] = [S]_I$ by diam ([S]) we will denote the maximum of diameters of its components. For an interval $[x^-, x^+]$ we set $right([x^-, x^+]) = x^+$ and $left([x^-, x^+]) = x^-$. For a set $X \subset \mathbb{R}^d$ by int X we denote an interior of X.

Taylor coefficients for $x(t,x_0)$ and $V(t,x_0)$ 2.2

Let $\Phi(h,x,p)$ denotes the Taylor method of order p for equation (1). For a description of a procedure for generation of Φ for an arbitrary order for a wide class of functions the reader is referred to [Mo, Ra]. The basic idea of this procedure can be explained as follows. Let us set $x(t, x_0) = \varphi(t, x_0)$. By differentiation with respect to t of (1) and (2) we obtain

$$\frac{d^2}{dt^2}x(t,x_0) = \frac{d}{dt}f(x(t,x_0)) = df(x(t,x_0)) \cdot f(x(t,x_0))$$

$$\frac{d^2}{dt^2}V(t,x_0) = \frac{d}{dt}\left(df(x(t,x_0)) \cdot V(t,x_0)\right) =$$

$$df^2(x(t,x_0))(f(x(t,x_0),f(x(t,x_0)) + df(x(t,x_0)) \cdot df(x(t,x_0)) \cdot V(t,x_0)).$$

We see that the second derivatives with respect to t of $x(t, x_0)$ and $V(t, x_0)$ are functions of $x(t,x_0)$ and $V(t,x_0)$, only. Hence there exists functions $a_1: \mathbb{R}^n \to \mathbb{R}^n$ and $b_1: \mathbb{R}^n \times \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$ such that

$$\frac{d^2}{dt^2}x(t,x_0) = \frac{d}{dt}f(x(t,x_0)) = a_1(x(t,x_0))$$
 (4)

$$\frac{d^2}{dt^2}V(t,x_0) = \frac{d}{dt}\left(df(x(t,x_0)) \cdot V(t,x_0)\right) = b_1(x(t,x_0),V(t,x_0)) \tag{5}$$

An easy induction shows that in general for $i \geq 2$ we have

$$\frac{d^{i}}{dt^{i}}x(t,x_{0}) = \frac{d^{i-1}}{dt^{i-1}}f(x(t,x_{0})) = a_{i-1}(x(t,x_{0}))$$
 (6)

$$\frac{d^{i}}{dt^{i}}V(t,x_{0}) = \frac{d^{i-1}}{dt^{i-1}}\left(df(x(t,x_{0}))\cdot V(t,x_{0})\right) = b_{i-1}(x(t,x_{0}),V(t,x_{0}))\tag{7}$$

for some functions $a_i: \mathbb{R}^n \to \mathbb{R}^n$ and $b_i: \mathbb{R}^n \times \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$. In the sequel we will use the following notation

$$\frac{d^i}{dt^i}f = a_i \tag{8}$$

$$\frac{d^i}{dt^i} \left(\frac{\partial f}{\partial x} V \right) = b_i \tag{9}$$

In this notation the symbols $\frac{d^i}{dt^i}f$ and $\frac{d^i}{dt^i}\left(\frac{\partial f}{\partial x}V\right)$ are the functions of x and V. Explicit formulae for Taylor coefficients for polynomials of degree 2 are given in the Appendix.

2.3 An outline of algorithms

Before we present the Lohner algorithm and our C^1 -modification of it we would like to stress the main points in the Lohner original algorithm [Lo]

- Even to perform C^0 -computations one needs some kind of a C^1 -data, because a direct evaluation of $\Phi(h, x_0, p)$ using an interval arithmetic leads to the wrapping effect, which allows to integrate equation (1) for a very short time, only.
- The C^1 -information about φ is obtained by computing a partial derivative of an explicitly given $\Phi(h, x, p)$ instead of estimating $\frac{\partial \varphi(h, x)}{\partial x}$.
- The rearrangement computations together with the knowledge of $\frac{\partial \Phi(h,x,p)}{\partial x}$ reduce considerably the wrapping effect.

Obviously to have a rigorous procedure one needs also to take care of the errors introduced by the finite computer arithmetic (round-off errors) and the discretization error of the numerical method used (the Taylor method in the Lohner algorithm). The round-off errors are taken care of by the interval arithmetic (see [Lo, MZ] and references given there).

The basic idea of modification of an original Lohner algorithm, which leads to a C^1 -Lohner algorithm presented here, is the realization that $\frac{\partial \Phi(h,x,p)}{\partial x}$ is also a Taylor expansion for $\frac{\partial \varphi(h,x)}{\partial x}$, hence with a little additional computational effort we can turn a C^0 -algorithm into a C^1 -algorithm. More precisely we have the following

Lemma 1 Consider the problem (1,2,3). Let h > 0. Assume that $[W_1] \subset \mathbb{R}^n$ is a compact and convex set such that

$$\varphi([0,h],[x_0]) \subset [W_1] \tag{10}$$

and $[W_3] \subset \mathbb{R}^{n \times n}$ is a compact and convex set, such that

$$V([0,h],[x_0]) \subset [W_3]. \tag{11}$$

Then

- $\frac{\partial \varphi}{\partial x}(t,x) = V(t,x)$ for $t \in [0,h]$ and $x \in [x_0]$
- $V(h,[x_0]) \subset \frac{\partial \Phi(h,[x_0],p)}{\partial x} + \frac{h^{p+1}}{(p+1)!} \left(\frac{d^p}{dt^p} \left(\frac{\partial f}{\partial x}V\right)([W_1],Id)\right) \cdot [W_3]$

Let us remind the reader (see section 2.2), that the symbol $\frac{d^p}{dt^p} \left(\frac{\partial f}{\partial x} V \right)$ is a function of x and V, hence it makes sense to plug-in $[W_1]$ for x and Id for V. **Proof:** The first assertion is obvious.

To prove second one we show that it is a Taylor expansion for V of order p plus a remainder term.

Observe that by the definition of Φ it follows that

$$\Phi(h, x, p) = \sum_{i=0}^{p} \frac{\partial^{i} \varphi(0, x)}{\partial t^{i}} \frac{h^{i}}{i!}$$
(12)

We differentiate the above formula with respect to x to obtain

$$\frac{\partial \Phi(h, x, p)}{\partial x} = \sum_{i=0}^{p} \frac{\partial^{i}}{\partial t^{i}} \frac{\partial \varphi(0, x)}{\partial x} \frac{h^{i}}{i!} = \sum_{i=0}^{p} \frac{d^{i}}{dt^{i}} V(0, x) \frac{h^{i}}{i!}. \tag{13}$$

It remains to compute an enclosure for the remainder term $[R] \subset \mathbb{R}^{n \times n}$ given by

$$[R]_{ij} = \frac{h^{p+1}}{(p+1)!} \frac{d^{p+1}}{dt^{p+1}} V_{ij}(\theta_{ij}h, x)$$
(14)

for i, j = 1, ..., n and $x \in [x_0]$, where $\theta_{ij} \in [0, 1]$ depends on x.

We will derive a different expression for the remainder term. Observe that for $t,s\geq 0$ we have

$$V(t+s,x) = V(s,\varphi(t,x)) \cdot V(t,x). \tag{15}$$

Hence after taking m derivatives with respect to s we obtain for s=0 the following identity

$$\frac{d^m}{dt^m}V(t,x) = \left(\frac{d^m}{dt^m}V(0,\varphi(t,x))\right) \cdot V(t,x). \tag{16}$$

Hence for m = p + 1, taking into account that $\varphi(\theta_{ij}h, x) \subset [W_1]$, $V(t, x) \subset [W_3]$ for $x \in [x_0]$, and equations (7) and (9) we obtain

$$[R] \subset \frac{h^{p+1}}{(p+1)!} \left(\frac{d^p}{dt^p} \left(\frac{\partial f}{\partial x} V \right) ([W_1], \mathrm{Id}) \right) \cdot [W_3]$$
 (17)

Remark 2 Observe that we can enclosure the remainder term for $V(h, [x_0])$ in second assertion of Lemma 1 by

$$[R] = \frac{d^p}{dt^p} \left(\frac{\partial f}{\partial x} V \right) ([W_1], [W_3]) \frac{h^{(p+1)}}{(p+1)!}, \tag{18}$$

but the formula given there is cheaper to compute and gives better bounds.

Let us fix p_e and p_v being respectively the orders for the Taylor methods used to solve equations (1) and (2) respectively. For the C_2^1 -algorithm we require that $p_v \geq p_e$.

In the description below the objects with an index k refer to the current values and those with an index k + 1 are the values after the next time step.

One step of the Lohner algorithms is a shift along the trajectory of system (1-2) with following input and output data:

Input data:

- t_k a current time
- h_k a time step
- $[x_k] \subset \mathbb{R}^n$, such that $\varphi(t_k, [x_0]) \subset [x_k]$
- (for C^1 -algorithms, only) $[V_k] \subset \mathbb{R}^{n \times n}$, such that $\frac{\partial \varphi}{\partial x}(t_k, [x_0]) \subset [V_k]$

Output data:

- $t_{k+1} = t_k + h_k$ a new current time
- $[x_{k+1}] \subset \mathbb{R}^n$, such that $\varphi(t_{k+1}, [x_0]) \subset [x_{k+1}]$
- (for C^1 -algorithms, only) $[V_{k+1}] \subset \mathbb{R}^{n \times n}$, such that $\frac{\partial \varphi}{\partial x}(t_{k+1}, [x_0]) \subset [V_{k+1}]$

We do not specify here a form (a representation) of sets $[x_k]$, and $[V_k]$. They can be interval sets, balls, doubletons etc. (see [MZ]). This issue is very important in handling the wrapping effect and will be discussed in detail in section 3.

One step of the algorithm consists from the following parts:

Part 1a. A computation of a rough enclosure $[W_1]$ for equation (1).

 $[W_1]$ is a compact and convex set such that

$$\varphi([0, h_k], [x_k]) \subset [W_1] \tag{19}$$

Part 1b. (Required for C_1^1 -algorithm). A computation of a rough enclosure $[W_2]$ for equation (1).

 $[W_2]$ is a compact and convex set, such that

$$\varphi([0, h_k], m([x_k])) \subset [W_2] \tag{20}$$

Part 2. (Required for C^1 -algorithms). A computation of a rough enclosure $[W_3]$ for equation (2).

 $[W_3]$ is a compact and convex set, such that

$$V([0, h_k], [x_k]) \subset [W_3]$$
 (21)

Part 3. A computation of $\frac{\partial \Phi}{\partial x}$ and (for C^1 -algorithms) $[V_{k+1}]$.

Part 4. A computation of $[x_{k+1}]$

2.4 Part 1 - a computation of a rough enclosure for equation (1)

Let $[Y] = [Y]_I$ be an interval set, such that $[x_k] \subset [Y]$. It is easy to see that, if

$$[[x_k] + [0, h_k]f([Y])]_I \subset \text{int}[Y]$$
 (22)

holds, then

$$\varphi([0, h_k], [x_k]) \subset [W_1] = [[x_k] + [0, h_k]f([Y])]_I, \tag{23}$$

where by $[[x_k] + [0, h_k]f([Y])]_I$ we denote the interval enclosure of the set $[x_k] + [0, h_k]f([Y])$.

Equation (22) suggests an iterative procedure. We can start with some $[Y_0]$ such that $[x_k] \subset [Y_0]$ and then set $[Y_{i+1}] = [[x_k] + [0, h_k]f([Y_i])]_I$, till (22) holds. This procedure does not always work, for example usually h_k cannot be too large for this procedure to succeed.

Sometimes, if some a-priori bounds, B, for the solutions of (1) are known we can take these bounds as $[W_1]$. To tighten these bounds we can refine $[W_1]$ as follows

$$[W_1] = B \cap [[x_k] + [0, h_k]f(B)]_I. \tag{24}$$

2.5 Part 2 - a computation of a rough enclosure for the variational part

In this section by ||x|| we denote an arbitrary norm.

In order to present and justify the procedure for producing a rough enclosure for the variational part we need to recall a notion of the logarithmic norm of a square matrix.

Definition 1 [HNW, Def. I.10.4] Let Q be a square matrix, then we call

$$\mu(Q) = \lim_{h>0, h\to 0} \frac{\|Id+hQ\|-1}{h}$$

the logarithmic norm of Q.

Theorem 3 [HNW, Th. I.10.5] The logarithmic norm is obtained by the following formulas

• for the Euclidean norm

$$\mu(Q) = the largest eigenvalue of 1/2(Q + Q^T).$$

• for the max norm $||x|| = \max_k |x_k|$

$$\mu(Q) = \max_{k} \left(q_{kk} + \sum_{i \neq k} |q_{ki}| \right)$$

• for the norm $||x|| = \sum_k |x_k|$

$$\mu(Q) = \max_{i} \left(q_{ii} + \sum_{k \neq i} |q_{ki}| \right)$$

The following theorem was proved in [HNW] (Theorem I.10.6)

Theorem 4 Consider the differential equation

$$\frac{dx}{dt} = f(t, x), \qquad f \in \mathcal{C}^1, \quad x \in \mathbb{R}^n.$$
 (25)

Let $t_0 < t_1 < \ldots < t_k = t_N$. Let x(t) be any solution of (25) on the interval. $[t_0, t_N]$. Let $\nu(t)$ denote the Euler polygon, so that

$$\nu'(t) = f(t_i, x_i), \quad \text{for } t_i < t < t_{i+1}, \quad i = 0, \dots, N-1.$$
 (26)

Suppose that we have the estimates for $t_0 \le t \le t_N$

$$\mu\left(\frac{\partial f}{\partial x}(t,\eta)\right) \leq l(t), \quad for \ \eta \in [x(t),\nu(t)]$$
 (27)

$$\|\nu'(t) - f(t, \nu(t))\| \le \delta(t) \tag{28}$$

$$\|\nu(t_0) - x(t_0)\| \le \rho$$
 (29)

Then for $t_N \ge t > t_0$ we have

$$||x(t) - \nu(t)|| \le e^{L(t)} \left(\rho + \int_{t_0}^t e^{-L(s)} \delta(s) ds\right),$$
 (30)

where $L(t) = \int_{t_0}^{t} l(s)ds$.

In fact the proof of above given in [HNW] is valid for any function ν , which is piecewise \mathcal{C}^1 . Hence we can take $\nu(t)$ to be also the solution of (25) in above theorem. In this situation $\delta(t) = 0$ and we obtain the following

Theorem 5 Let Z be a convex set and $\mu(\frac{\partial f}{\partial x}(x)) \leq l$ for $x \in Z$. Suppose that $\varphi(t,x) \in Z$ and $\varphi(t,y) \in Z$ for all $t \in [0,h]$. Then

$$\|\varphi(h,y) - \varphi(h,x)\| \le e^{hl} \|y - x\|$$
$$\|\frac{\partial \varphi(t,x)}{\partial x}\| \le e^{tl}, \quad for \ t \in [0,h]$$

The enclosure procedure can be formulated as follows:

Input parameters:

- h_k a time step
- $[x_k] \subset \mathbb{R}^n$ and $[V_k] \subset \mathbb{R}^{n \times n}$

• $[W_1] \subset \mathbb{R}^n$ - compact and convex, such that $\varphi([0,h_k],[x_k]) \subset [W_1]$

On **output** we compute $[W_3]$ as follows:

- 1. $l = \mu(\frac{\partial f}{\partial x}([W_1]))$
- **2.** We define an interval matrix $[W] \subset \mathbb{R}^{n \times n}$ by $[W_{ij}] = [\pm \max(e^{l[0,h_k]})]$ $i,j = 1,\ldots,n$

3.
$$[W_3] = \left(Id + \left[[0, h_k] \cdot \frac{\partial f}{\partial x}([W_1])\right]_I \cdot [W]\right) \cap [W]$$

From Theorem 5 it follows that $V([0, h_k], [x_k]) \subset [W]$, where [W] is defined in the second step of the above procedure. The next step is an attempt to refine this enclosure by using equation (2).

2.6 Part 3 - A computation of the variational part

Input parameters:

- h_k a time step
- $[x_k] \subset \mathbb{R}^n$ and $[V_k] \subset \mathbb{R}^{n \times n}$
- $[W_1] \subset \mathbb{R}^n$ compact and convex, such that $\varphi([0, h_k], [x_k]) \subset [W_1]$
- (for C^1 -algorithms) $[W_3] \subset \mathbb{R}^{n \times n}$ such that $V([0, h_k], [x_k]) \subset [W_3]$

From the linearity of equation (2) with respect to V it follows that

$$V(t_k + h_k, [x_0]) \subset V(h_k, [x_k]) \cdot [V_k],$$

hence to compute $[V_{k+1}]$ it is enough to compute bounds for $V(h_k, [x_k])$, which we will denote $[J_k]$. To control the Lipschitz part of error for the x-variable we will use the matrix $[A_k]$, which for the C_1^1 -algorithm is equal to $[J_k]$ (the partial derivative of the flow with respect to initial conditions) and for C_2^0 - and C_2^1 -algorithms we use instead the partial derivative of the Taylor expansion (this is an original Lohner approach).

To be more specific, we proceed as follows

 C_1^1 -algorithm: We set

$$[A_{k}] = [J_{k}] = Id + \sum_{i=1}^{p_{v}} \frac{d^{(i-1)}}{dt^{(i-1)}} \left(\frac{\partial f}{\partial x}V\right) ([x_{k}], Id) \frac{h_{k}^{i}}{i!} + \frac{h_{k}^{p_{v}+1}}{(p_{v}+1)!} \left(\frac{d^{p_{v}}}{dt^{p_{v}}} \left(\frac{\partial f}{\partial x}V\right) ([W_{1}], Id)\right) \cdot [W_{3}]$$
(31)

From Lemma 1 it follows that we have

$$\frac{\partial \varphi}{\partial x}(h_k, [x_k]) = V(h_k, [x_k]) \subset [J_k] = [A_k]. \tag{32}$$

 C_2^1 -algorithm: We set

$$[A_k] = Id + \sum_{i=1}^{p_e} \frac{d^{(i-1)}}{dt^{(i-1)}} \left(\frac{\partial f}{\partial x} V\right) ([x_k], Id) \frac{h_k^i}{i!}.$$
 (33)

The remainder of the Taylor expansion of the order p_v plus the error term are given by

$$[\Delta A_k] = \sum_{i=p_e+1}^{p_v} \frac{d^{(i-1)}}{dt^{(i-1)}} \left(\frac{\partial f}{\partial x}V\right) ([x_k], Id) \frac{h_k^i}{i!} + \frac{h_k^{p_v+1}}{(p_v+1)!} \left(\frac{d^{p_v}}{dt^{p_v}} \left(\frac{\partial f}{\partial x}V\right) ([W_1], Id)\right) \cdot [W_3]$$
(34)

Finally we set

$$[J_k] = [A_k] + [\Delta A_k] \tag{35}$$

Observe that by Lemma 1 we have

$$\begin{array}{ccc} \frac{\partial \Phi}{\partial x}(h,[x_k],p_e) & \subset & [A_k] \\ \\ \frac{\partial \varphi}{\partial x}(h_k,[x_k]) & = & V(h_k,[x_k]) \subset [J_k]. \end{array}$$

On output:

• the interval matrix $[A_k]$, such that for C^0 - and C_2^1 algorithms we have

$$\frac{\partial \Phi}{\partial x}(h_k, [x_k], p_e) \subset [A_k] \tag{36}$$

and for the C_1^1 -algorithm we have

$$\frac{\partial \varphi}{\partial x}(h_k, [x_k]) \subset [A_k]. \tag{37}$$

• (for C^1 -algorithms, only) the interval matrix $[V_{k+1}]$, such that

$$\frac{\partial}{\partial x}\varphi(h_k, [x_k]) \subset [J_k] \tag{38}$$

$$V(t_k + h_k, [x_0]) \subset [V_{k+1}] = [J_k] \cdot [V_k]$$
(39)

We do not specify here, how we evaluate the product $[J_k] \cdot [V_k]$. This depends on the representation of $[V_k]$ and is discussed in Section 3.

Let us stress here that what we add in C^1 -algorithms, when compared to the C^0 -algorithm, is only the computation of the error term for $[J_k]$ plus an evaluation of $[J_k] \cdot [V_k]$, because the Taylor expansion for V is already computed in $[A_k]$, which is also is present in the C^0 -algorithm.

2.7 Part 4 - a moving forward with x

Input parameters for C^0 - and C_2^1 -algorithm

- h_k a time step
- $[x_k] \subset \mathbb{R}^n$ a current estimate for $\varphi(t_k, [x_0])$
- $[W] \subset \mathbb{R}^n$ a compact and convex set, such that $\varphi([0, h_k], [x_k]) \subset [W]$ (this is the set $[W_1]$ obtained in 1a)
- $[A_k] \subset \mathbb{R}^{n \times n}$, such that $\frac{\partial \Phi}{\partial x}(h_k, [x_k], p_e) \subset [A_k]$

Input parameters for C_1^1 -algorithm

- h_k a time step
- $[x_k] \subset \mathbb{R}^n$ a current estimate for $\varphi(t_k, [x_0])$
- $[W] \subset \mathbb{R}^n$ a compact and convex set, such that $\varphi([0, h_k], \mathbf{m}([x_k])) \subset [W]$ (this is the set $[W_2]$ obtained in 1b)
- $[A_k] \subset \mathbb{R}^{n \times n}$, such that $\frac{\partial \varphi}{\partial x}(h_k, [x_k]) \subset [A_k]$

On **output** we set

$$[x_{k+1}] = \Phi(h_k, \mathbf{m}([x_k]), p_e) + \frac{d^{p_e}}{dt^{p_e}} f([W]) \frac{h_k^{p_e+1}}{(p_e+1)!} + [A_k]([x_k] - \mathbf{m}(x_k)).$$
(40)

3 The rearrangement computations.

It is well known that the straightforward interval evaluation of the products of matrices and vectors leads immediately to the so-called *wrapping effect* (see for example [Lo, NJ, AZ]). As it will follow from the discussion below we can avoid it to some extend, by treating the products appearing in the algorithm carefully. We will refer to this part of the algorithm as the rearrangement computations.

3.1 Evaluation of equation (40)

To discuss various methods of an evaluation of equation (40) following [Lo, Lo1] we decompose $[x_k]$ as follows

$$[x_k] = x_k + [r_k], \quad \text{where} \quad x_k = m([x_k]), [r_k] = [x_k] - x_k$$
 (41)

We set

$$x_{k+1} = m \left(\Phi(h_k, \mathbf{m}([x_k]), p_e) + \frac{d^{p_e}}{dt^{p_e}} f([W]) \frac{h_k^{p_e+1}}{(p_e+1)!} \right)$$
$$[z_{k+1}] = \Phi(h_k, m([x_k]), p_e) + \frac{d^{p_e}}{dt^{p_e}} f([W]) \frac{h_k^{p_e+1}}{(p_e+1)!} - x_{k+1}$$

With these notations equation (40) becomes

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}] \tag{42}$$

Evaluation 1. In [MZ] terminology this approach is called an interval set. This is a direct evaluation of (42) using interval arithmetic. This method is simple and fast, but usually produces very bad bounds due to the wrapping effect.

To avoid the wrapping effect Lohner proposed the following: instead of representing $[r_k]$ as an interval vector, he proposed to use parallelograms (interval vectors in other coordinate systems) i.e. $[r_k] = B_k[\hat{r}_k]$, where B_k are nonsingular matrices and $[\hat{r}_k]$ are interval vectors. Equation (42) becomes

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}] = B_{k+1} \left(B_{k+1}^{-1}[A_k]B_k[\hat{r}_k] + B_{k+1}^{-1}[z_{k+1}] \right)$$
(43)

In computer calculations it is usually impossible to find an exact inverse of a given matrix. So in fact we deal with interval matrices $[B_i]$ and $[B_i^{-1}]$.

Finally we calculate $[\hat{r}_k]$ as follows

$$[r_0] = [B_0][\hat{r}_0], \quad [B_0] = \{Id\}$$
 (44)

$$[r_0] = [B_0][\hat{r}_0], \quad [B_0] = \{Id\}$$

$$[\hat{r}_{k+1}] = ([B_{k+1}^{-1}][A_k][B_k])[\hat{r}_k] + [B_{k+1}^{-1}][z_{k+1}]$$
(45)

$$[r_{k+1}] = [B_{k+1}][\hat{r}_{k+1}] \tag{46}$$

It should be stressed that only $[\hat{r}_k]$ is computed using the interval arithmetic. When evaluating r.h.s of equation (45) we do first matrix multiplications as indicated by brackets. This is the place where we can reduce the wrapping effect, if we make a good choice of $[B_k]$'s. We evaluate formula (46) to compute rough enclosures and an at the end of computations (while considering the intersection of the orbit of $[x_0]$ with a Poincaré section).

Evaluation 2. In the [MZ] terminology this approach is called a parallelepiped. We choose $B_{k+1} \in [A_k][B_k]$. This is not a method recommended for general applications. The main problem with this method is the need of calculating the inverse of a matrix.

Evaluation 3. In the [MZ] terminology this approach is called a cuboid. Choose a matrix $U \in [A_k][B_k]$, we perform an approximate floating-point QR-decomposition of U. Let the matrix Q be a Q-factor from this decomposition. The matrix Q is very close to an orthogonal one. Next, we apply an interval Gram-Schmidt procedure to columns of Q to obtain a matrix $[Q_0]$. Observe that $[Q_0]$ contains an orthogonal matrix, Q_1 , hence $Q_1^{-1} = Q_1^T \in [Q_0]^T$. We set $B_{k+1} = Q_1$, $B_{k+1}^{-1} = Q_1^T$. This leads to

$$[B_{k+1}] = [Q_0], [B_{k+1}^{-1}] = [Q_0]^T.$$
 (47)

Slightly different approach (probably more efficient) was proposed originally by Lohner. Namely, instead of orthogonalizing of columns of Q he proposed to compute rigorously inverse of Q. Observe that since Q is almost orthogonal, the rigorous Q^{-1} can be obtained very easily with little cost.

Evaluation 4. In the [MZ] terminology this approach is called *a doubleton*. This method is designed to handle the situation, when the initial error is large in comparison to local errors produced in every step. Lohner proposed to separately keep track of the error originating from $[r_0]$ and the local errors produced in every step. An example of such a method is given by

$$[r_{k+1}] = [E_{k+1}][r_0] + [\tilde{r}_{k+1}] \tag{48}$$

where
$$[\tilde{r}_{k+1}] = [A_k][\tilde{r}_k] + [z_{k+1}]$$
 (49)

and
$$[E_{k+1}] = [A_k][E_k], \quad [E_0] = Id$$
 (50)

and $[\tilde{r}_k]$ is evaluated using any method described previously (preferably evaluation 3). It is easy to see that the matrix $[E_k]$ corresponds to $\frac{\partial \varphi(t_{k+1},\cdot)}{\partial x}$. We still have some wrapping effect in the product $[A_k][E_k]$, which becomes more and more important when we want to follow the trajectory for a longer time. To avoid this Lohner proposed the following

$$[r_{k+1}] = C_{k+1}[r_0] + [\tilde{r}_{k+1}] \tag{51}$$

where
$$[\tilde{r}_{k+1}] = [A_k][\tilde{r}_k] + [z_{k+1}] + ([A_k]C_k - C_{k+1})[r_0], \quad [\tilde{r}_0] = 0$$
 (52)

and
$$C_0 = Id$$
, $C_{k+1} \in [A_k]C_k$ (53)

and $[\tilde{r}_k]$ is evaluated using any method described previously (preferably evaluation 3).

The tests in [MZ] on the Rössler equation and the Lorenz equation show that the last approach - a doubleton is by far better than the previous ones.

3.2 Evaluation of equation (39)

To evaluate (39) we mimic the approach from the previous subsection.

Evaluation 1. The direct interval evaluation.

To discuss other evaluations let us decompose first the interval matrices $[V_k]$ into the center point and the 'remainder'

$$[V_k] = V_k + [\Delta V_k], \tag{54}$$

We can rewrite equation (39) as follows

$$V_{k+1} + [\Delta V_{k+1}] = [J_k]V_k + [J_k][\Delta V_k]$$
(55)

Let

$$V_{k+1} = m([J_k]V_k) \tag{56}$$

$$[Z_{k+1}] = [J_k]V_k - V_{k+1}. (57)$$

We have

$$[\Delta V_{k+1}] = [J_k] \cdot [\Delta V_k] + [Z_{k+1}] \tag{58}$$

We see that this equation has the same structure as equation (42), where $[\Delta V_k]$ corresponds to $[r_k]$, $[Z_{k+1}]$ to $[Z_{k+1}]$ and $[J_k]$ to $[A_k]$. Hence we can treat it with similar methods.

For any family of nonsingular matrices $[B_k]$ for k = 0, 1, ... we set $[\Delta V_k] = [B_k][\widetilde{\Delta V_k}]$. Equation (58) becomes

$$[\Delta V_{k+1}] = [B_{k+1}] \left([B_{k+1}^{-1}][J_k][B_k][\widetilde{\Delta V_k}] + [B_{k+1}^{-1}][Z_{k+1}] \right)$$
(59)

We define the following scheme for an evaluation of equation (58)

$$\begin{split} [\Delta V_k] &= [B_k] [\widetilde{\Delta V_k}] \\ [\widetilde{\Delta V_0}] &= 0, \quad [B_0] = Id \\ [\widetilde{\Delta V_{k+1}}] &= \left([B_{k+1}^{-1}] [J_k] [B_k] \right) [\widetilde{\Delta V_k}] + [B_{k+1}^{-1}] [Z_{k+1}] \end{split}$$

Evaluation 2. Choose B_{k+1} to be any matrix in $[J_k] \cdot [B_k]$.

Evaluation 3. Take any $U \in [J_k] \cdot [B_k]$, perform the QR-decomposition of U and set $[B_{k+1}] = [Q]$. Just as in the previous subsection this method appears to be better than the previous evaluations.

Evaluation 4. Since we start with a zero matrix ($[\Delta V_0] = 0$), there is no a Lipschitz part at the beginning and we apply any of the previous evaluations (preferably the 3-rd one) till ΔV_k become 'thick' (its diameter becomes larger than some threshold value). Suppose that this happens after k_0 steps. Then we switch to a doubleton representation as follows

$$[\Delta V_k] = C_k^V [\Delta V_0] + \overline{\Delta V_k}, \quad k \ge k_0$$

$$C_{k+1}^V \in [J_k] \cdot C_k^V, \quad \overline{\Delta V_{k+1}} = [J_k] \cdot [\overline{\Delta V_k}] + ([J_k] \cdot C_k^V - C_{k+1}^V) [\Delta V_0] + [Z_{k+1}].$$

We initiate the variables $C_{k_0}^V$, $[\Delta V_0]$, $\overline{\Delta V_{k_0}}$ and redefine $[B_{k_0}]$ as follows

$$[\Delta V_0] = [\widetilde{\Delta V_{k_0}}], \quad C_{k_0}^V = m([B_{k_0}]),$$

$$\overline{\Delta V_{k_0}} = ([B_{k_0}] - C_{k_0}^V)[\Delta V_0], \quad [B_{k_0}] = Id.$$

The interval matrix $[\overline{\Delta V_k}]$ is evaluated using any of the previous evaluation methods (preferably evaluation 3).

4 Rigorous estimates between time steps

The goal of this section is to answer the following question, which is very important in the computation of the Poincaré map:

How to estimate $\varphi(t,x)$ and $\frac{\partial \varphi}{\partial x}$ between time steps?

Obviously for this purpose we can use rough enclosures $[W_1]$ and $[W_3]$. Here we present a much more efficient and relatively cheap approach.

The following lemma tells us how well is $\varphi(\tau + t, x)$ for $t \in (0, h)$ approximated by the segment joining $\varphi(\tau, x)$ and $\varphi(\tau + h, x)$.

Lemma 6 Let $Z \subset \mathbb{R}^n$ be a convex set such that $\varphi(\tau + t, x) \in Z$ for $t \in [0, h]$, then

$$\left| \varphi_i(\tau + t, x) - \left((1 - \frac{t}{h}) \varphi_i(\tau, x) + \frac{t}{h} \varphi_i(\tau + h, x) \right) \right| \le \frac{h^2 \max_{z \in Z} \left| \sum_j \frac{\partial f_i}{\partial x_j}(z) \cdot f_j(z) \right|}$$
(60)

Proof: Without any loss of generality we can assume that $\tau=0$, hence $\varphi(\tau,x)=x$. Observe that we can represent the interval joining x and $\varphi(h,x)$ as follows

$$(1 - \frac{t}{h})x + \frac{t}{h}\varphi_i(h, x) = x + t\frac{\varphi(h, x) - x}{h}$$

$$\tag{61}$$

$$(1 - \frac{t}{h})x + \frac{t}{h}\varphi_i(h, x) = \varphi(h, x) - (1 - \frac{t}{h})(\varphi(h, x) - x)$$

$$(62)$$

We will use formula (61) for $t \in [0, h/2]$ and formula (62) $t \in [h/2, h]$.

Assume that $t \in [0, h/2]$. From the mean value theorem we obtain for some $\theta_1, \theta_2, \theta_3 \in [0, 1]$

$$\begin{split} |\varphi_i(t,x)-(x_i+t\frac{\varphi_i(h,x)-x_i}{h})| &= |(\varphi_i(t,x)-x_i)-t\frac{\varphi_i(h,x)-x_i}{h}| = \\ &= |t||f_i(\varphi(\theta_2t,x))-f_i(\varphi(\theta_1h,x))| \\ &= |t||\theta_2t-\theta_1h|\left|\sum_j\frac{\partial f_i}{\partial x_j}(\varphi(\theta_3h,x))\cdot f_j(\varphi(\theta_3h,x))\right| \leq \\ &\frac{h^2}{2}\left|\sum_j\frac{\partial f_i}{\partial x_j}(z)\cdot f_j(z)\right| \end{split}$$

where $z = \varphi(\theta_3 h, x) \in Z$.

Similarly for $t \in [h/2, h]$ we have

$$\begin{aligned} |\varphi_i(t,x) - (\varphi_i(h,x) - (1 - t/h)(\varphi_i(h,x) - x_i))| &= \\ |(\varphi_i(t,x) - \varphi_i(h,x)) + (1 - t/h)(\varphi_i(h,x) - x_i))| &= \\ |(t - h)f_i(\varphi_i(\theta_1 h, x) + (1 - t/h)hf_i(\varphi_i(\theta_2 h, x))| &= \\ |(h - t)|\theta_1 h - \theta_2 h| \left| \sum_j \frac{\partial f_i}{\partial x_j} f_j(z) \right| &\leq \frac{h^2}{2} \left| \sum_j \frac{\partial f_i}{\partial x_j} (z) \cdot f_j(z) \right| \end{aligned}$$

where $z = \varphi(\theta_3 h, x) \in Z$.

When we apply Lemma 6 to the system (1-2) then for r.h.s in equation (60) for V_{ij} we obtain the following expression

$$\sum_{l} \frac{\partial V'_{ij}}{\partial x_{l}} f_{l} + \sum_{lm} \frac{\partial V'_{ij}}{\partial V_{lm}} V'_{lm} = \sum_{kl} \frac{\partial^{2} f_{i}}{\partial x_{k} \partial x_{l}} V_{kj} f_{l} + \sum_{l} \frac{\partial f_{i}}{\partial x_{l}} V'_{lj} =$$

$$\sum_{kl} \frac{\partial^2 f_i}{\partial x_k \partial x_l} V_{kj} f_l + \sum_{lm} \frac{\partial f_i}{\partial x_l} \frac{\partial f_l}{\partial x_m} V_{mj}$$

Hence we have proved the following

Lemma 7 Let $Z \subset \mathbb{R}^n$ and $M \subset \mathbb{R}^{n \times n}$ be convex set such that $\varphi(\tau + t, x) \in Z$ and $V(\tau + t, x) \in M$ for $t \in [0, h]$, then

$$\left| V_{ij}(\tau + t, x) - \left((1 - \frac{t}{h}) V_{ij}(\tau, x) + \frac{t}{h} V_{ij}(\tau + h, x) \right) \right| \le \frac{h^2}{2} \max_{z \in Z, A \in M} \left| \sum_{kl} \frac{\partial^2 f_i}{\partial x_k \partial x_l} (z) A_{kj} f_l(z) + \sum_{lm} \frac{\partial f_i}{\partial x_l} (z) \frac{\partial f_l}{\partial x_m} (z) A_{mj} \right|$$

Lemmas 6 and 7 offer a justification for the following procedure for the estimation of $\varphi([0, h_k], [x_k])$ and $V(t_k + [0, h_k], [x_0])$

PROCEDURE:

Input parameters:

- h_k a time step
- $[x_k] \subset \mathbb{R}^n$, such that $\varphi(t_k, [x_0]) \subset [x_k]$
- $[x_{k+1}] \subset \mathbb{R}^n$ such that $\varphi(h_k, [x_k]) \subset [x_{k+1}]$
- $[W_1] \subset \mathbb{R}^n$ compact and convex, such that $\varphi([0, h_k], [x_k]) \subset [W_1]$
- (for C^1 algorithms) $[V_k] \subset \mathbb{R}^{n \times n}$, such that $V(t_k, [x_0]) \subset [V_k]$
- (for C^1 algorithms) $[V_{k+1}] \subset \mathbb{R}^{n \times n}$, such that $V(t_k + h_k, [x_0]) \subset [V_{k+1}]$
- (for C^1 algorithms) $[W_3] \subset \mathbb{R}^{n \times n}$ compact and convex, such that $V([0, h_k], [x_k]) \subset [W_3]$

Output:

We compute $[E_k] \subset \mathbb{R}^n$ such that

$$\varphi([0,h_k],[x_k]) \subset [E_k],$$

and for \mathcal{C}^1 -algorithms $[M_k] \subset \mathbb{R}^{n \times n}$ such that

$$V(t_k + [0, h_k], [x_0]) \subset [M_k].$$

We proceed as follows

• if $0 \in f_i([W_1])$, then

$$[E_k]_i := \text{hull}([x_k]_i, [x_{k+1}]_i) + [-1, 1] \cdot \frac{h_k^2}{2} \left| \sum_j \frac{\partial f_i}{\partial x_j}([W_1]) \cdot f_j([W_1]) \right|$$

• if $0 \notin f_i([W_1])_i$, then i-th coordinate is strictly monotone on $[W_1]$, hence

$$[E_k]_i = \text{hull}([x_k]_i, [x_{k+1}]_i)$$

For C^1 -algorithms:

We define

$$[W_4] = [W_3] \cdot [V_k]. \tag{63}$$

It is easy to see that $V(t_k + [0, h_k], [x_0]) \subset [W_4]$.

• if $V'_{ij}([W_1], [W_4]) = \sum_l \frac{\partial f_i}{\partial x_l}([W_1]) \cdot [W_4]_{lj}$ contains 0, then

$$[M_k]_{ij} = \text{hull}([V_k]_{ij}, [V_{k+1}]_{ij}) +$$

$$[-1, 1] \cdot \frac{h_k^2}{2} \left| \sum_{kl} \frac{\partial^2 f_i}{\partial x_k \partial x_l} ([W_1]) \cdot [W_4]_{kj} \cdot f_l([W_1]) +$$

$$\sum_{lm} \frac{\partial f_i}{\partial x_l} ([W_1]) \cdot \frac{\partial f_l}{\partial x_m} ([W_1]) \cdot [W_4]_{mj} \right|$$

• if $V'_{ij}([W_1], [W_4])$ does not contain 0, then $V_{ij}(t_k + t, [x_0])$ is strictly monotone for $t \in [0, h_k]$, hence we can set

$$[M_k]_{ij} = \text{hull}([V_k]_{ij}, [V_{k+1}]_{ij}).$$

Poincaré map 5

The goal of this section is to show how from the bounds for $\varphi(t,x)$ and $\frac{\partial \varphi}{\partial x}$

obtained by C^0 - and C^1 -Lohner algorithms we can compute P(x) and $\frac{\partial P}{\partial x}$. In Section 5.1 we derive the formulas, which express $\frac{\partial P}{\partial x}$ in terms of $\frac{\partial \varphi}{\partial x}$. In Section 5.2 we discuss in details the procedure which allows to compute P and $\frac{\partial P}{\partial x}$ from the data obtained from the Lohner algorithm.

In Section 5.3 we discuss the issue of errors related to the computation of intersection of the trajectory with a section. Insights gained in this section are then used in Section 5.4 to describe an efficient time step selection scheme near

Let $\alpha: \mathbb{R}^n \to \mathbb{R}$ be a \mathcal{C}^1 function. We define a section, Θ , by the

$$\Theta = \{ x \mid \alpha(x) = 0, \qquad f(x) \cdot \nabla \alpha(x) > 0 \}. \tag{64}$$

We assume that Θ is a local section for equation (1).

For $x \in \mathbb{R}^n$ by $t_p(x)$ we will denote the return time to Θ . This means that

$$\varphi(t_p(x), x) \in \Theta. \tag{65}$$

The Poincaré map $P:\Theta\supset \mathrm{dom}\,(P)\to\Theta$ can be seen as a restriction the section of the map $\tilde{P}:\mathbb{R}^n\supset U\to\mathbb{R}^n$ given by

$$\tilde{P}(x) = \varphi(t_p(x), x). \tag{66}$$

From now on we will not distinguish between the map \tilde{P} and P, and we will use the same symbol P to denote both of them. Hence we effectively treat a Poincaré map as a map defined on some open subset in \mathbb{R}^n for two reasons, we want to avoid any particular coordinate system on Θ and we want to allow for maps between the different sections.

To infer the derivatives of $P: \Theta \to \Theta$ we have consider how Θ is embedded in \mathbb{R}^n . For example, when $\alpha(x) = x_1 - C$ and we use (x_2, \ldots, x_n) to represent the points on Θ , then we just drop the first row and the first column from the matrix $\frac{\partial \tilde{P}}{\partial x}$.

5.1 A formula for partial derivatives of Poincaré map

The Poincaré map P is defined by

$$P(x) = \varphi(t_P(x), x), \tag{67}$$

where $t_P: \mathbb{R}^n \to \mathbb{R}$ satisfies the following equation

$$\alpha(\varphi(t_p(x), x)) = 0. \tag{68}$$

Since Θ is a local section, it follows easily from the implicit function theorem that t_p is a smooth function. We compute now the derivatives of t_p . We differentiate equation (68) with respect to x_j for j = 1, ..., n to obtain

$$\sum_{i=1}^{n} \frac{\partial \alpha}{\partial x_i} \left(f_i \frac{\partial t_P}{\partial x_j} + \frac{\partial \varphi_i}{\partial x_j} \right) = 0$$

$$(\nabla \alpha \cdot f) \frac{\partial t_P}{\partial x_j} + \sum_{i=1}^n \frac{\partial \alpha}{\partial x_i} \frac{\partial \varphi_i}{\partial x_j} = 0$$

Hence

$$\frac{\partial t_P}{\partial x_j} = -\frac{1}{\nabla \alpha \cdot f} \sum_{i=1}^n \frac{\partial \alpha}{\partial x_i} \frac{\partial \varphi_i}{\partial x_j}$$
 (69)

Now we can compute $\frac{\partial P_i}{\partial x_j}$

$$\frac{\partial \varphi_i(t_P(x), x)}{\partial x_j} = f_i \frac{\partial t_P}{\partial x_j} + \frac{\partial \varphi_i}{\partial x_j} = \frac{\partial \varphi_i}{\partial x_j} - \frac{f_i}{\nabla \alpha \cdot f} \sum_{k=1}^n \frac{\partial \alpha}{\partial x_k} \frac{\partial \varphi_k}{\partial x_j}$$
(70)

For example if $\alpha(x) = x_1 - C$ we obtain

$$\frac{\partial P_i}{\partial x_j} = -\frac{f_i}{f_1} \frac{\partial \varphi_1}{\partial x_j} + \frac{\partial \varphi_i}{\partial x_j} \tag{71}$$

Hence we have proved the following

Lemma 8

$$\frac{\partial P_i}{\partial x_j}(x) = \frac{\partial \varphi_i}{\partial x_j}(t_p(x), x) +$$

$$-\frac{f_i}{\nabla \alpha \cdot f} \left(\varphi(t_p(x), x) \right) \cdot \sum_{k=1}^n \frac{\partial \alpha}{\partial x_k} \left(\varphi(t_p(x), x) \right) \frac{\partial \varphi_k}{\partial x_j}(t_p(x), x)$$
(72)

5.2Computation of Poincaré map

In this section we describe how from the data supplied by the Lohner algorithm we can obtain $P([x_0])$ and $\frac{\partial P}{\partial x}([x])$. In this section we assume that we have a prescribed sequence of time steps h_k . A proposal for an efficient time step selection scheme near the Poincaré section is given in Section 5.4.

Let us set $t_k = \sum_{i=0}^{k-1} h_i$, where h_i is the time step used in (i+1)-th step of the Lohner algorithm.

From the Lohner algorithm we have

- **1.** a sequence $[x_{N+k}] \subset \mathbb{R}^n$, $k = 0, \ldots, s$, such that $\varphi(t_{N+k}, [x_0]) \subset [x_{N+k}]$
- **2.** a sequence $[V_{N+k}] \subset \mathbb{R}^{n \times n}$, $k = 0, \ldots, s$, such that $\frac{\partial \varphi}{\partial x}(t_{N+k}, [x_0]) \subset [V_{N+k}]$, such that the following conditions are satisfied

$$\varphi((0, t_N], [x_0]) \cap \Theta = \emptyset \tag{73}$$

$$\alpha([x_N]) < 0 \tag{74}$$

$$\alpha([x_{N+s}]) > 0 \tag{75}$$

For k = 0, ..., s-1 we define $[E_{N+k}] \subset \mathbb{R}^n$, $[M_{N+k}] \subset \mathbb{R}^{n \times n}$ as the output of the procedure described in Section 4. We have

$$\varphi([t_{N+k}, t_{N+k+1}], [x_0]) \subset \varphi([0, h_{N+k}], [x_{N+k}]) \subset [E_{N+k}] \tag{76}$$

$$\varphi([t_{N+k}, t_{N+k+1}], [x_0]) \subset \varphi([0, h_{N+k}], [x_{N+k}]) \subset [E_{N+k}]$$

$$\frac{\partial \varphi}{\partial x}([t_{N+k}, t_{N+k+1}], [x_0]) = V([t_{N+k}, t_{N+k+1}], [x_0]) \subset [M_{N+k}]$$
(76)

We set

$$\langle P \rangle = \bigcup_{k=0}^{s-1} [E_{N+k}] \tag{78}$$

$$\langle V \rangle = \bigcup_{k=0}^{s-1} [M_{N+k}]. \tag{79}$$

The sums in above equations are realized by taking the interval enclosures. We have

$$\varphi([t_N, t_{N+s}], [x_0]) \subset \langle P \rangle \tag{80}$$

$$\varphi([t_N, t_{N+s}], [x_0]) \subset \langle P \rangle$$

$$\frac{\partial \varphi}{\partial x}([t_N, t_{N+s}], [x_0]) \subset \langle V \rangle.$$
(80)

Assume now that on $\langle P \rangle$ we have

$$\nabla \alpha(\langle P \rangle) \cdot f(\langle P \rangle) > 0. \tag{82}$$

From the above equation it follows that $\alpha(t) = \alpha(\varphi(t, x))$ is an increasing function for $x \in \langle P \rangle$. Hence from equations (73-75), (80) and (81) it follows immediately that for all $x \in [x_0]$ the Poincaré map, P, is well defined and

$$t_P([x_0]) \subset (t_N, t_{N+s}) \tag{83}$$

$$P([x_0]) \subset [P] := \langle P \rangle \cap \Theta$$
 (84)

$$\frac{\partial \varphi}{\partial x}(t_P(x), x) \in \langle V \rangle, \quad \forall x \in [x_0].$$
 (85)

Finally from Lemma 8 it follows that

$$\frac{\partial P_i}{\partial x_j}([x_0]) \subset \langle dP \rangle_{ij} := \langle V \rangle_{ij} - \frac{f_i}{\nabla \alpha \cdot f}([P]) \cdot \sum_{k=1}^n \frac{\partial \alpha}{\partial x_k}([P]) \langle V \rangle_{kj}. \tag{86}$$

Let us remind the reader that the map P in the above formula is treated as map $P: \mathbb{R}^n \to \mathbb{R}^n$ (see the beginning of Section 5). To infer the derivatives of a Poincaré map $P: \Theta \to \Theta$ we have consider how Θ is embedded in \mathbb{R}^n . For example, when $\alpha(x) = x_1 - C$ and we use (x_2, \ldots, x_n) to represent the points on Θ , then we just drop the first row and the first column from the matrix $\langle dP \rangle$ defined in equation (86).

5.3 Estimates for the section error

Let us consider a planar example. We assume that we have a section Θ defined by $\alpha(x)=x_1-C=0$ and near Θ the flow is represented by the following system of equations

$$x_1' = 1, \quad x_2' = a, \qquad a \ge 0, \quad a \in \mathbb{R}$$
 (87)

It is easy to see that the trajectory of a point (x_1, x_2) , where $x_1 < 0$ will intersects the section Θ at the point $P(x_1, x_2) = (0, a|x_1| + x_2)$ and $t_p(x_1, x_2) = |x_1|$.

Let $[x] = [x_1^-, x_1^+] \times [x_2^-, x_2^+]$, where $[x_1^-, x_1^+] < 0$. We have

$$\dim (t_n([x])) = x_1^+ - x_-^1 \tag{88}$$

$$P([x]) = \{0\} \times [a|x_1^+| + x_2^-, a|x_1^-| + x_2^+]. \tag{89}$$

Consider now the computation of P([x]) using the method described in Section 5.2. For this end assume that $[x_N] = [x]$ and the sum in equation (67) is realized as the interval enclosure, then we have

$$[x_1^-, x_1^+ + t_{N+s} - t_N] \times [x_2^-, x_2^+ + a(t_{N+s} - t_N)] \subset \langle P \rangle$$

$$\{0\} \times [x_2^-, x_2^+ + a(t_{N+s} - t_N)] \subset [P].$$

Hence we obtain

$$\operatorname{diam}([P]) - \operatorname{diam}(P([x_N])) = a \cdot ((t_{N+s} - t_N) - \operatorname{diam}(t_P([x_N]))) \tag{90}$$

The above equation gives us the difference between the computed image and the true image of the Poincaré map. We will call this difference a section error and we will denote it by ΔS . In general situation ΔS is a (n-1)-dimensional vector and ΔS_i is a section error for the *i*-th coordinate on section.

A higher dimensional generalization of the above example leads to the following formula (for small boxes $[x_N]$ and sections given by $\alpha(x) = x_j - C$) and the considerations given in Section 4

$$\Delta S_i \approx \frac{f_i}{f_1} \cdot ((t_{N+s} - t_N) - \text{diam}(t_p([x_N]))) + Ch^2,$$
 (91)

where $\frac{f_i}{f_1}$ should be evaluated on $P([x_N])$, h is the time step used close the section Θ and C is some constant depending on f (see Lemma 6).

From the above formula we see that in order to minimize the section error we can do three things

- 1. Take small time steps close to Θ , to minimize the Ch^2 term.
- **2.** Choose the section Θ to be as orthogonal to the flow as possible (to make $\frac{f_i}{f_1}$ small). In this case it is reasonable to use a different coordinates, y, locally close to the section Θ , so that in new coordinates $\tilde{\alpha}(y) = y_1 C$ and the flow is very close to the parallel flow $y'_1 = \tilde{f}_1(y_1, \ldots, y_n), \ y'_i = 0$ for i > 1.
- **3.** Minimize $t_{N+s} t_N$ to make it as close as possible to $t_p([x_N])$. This is issue is addressed in Section 5.4.

5.4 The choice of time steps close to the section

Let us first estimate the diameter of the Poincaré return time, $t_p([x_0]) = t_p([x_N])$. If we assume that $[x_N]$ is small and we are very close to Θ , then we can assume that $\frac{d}{dt}\alpha(\varphi(t,x)) = \nabla\alpha \cdot f(x)$ is approximately constant, while our trajectory is crossing the section. For simplicity we also assume that $\operatorname{diam}(\alpha(\varphi(t,[x_N])))$ is also constant. From this we obtain the following estimate

$$t_p([x_N]) \approx h_C = \frac{\operatorname{diam}(\alpha([x_N]))}{\nabla \alpha \cdot f(x)},$$
 (92)

where x is any point in $[x_N]$. The number h_C will be called in the sequel the estimated crossing time.

Similar considerations allows one to make nonrigorous, but reasonably good guesses about the time need to get very close to section and the time need to get past the section, but very close to it.

A TIME STEP SELECTION SCHEME CLOSE TO THE SEC-

Let h > 0, D > 1 (we used D = 12, D = 36 in our implementation) and $\epsilon > 0$ (this should be a small number, we used $\epsilon = 10^{-2}$)

1. We compute $[x_k]$, $[V_k]$ $k=1,\ldots,N-1$ using Lohner algorithm with a constant time step $h_k = h$ as long as equation

$$\varphi([0, h_k], [x_k]) \cap \Theta = \emptyset, \tag{93}$$

is satisfied. For the N-th step we have

$$\varphi([0, h_{N-1}], [x_{N-1}]) \cap \Theta \neq \emptyset, \tag{94}$$

2. We discard the data obtained for the N-th step. We find a new value for h_{N-1} , such that the Lohner algorithm applied to $[x_{N-1}]$ gives

$$\alpha([x_N])$$
 < 0, (95)

$$-\epsilon \operatorname{diam}\left(\alpha([x_N])\right) < \operatorname{right}\left(\alpha([x_N])\right)$$
 (96)

Obviously if we are doing C^1 -computation we have to recompute $[V_N]$.

- **3.** We set $\bar{h} = \min(\frac{h}{D}, h_C)$. This will be our time step, while we will be crossing the section.
- **4.** With $h_{N+k} = \bar{h}$ for $k = 0, \ldots$ we continue to compute $[x_{N+k}]$ (and $[V_{N+k}]$) until for k = s we have

$$\alpha([x_{N+s}]) > 0. \tag{97}$$

5. We check if the following condition holds

$$\operatorname{left}\left(\alpha([x_{N+s}])\right) < \epsilon \cdot \operatorname{diam}\left([x_{N+s-1}]\right) \tag{98}$$

If the above condition is not true, then we discard the value of $[x_{N+s}]$ (and $[V_{N+s}]$). We decrease the value of h_{N+s-1} and we recompute $[x_{N+s}]$ (and $[V_{N+s}]$), until equations (97) and (98) are satisfied.

Observe that from conditions (96) and (98) it follows that we overestimate the diameter of the Poincaré return time, $t_p([x_N])$ by the factor approximately equal to $1 + 2\epsilon$.

Point 3 is necessary in case when $[x_N]$ is relatively large, so that the estimated crossing time becomes unacceptable for us (either the term h^2C in equation (91) becomes to large or the enclosure procedures cannot be completed). In this case we just use the previous time step divided by D. In this case we will cross the section in several time steps. When $[x_N]$ is small we cross the section in one or two steps.

6 Remarks and discussion

6.1 A cost comparison of C^0 - and C^1 -algorithms

Let us observe that, the C^0 - and C_2^1 -algorithms are identical on the x-variables, i.e. for the same order and $[x_0]$, the sequence of time steps h_k and the same rough enclosure procedure they return the same estimate for $\varphi(t,[x_0])$. This is not the case for the C_1^1 -algorithm, because instead of the partial derivative of the Taylor method, the partial derivative of the flow is used.

With respect to a cost for the same order observe that C^1 -algorithms add the following

- 1. the computation of an enclosure $[W_2]$ (for C_1^1 -algorithm, only)
- 2. the computation of the error term of the Taylor method for equation (2) (all derivatives of V up to order $p_v + 1$) (if $p_v \ge p_e$ then this is the most expensive part of the algorithm)
- **3.** the rearrangement computations of V.

From the items listed above 1 and 3 appear to be quite cheap when compared to the second one. Hence we expect that the C^1 -algorithm with $p_v = p_e = r$ will run in the time comparable to C^0 -algorithm with the order $p_e = r - 1$. We tested it on Poincaré maps for the Rössler equation and the Galerkin projection of KS-equations described in section 7. These tests show that the computation times of the C^1 -algorithm with $p_v = p_e = r$ are usually less that twice the computation time for the C^0 -algorithm with the same time step and with the order $p_e = r + 1$. The test was performed over the orders $3, 4, \ldots, 9$.

6.2 Remarks on a direct integration of the system (1-2) using C^0 -Lohner algorithm

As it was mentioned in the introduction one can do a C^1 -computation by simply applying the original Lohner algorithm to the system of equations (1-2).

Observe that the dimension of the phase space for this system is $n + n^2$, where n is the dimension appearing in equation (1). This has an immediate consequence for the computation time of the Taylor expansion. For example from the formulas given in the Appendix it follows that for a second degree polynomial and an order p the computation time has a leading term $C(p)n^4$, where C is constant depending of the order only. Hence one can expect that the proposed algorithm will be about $(n+1)^4$ -times faster.

But there is also one even more important issue. It turns out that the Lohner algorithm applied to system (1-2) performs quite poorly with respect to controlling the growth of the computed image. For example we weren't able using this approach to compute any of the Poincaré maps considered in section 7. Apparently, the QR-decomposition for the system (1-2), which plays a crucial role in controlling the wrapping effect by choosing a good coordinate frame, become very quickly dominated by the variational variables (the V-variables).

This produces a huge wrapping effect in x-variables and leads to meaningless results, i.e. the computed rigorous bounds are so large, that become impractical or the program returns overflow. There is an obvious cure to this problem: do the QR-decomposition separately for x-variables and for the variational part. This is what we are doing in the proposed C^1 -algorithm.

7 Applications - Proofs of an existence of periodic orbits for ODEs

In this section we report on some numerical experiments using the proposed C^1 -Lohner algorithm for a computation of a Poincaré map,P, for some ODE's defined by second degree polynomial vector fields. For this class of ODE's we implemented the C_1 -Lohner algorithm in C++ (we used Borland C++ 5.01 compiler). The iterative formulas we used to obtain the Taylor coefficients are given in the Appendix. The computations were performed on PC Pentium III 733 MHZ machine. The orders p_v and p_e were equal. We used always a fixed time step,h, but close to a Poincaré section we reduced h significantly (see Section 5 for more details).

7.1 Interval Newton method for maps

The goal of this subsection is to recall the interval version of the Newton method (see [A] and the references given there) for finding zeros of a function $f: \mathbb{R}^n \to \mathbb{R}^n$.

The following theorem was proved in [A, Thm. 1]

Theorem 9 Let $f: \mathbb{R}^n \to \mathbb{R}^n$ be a C^1 function. Let $X = \prod_{i=1}^n [a_i, b_i]$, $a_i < b_i$. Assume the interval enclosure of Df(X), $[Df(X)]_I$, is invertible. Let $x_0 \in X$ and we define

$$N(x_0, X) = -[Df(X)]_I^{-1} f(x_0) + x_0$$
(99)

Then

- **0.** if $x_1, x_2 \in X$ and $f(x_1) = f(x_2)$, then $x_1 = x_2$
- **1.** if $N(x_0, X) \subset X$, then $\exists ! x^* \in X$ such that $f(x^*) = 0$
- **2.** if $x_1 \in X$ and $f(x_1) = 0$, then $x_1 \in N(x_0, X)$
- **3.** if $N(x_0, X) \cap X = \emptyset$, then $f(x) \neq 0$ for all $x \in X$

When looking for the fixed point of the map P we set f = I - P, hence the set $N(x_0, X)$ will be given by

$$N(x_0, X) = -[I - DP(X)]_I^{-1}(x_0 - P(x_0)) + x_0$$
(100)

We can formulate an interval Newton algorithm for finding fixed points of the map P as follows.

INTERVAL NEWTON ALGORITHM. Let X be a product of intervals. We define the function $N(x_0, X)$ as follows

$$x_0 = \operatorname{mid}(X), \qquad N(x_0, X) = -[I - DP(X)]_I^{-1}(x_0 - P(x_0)) + x_0$$
 (101)

Step 1. Compute $N(x_0, X)$.

Step 2. If $N(x_0, X) \subset X$, then return success.

Step 3. If $X \cap N(x_0, X) = \emptyset$, then return **fail**. There are no fixed points in X.

Step 4. If $X \subset N(x_0, X)$, then we modify the computation parameters. For example decrease a time step, eventually increase the order of the algorithm used to compute P. Go to step 1.

Step 5. Define a new X by $X := X \cap N(x_0, X)$ and go to step 1.

7.2 Rössler equations

The Rössler equations [R] are given by

$$x' = -(y+z) y' = x + 0.2y z' = 0.2 + z(x - a),$$
 (102)

where a is a real parameter. We focus here at the values of a=2.2, where numerical simulations strongly suggest an existence of an attracting limit cycle and a=5.7, where numerical simulations suggest an existence of a strange attractor.

We investigate the Poincaré map on a section $\Pi = \{x = 0, y < 0\}$. In the sequel we will denote this map by P. On Π we will use (y, z) as the coordinates. All data for the Rössler equation presented in subsections 7.3 and 7.4 are expressed in these coordinates.

7.3 Rössler equations for a = 2.2, a proof of an existence of an attracting periodic orbit

For a=2.2 numerical simulations suggest an existence of an attracting limit cycle γ , which gives rise to an attracting fixed point, $x_0 \approx (-3.9205, 0.063858)$, for P on Π . An existence of such periodic orbit (using a topological method based on the Conley index) was recently proved with a computer assistance by Pilarczyk [P] (the computation time was around 2 hours). The fact that the orbit is actually attracting was not established there.

Using x_0 obtained by an iteration of a nonrigorous Newton method, as the starting location of the fixed point, we verified (for the first iterate of the interval

Newton method) that $N(x_0, X) \subset X$, where $X = x_0 + [-2.5 \cdot 10^{-2}, 2.5 \cdot 10^{-2}]^2$. The time step was $h = 10^{-2}$ and the order of the numerical method was p = 4. Below we list some data from this computation

$$N(x_0, X) = x_0 + \left\{ 2.287225 \cdot 10^{-8} + \left[-1.094486 \cdot 10^{-7}, \ 1.094486 \cdot 10^{-7} \right] \right\} \times \left\{ -1.273267 \cdot 10^{-10} + \left[-6.702682 \cdot 10^{-9}, \ 6.702682 \cdot 10^{-9} \right] \right\} \subset X$$

For $x_0 - P(x_0)$ we obtained

$$\begin{array}{lcl} x_0 - P(x_0) & = & [-3.672362 \cdot 10^{-8}, \ 2.247709 \cdot 10^{-8}] \times \\ & & [-8.317404 \cdot 10^{-10}, \ 8.398115 \cdot 10^{-10}] \\ \mathrm{diam}(x_0 - P(x_0)) & = & 5.920072 \cdot 10^{-8} \end{array}$$

We obtained the following values for all entries of DP(X)

$$DP(X)_{11} = [-1.786834, 4.775295 \cdot 10^{-1}]$$

 $DP(X)_{12} = [1.998447, 4.929028]$
 $DP(X)_{21} = [-4.231020 \cdot 10^{-2}, 4.040204 \cdot 10^{-2}]$
 $DP(X)_{22} = [-3.912754 \cdot 10^{-2}, 6.046568 \cdot 10^{-2}]$
 $diam(DP(X)) = 2.930582$

The computation times were 5 seconds for DP(X) and 3 seconds for $P(x_0)$.

The reader may notice that the diameter of the computed DP(X) is quite large, hence with these data we cannot establish that the fixed point found is attracting.

It turns out that increasing order of the method, while keeping the size of X constant and the time step h constant, still gives the diameter of DP(X) of the same size.

To prove that we have here an attracting fixed point for P one needs either to perform the next iterate of the interval Newton algorithm with the set $N(x_0, X)$ obtained above or to choose a smaller starting set. Below we present an example of such set.

For the initial $X = x_0 + [-1, 1]^2 \cdot 10^{-6}$, $h = 10^{-2}$ and p = 4 we obtain

$$N(x_0, X) \subset x_0 + \left\{ 4.546329 \cdot 10^{-9} + \left[-2.075644 \cdot 10^{-8}, \ 2.075644 \cdot 10^{-8} \right] \right\} \times \left\{ -1.358635 \cdot 10^{-11} + \left[-8.82068 \cdot 10^{-10}, \ 8.82068 \cdot 10^{-10} \right] \right\} \subset X$$

For $x_0 - P(x_0)$ we obtained

$$x_0 - P(x_0) = ([-3.672362, 2.247709] \cdot 10^{-8}) \times ([-8.317404, 8.398115] \cdot 10^{-10})$$

 $\operatorname{diam}(x_0 - P(x_0)) = 5.920072 \cdot 10^{-8}$

The entries of DP(X) are

$$DP(X)_{11} = [-5.568081 \cdot 10^{-1}, -5.567340 \cdot 10^{-1}]$$

```
DP(X)_{12} = [3.377049, 3.377150]

DP(X)_{21} = [-2.063501 \cdot 10^{-3}, -2.061059 \cdot 10^{-3}]

DP(X)_{22} = [1.246689 \cdot 10^{-2}, 1.247005 \cdot 10^{-2}]

diam(DP(X)) = 1.019493 \cdot 10^{-4}
```

The eigenvalues of DP(X) are given by

```
\lambda_1 = [-9.0097845007 \cdot 10^{-5}, 7.6326532192 \cdot 10^{-6}]

\lambda_2 = [-5.4431024142 \cdot 10^{-1}, -5.4421251092 \cdot 10^{-1}]
```

Hence the fixed point found is attracting.

7.4 Rössler equations for a = 5.7, a proof of an existence of an unstable periodic orbit

The goal of this section is to show that the proposed C^1 -Lohner algorithm works well enough to obtain an existence of an unstable fixed point.

For the parameter value a=5.7 numerical simulations suggest an existence of a strange attractor. In [Z1] (see also [Z2]) it was proved with a computer assistance that the Poincaré map, P, has a symbolic dynamics on there symbols. In particular it follows from [Z1] that there exists a fixed point $x^* \in [-9, -7] \times [-0.02, 0.08]$ for P. Below using the C^1 -Lohner algorithm and the interval Newton method we find coordinates of this point which much better precision.

For $x_0 \approx (-8.38095, 0.0295902)$, $X = x_0 + [-10^{-3}, 10^{-3}]^2$, $h = 10^{-2}$ and p = 4 we were able to verify that

$$N(x_0, X) = x_0 + \left\{ -4.327904 \cdot 10^{-8} + \left[-3.322230 \cdot 10^{-7}, \ 3.322230 \cdot 10^{-7} \right] \right\} \times \left\{ -3.937174 \cdot 10^{-8} + \left[-6.728499 \cdot 10^{-9}, \ 6.728499 \cdot 10^{-9} \right] \right\} \subset X$$

For $x_0 - P(x_0)$ we obtained the following values

$$x_0 - P(x_0) = [-1.038311 \cdot 10^{-6}, 1.176263 \cdot 10^{-6}] \times$$

 $[3.310963 \cdot 10^{-8}, 4.566477 \cdot 10^{-8}]$
diam $(x_0 - P(x_0)) = 2.214574 \cdot 10^{-6}$

The computed bounds for DP(X) are given by

```
DP(X)_{11} = [-2.438481, -2.372972]

DP(X)_{12} = [1.946089, 1.988827]

DP(X)_{21} = [-1.334871 \cdot 10^{-3}, -8.601484 \cdot 10^{-4}]

DP(X)_{22} = [7.680544 \cdot 10^{-4}, 1.019349 \cdot 10^{-3}]

diam(DP(X)) = 6.550938 \cdot 10^{-2}
```

The eigenvalues of DP(X) are

$$\lambda_1 = [-3.3231261746 \cdot 10^{-2}, 3.3213281643 \cdot 10^{-2}]$$

 $\lambda_2 = [-2.4380463797, -2.3716018363]$

Hence the fixed point found is hyperbolic with one stable and one unstable direction.

7.5 A 14-dimensional Galerkin projection of Kuramoto-Sivashinsky equations

The Kuramoto-Sivashinsky equation [KT, S] (we will use shortcut KS equation in the sequel) introduced in the context of a wave front propagation is given by

$$u_t = -\nu u_{xxxx} - u_{xx} + 2uu_x$$
 $(t, x) \in [0, \infty) \times (-\pi, \pi), \quad \nu > 0.$ (103)

Assuming odd and periodic boundary conditions KS-equation can be reduced (see [ZM]) to the following infinite system of ordinary differential equations for the coefficients of the Fourier expansion of u

$$\dot{a}_k = k^2 (1 - \nu k^2) a_k - k \sum_{n=1}^{k-1} a_n a_{k-n} + 2k \sum_{n=1}^{\infty} a_n a_{n+k} \quad k = 1, 2, 3, \dots$$
 (104)

We will refer to coordinates a_k as modes. In this paper we focus on $\nu = 0.127$. For this parameter value numerical simulations suggests an existence of an attracting limit cycle, whose projection (a_1, a_3) is an ellipse on which the point moves in the clockwise direction.

We focus on the following two sections

$$\Theta_1$$
: angle $-\pi/4$ in the (a_1, a_3) plane: $a_1 + a_3 = 0$, $a_1 > 0$, $a_1' + a_2' < 0$

$$\Theta_2$$
: angle $-5\pi/4$ in the (a_1, a_3) plane: $a_1 + a_3 = 0$, $a_1 < 0$, $a_1' + a_3' > 0$

On these sections we use the following coordinates: $(c_1, c_2, c_3, c_4, ...) = (\sqrt{a_1^2 + a_3^2}, a_2, a_4, a_5, ...)$. We will call them section coordinates.

Let R be a map which leaves even modes and changes sign of odd modes: $a_{2k} \to a_{2k}$ and $a_{2k+1} \to -a_{2k+1}$. It is easy to see that R leaves the system (104) invariant (R is the symmetry of the equations) and sections Θ_1 and Θ_2 are mapped one onto another by this symmetry.

Let $P_{1\to 2}: \Theta_1 \to \Theta_2$ and $P_{2\to 1}: \Theta_2 \to \Theta_1$ denote the Poincaré maps between sections Θ_1 and Θ_2 . We have

$$P_{2\to 1} = RP_{1\to 2}R\tag{105}$$

For the full Poincaré map on section Θ_1 we obtain that

$$P = P_{2\to 1}P_{1\to 2} = RP_{1\to 2}RP_{1\to 2} = (RP_{1\to 2})^2.$$
(106)

Hence any fixed point for $RP_{1\rightarrow 2}$ is a fixed point for P.

For $\nu=0.127$ and the dimension of the Galerkin projection d=14 we have the following approximate fixed point for $RP_{1\rightarrow 2}$ (expressed in section coordinates)

$$x_0 = (0.548852, 1.32064, -0.34417, 0.106402, 0.0322448, -0.0153075, -0.00196743, 0.00166589, 2.79272 \cdot 10^{-5}, -0.000147416, 1.04171 \cdot 10^{-5}, 1.11144 \cdot 10^{-5}, -1.76484 \cdot 10^{-6})$$

We started the interval Newton algorithm with the following parameters

$$\delta = 10^{-5}, \quad X = x_0 + [-\delta, \delta]^{d-1}$$

$$p = 4, \qquad h = \frac{1}{2d^2(\nu d^2 - 1)} \approx 0.000106773$$

and were able to check the assumptions of Theorem 9 and show that the fixed point found is attracting. Below we give some numerical data from these computations.

$$\begin{split} N(x_0,X) &= x_0 + (-4.799947 \cdot 10^{-7} + [-2.301085 \cdot 10^{-7}, \ 2.301085 \cdot 10^{-7}], \\ &\quad 4.638543 \cdot 10^{-7} + [-1.421597 \cdot 10^{-7}, \ 1.421597 \cdot 10^{-7}], \\ &\quad -3.642497 \cdot 10^{-7} + [-1.266866 \cdot 10^{-7}, \ 1.266866 \cdot 10^{-7}], \\ &\quad -4.326831 \cdot 10^{-8} + [-5.090406 \cdot 10^{-8}, \ 5.090406 \cdot 10^{-8}], \\ &\quad 7.367633 \cdot 10^{-8} + [-3.519784 \cdot 10^{-8}, \ 3.519784 \cdot 10^{-8}], \\ &\quad -2.027772 \cdot 10^{-9} + [-9.687707 \cdot 10^{-9}, \ 9.687707 \cdot 10^{-9}], \\ &\quad -1.034572 \cdot 10^{-8} + [-7.233898 \cdot 10^{-9}, \ 7.233898 \cdot 10^{-9}], \\ &\quad 1.377686 \cdot 10^{-9} + [-1.960368 \cdot 10^{-9}, \ 1.960368 \cdot 10^{-9}], \\ &\quad 1.100782 \cdot 10^{-9} + [-1.555556 \cdot 10^{-9}, \ 1.555556 \cdot 10^{-9}], \\ &\quad -2.520153 \cdot 10^{-10} + [-5.082655 \cdot 10^{-10}, \ 5.082655 \cdot 10^{-10}], \\ &\quad -8.833202 \cdot 10^{-11} + [-7.110429 \cdot 10^{-10}, \ 7.110429 \cdot 10^{-10}], \\ &\quad 3.422440 \cdot 10^{-11} + [-7.501527 \cdot 10^{-10}, \ 7.501527 \cdot 10^{-10}], \\ &\quad 9.362639 \cdot 10^{-12} + [-2.636542 \cdot 10^{-9}, \ 2.636542 \cdot 10^{-9}]) \subset x_0 + X \end{split}$$

The rigorous bound for the matrix norm of $DRP_{1\rightarrow 2}(X)$ corresponding to the norm $||x||_m = \max_i |x_i|$ is

$$||DRP_{1\to 2}(X)||_m = \max_{i=1,\dots,d-1} \sum_{i} |DRP_{1\to 2}(X)_{ij}| < 0.82,$$
 (107)

which shows that the fixed point found is attracting.

In Tables 1 and 2 we list two first rows and columns $DRP_{1\to 2}$ to give the reader the feeling about the sizes of the obtained bounds. The entries $DRP_{1\to 2}(X)_{ij}$ are decaying as i and j increases. For the diameter we have

$$diam(DRP_{1\to 2}) = 2.538517 \cdot 10^{-1}$$

Table 1: Two first rows of $DRP_{1\rightarrow 2}(X)$

j	$DRP_{1\to 2}(X)_{1j}$	$DRP_{1\to 2}(X)_{2j}$
1	$[4.450702, 6.989218] \cdot 10^{-1}$	$[-5.042949, -4.544209] \cdot 10^{-1}$
2	$[0.8580582, 7.208375] \cdot 10^{-2}$	$[6.742856, 7.952010] \cdot 10^{-2}$
3	$[-2.103405 \cdot 10^{-2}, 1.077716 \cdot 10^{-3}]$	$[4.114357 \cdot 10^{-2}, \ 4.521749 \cdot 10^{-2}]$
4	$[7.242173 \cdot 10^{-3}, 1.785252 \cdot 10^{-2}]$	$\left[-1.489896 \cdot 10^{-2}, -1.274972 \cdot 10^{-2} \right]$
5	$[-4.405318 \cdot 10^{-3}, -2.183634 \cdot 10^{-3}]$	$[4.344733 \cdot 10^{-3}, 4.762542 \cdot 10^{-3}]$
6	$[-7.412482 \cdot 10^{-4}, -5.316928 \cdot 10^{-4}]$	$[1.905524 \cdot 10^{-4}, 2.181210 \cdot 10^{-4}]$
7	$[1.844130 \cdot 10^{-5}, 1.331995 \cdot 10^{-4}]$	$\left[-1.752168 \cdot 10^{-4}, -1.579311 \cdot 10^{-4} \right]$
8	$[-4.380603 \cdot 10^{-5}, 8.325807 \cdot 10^{-6}]$	$[3.447287 \cdot 10^{-5}, 4.318816 \cdot 10^{-5}]$
9	$[1.565435 \cdot 10^{-6}, 2.055378 \cdot 10^{-5}]$	$\left[-1.268904 \cdot 10^{-5}, -9.857161 \cdot 10^{-6} \right]$
10	$[-3.177638 \cdot 10^{-6}, 4.527249 \cdot 10^{-6}]$	$[-7.197865 \cdot 10^{-7}, 2.291789 \cdot 10^{-7}]$
11	$[-3.236594 \cdot 10^{-6}, 1.487707 \cdot 10^{-6}]$	$[6.155755 \cdot 10^{-7}, 1.206583 \cdot 10^{-6}]$
12	$[-1.415723 \cdot 10^{-6}, 1.494335 \cdot 10^{-6}]$	$[-2.936788 \cdot 10^{-7}, 4.853580 \cdot 10^{-8}]$
13	$[-9.496676 \cdot 10^{-7}, 1.017148 \cdot 10^{-6}]$	$[-1.434915 \cdot 10^{-7}, 8.756737 \cdot 10^{-8}]$

and it is reached for (1,1) entry.

Table 3 contains the computed bounds for $x_0 - RP_{1\rightarrow 2}(x_0)$.

The period of the fixed point found is approximately equal to 2.242. The computation times were 1540 seconds (25.7 minutes) and 628 seconds (10.5 minutes) for C^{1} - and C^{0} -computations, respectively.

We performed a similar computation for d=7,8,9-dimensional Galerkin projection and each time we obtained a proof of an existence of an attracting fixed point. For a comparison, for d=7 the computation times for $h=5\cdot 10^{-4}$, $\delta=10^{-5}$ were 52 and 25 seconds for C^1 - and C^0 -computations, respectively.

8 Conclusions and future directions

It is quite obvious that one can hope to improve the algorithm proposed here, in terms of bounds produced at a given computation cost, by constructing much better rough enclosures (for example by using a low order Taylor method - (see [Lo])) or by introducing a smart time step selection scheme.

But it appears to us that major improvements can be obtained if one will be able to control the Lipschitz part of the error (as it was discussed in the introduction). Another possible huge improvement should be possible if one will be able to evaluate the Taylor formula (or any other formula used as a numerical method) in a way, which will allow for as many cancellations of various terms as possible, so that the computed range using interval arithmetic will be close to the ideal one. To explain what we mean let us consider the computation of

Table 2: Two first columns of $DRP_{1\rightarrow 2}(X)$

i	$DRP_{1\rightarrow 2}(X)_{i1}$	$DRP_{1\rightarrow 2}(X)_{i2}$
1	$[4.450702 \cdot 10^{-1}, 6.989218 \cdot 10^{-1}]$	$[8.580582 \cdot 10^{-3}, 7.208375 \cdot 10^{-2}]$
2	$\left[-5.042949 \cdot 10^{-1}, -4.544209 \cdot 10^{-1} \right]$	$\left[6.742856 \cdot 10^{-2}, 7.952010 \cdot 10^{-2}\right]$
3	$[3.448295 \cdot 10^{-1}, 4.253800 \cdot 10^{-1}]$	$\begin{bmatrix} -5.718379 \cdot 10^{-2}, -3.723603 \cdot 10^{-2} \end{bmatrix}$
4	$[2.070086 \cdot 10^{-2}, 1.004633 \cdot 10^{-1}]$	$[5.415046 \cdot 10^{-3}, 2.537533 \cdot 10^{-2}]$
5	$[-9.715707 \cdot 10^{-2}, -6.493140 \cdot 10^{-2}]$	$[2.745561 \cdot 10^{-3}, 1.070263 \cdot 10^{-2}]$
6	$[-8.989916 \cdot 10^{-3}, 8.344327 \cdot 10^{-3}]$	$\begin{bmatrix} -5.325052 \cdot 10^{-3}, -1.055837 \cdot 10^{-3} \end{bmatrix}$
7	$[6.416967 \cdot 10^{-3}, 1.640791 \cdot 10^{-2}]$	$[-1.843014 \cdot 10^{-3}, 6.005894 \cdot 10^{-4}]$
8	$\left[-2.897343 \cdot 10^{-3}, 6.205670 \cdot 10^{-4} \right]$	$[2.720738 \cdot 10^{-5}, 8.916281 \cdot 10^{-4}]$
9	$\left[-2.582180 \cdot 10^{-3}, 2.064264 \cdot 10^{-4} \right]$	$[-3.203044 \cdot 10^{-4}, 3.720348 \cdot 10^{-4}]$
10	$\left[-2.153901 \cdot 10^{-4}, 6.846829 \cdot 10^{-4} \right]$	$[-1.697652 \cdot 10^{-4}, 6.874759 \cdot 10^{-5}]$
11	$\left[-5.261595 \cdot 10^{-4}, 7.236297 \cdot 10^{-4} \right]$	$[-1.706955 \cdot 10^{-4}, 1.737552 \cdot 10^{-4}]$
12	$\left[-6.866004 \cdot 10^{-4}, 6.194646 \cdot 10^{-4} \right]$	$[-1.857865 \cdot 10^{-4}, 1.971323 \cdot 10^{-4}]$
13	$\left[-2.308010 \cdot 10^{-3}, 2.286113 \cdot 10^{-3} \right]$	$\left[-6.751461 \cdot 10^{-4}, 6.790530 \cdot 10^{-4} \right]$

 e^{-x} using a series expansion

$$e^{-x} = 1 - x + x^2/2! - x^3/3! + \dots$$
 (108)

Assume that we want to compute $e^{-[0,h]}$, for some h>0. It is easy see that the direct interval evaluation of (108) will give us an interval containing $[e^{-h}, \cosh(h)]$, because to compute a possible upper bound we insert x=0 for the odd powers and x=h for the even powers. One can imagine that much worse things may happen in a higher dimensional situation, when we evaluate the higher order terms of the Taylor method, which are complicated expressions, on a rough enclosure, which in many applications can have a considerable diameter. An example of an approach, which deals well with this problem for the Euler method was presented in [T, T1], where monotonicity properties of the vector field were exploited.

Let me finish with pointing out two important directions in the context applications of rigorous numerics to the dynamics of ODE's and PDE's, which apparently require a development of new efficient algorithms.

Bifurcations of periodic orbits for ODE's The C^1 -algorithm developed here should allow to trace rigorously branches of periodic orbits for ODE's, but to treat a rigorously bifurcation point one needs some C^2 -information, which clearly requires an efficient C^2 -algorithm for ODE's.

The dynamics of dissipative PDEs The dynamics of many important PDE's (for example the Navier-Stokes equations) is effectively finite dimensional (see for example [ZM] and references given there). The tools developed in

Table 3: The bounds for $x_0 - RP_{1\rightarrow 2}(x_0)$

i	$x_{0,i} - RP_{1\to 2}(x_0)_i$
1	$[2.100324 \cdot 10^{-7}, 2.120372 \cdot 10^{-7}]$
2	$\begin{bmatrix} -2.094023 \cdot 10^{-7}, -2.085218 \cdot 10^{-7} \end{bmatrix}$
3	$[1.639110 \cdot 10^{-7}, 1.647684 \cdot 10^{-7}]$
4	$[1.873067 \cdot 10^{-8}, 1.925487 \cdot 10^{-8}]$
5	$[-3.372191 \cdot 10^{-8}, -3.350485 \cdot 10^{-8}]$
6	$[8.123026 \cdot 10^{-10}, 8.859718 \cdot 10^{-10}]$
7	$[4.608611 \cdot 10^{-9}, 4.645857 \cdot 10^{-9}]$
8	$\begin{bmatrix} -5.926317 \cdot 10^{-10}, -5.824013 \cdot 10^{-10} \end{bmatrix}$
9	$\left[-4.717564 \cdot 10^{-10}, -4.629766 \cdot 10^{-10} \right]$
10	$[1.055226 \cdot 10^{-10}, 1.099981 \cdot 10^{-10}]$
11	$[3.324677 \cdot 10^{-11}, 4.100305 \cdot 10^{-11}]$
12	$\begin{bmatrix} -1.666509 \cdot 10^{-11}, -1.160854 \cdot 10^{-11} \end{bmatrix}$
13	$\left[-6.625590 \cdot 10^{-12}, 1.340692 \cdot 10^{-12} \right]$

[ZM] promise that one can exploit this finite-dimensionality to perform rigorous computations for these equations. For this end one needs to develop an efficient algorithm for solving ODE's with a controlled perturbation.

9 Appendix. Iterative formulas for the Taylor method for second degree polynomial

Consider the ordinary differential equation

$$x' = f(x), \quad , x \in \mathbb{R}^n, \quad f \text{ is a polynomial of degree 2}$$
 (109)

and let $\varphi(t, x_0)$ be a local flow induced by (109).

Theorem 10 Let $x^{(s)} = x^{(s)}(t, x_0) = \frac{d^s}{dt^s} \varphi(t, x_0)$, then

$$x_i^{(1)} = f_i (110)$$

$$x_i^{(2)} = \sum_{j=1}^n \frac{\partial f_i}{\partial x_j} x_j^{(1)}$$

$$(111)$$

$$x_i^{(r)} = \sum_{j=1}^n \frac{\partial f_i}{\partial x_j} x_j^{(r-1)} + \sum_{j,k=1}^n \frac{\partial^2 f_i}{\partial x_j x_k} a_{rkj} \quad \text{if } r > 2$$
 (112)

where

$$a_{rkj} = \left\{ \sum_{s=0}^{r-3} {r-2 \choose s} x_k^{(r-2-s)} x_j^{(1+s)} \right\}.$$
 (113)

In above formulas the functions f_i , $\frac{\partial f_i}{\partial x_j}$ and $\frac{\partial^2 f_i}{\partial x_j x_k}$ are all evaluated at $x = \varphi(t, x_0)$.

Proof: The formula for $r \leq 3$ is obviously satisfied. So suppose that the formula holds for r-1 and we will show it for r. The term involving $\frac{\partial f_i}{\partial x_j}$ is obviously correct.

Consider now the coefficient of the term $x_k^{(r-2-s)}x_j^{(1+s)}$. If s=0 then this coefficient may result only from the differentiation of $x_k^{(r-3)}x_j^{(1)}$ which was multiplied by $\binom{r-3}{0} = \binom{r-2}{0}$.

For $0 < s \le r-1-3$ we have two possibilities of obtaining $x_k^{(r-2-s)}x_j^{(1+s)}$: we differentiate either x_k or x_j . This gives us the coefficient $\binom{r-3}{s-1} + \binom{r-3}{s-1} = \binom{r-2}{s}$.

For s=r-3 we have the coefficient $\binom{r-3}{r-4}$ from the last term in the sum over s and we have to add to it $1=\binom{r-3}{r-3}$ which arises from the differentiation of $\frac{\partial f_i}{\partial x_j}x_j^{(r-2)}$. Hence we obtain a coefficient $\binom{r-2}{r-3}$.

By taking partial derivatives of $x_i^{(r)}(t,x_0)$ we obtain easily the following

Theorem 11 Let $D_b x_i^{(r)} = D_b x_i^{(r)}(t,x) := \frac{\partial x_i^{(r)}}{\partial x_b}(t,x)$. We have

$$D_b x_i^{(1)} = \sum_{k=1}^n \frac{\partial f_i}{\partial x_k} D_b x_k^{(0)} \tag{114}$$

$$D_b x_i^{(2)} = \sum_{j,k=1}^n \frac{\partial^2 f_i}{\partial x_j \partial x_k} x_j^{(1)} D_b x_k^{(0)} + \sum_{j=1}^n \frac{\partial f_i}{\partial x_j} D_b x_j^{(1)}$$
(115)

and for r > 2

$$D_b x_i^{(r)} = \sum_{j,k=1}^n \frac{\partial^2 f_i}{\partial x_j \partial x_k} x_j^{(r-1)} D_b x_k^{(0)} + \sum_{j=1}^n \frac{\partial f_i}{\partial x_j} D_b x_j^{(r-1)} + \sum_{j,k=1}^n \frac{\partial^2 f_i}{\partial x_j x_k} D_b a_{rkj},$$

where

$$a_{rkj} = \sum_{s=0}^{r-3} {r-2 \choose s} x_k^{(r-2-s)} x_j^{(1+s)}$$

$$D_b a_{rkj} = \sum_{s=0}^{r-3} {r-2 \choose s} \left\{ D_b(x_k^{(r-2-s)}) \cdot x_j^{(1+s)} + x_k^{(r-2-s)} \cdot D_b(x_j^{(1+s)}) \right\}$$

In above formulas the functions f_i , $\frac{\partial f_i}{\partial x_j}$ and $\frac{\partial^2 f_i}{\partial x_j x_k}$ are all evaluated at $\varphi(t,x)$.

Observe that $V_{ib}(t,x) = \frac{\partial \varphi_i}{\partial x_b}(t,x)$ is in the notation used in above theorem equal to $D_b x_i^{(0)}(t,x)$.

It is clear from the expressions given in Theorems 10 and 11, that to compute the functions $x^{(s)}$ and $D_b x^{(s)}$ it is enough to specify $x^{(0)} = \varphi(t, x_0)$ and $D_b x_i^{(0)} = \frac{\partial \varphi_i}{\partial x_b}(t, x_0)$.

The functions $\frac{d^i}{dt^i}f$ and $\frac{d^i}{dt^i}\left(\frac{\partial f}{\partial x}V\right)$ used in Section 2 are given by

$$\left(\frac{d^s}{dt^s}f\right)(x_0) = x^{(s+1)}(x_0)$$

$$\left(\frac{d^s}{dt^s}\left(\frac{\partial f}{\partial x}V\right)\right)_{ib}(x_0, V_0) = D_b x_i^{(s+1)}(x_0, V_0),$$

where $x_0 \in \mathbb{R}^n$ and $V_0 \in \mathbb{R}^{n \times n}$.

The derivative of the Taylor method of order p and a time step h is given by

$$\frac{\partial}{\partial x_b} \Phi_i(h, x, p) = \delta_{ib} + \sum_{s=1}^p \left(\frac{d^{s-1}}{dt^{s-1}} \left(\frac{\partial f}{\partial x} V \right) \right)_{ib} (x, \operatorname{Id}) \frac{h^s}{s!} = \delta_{ib} + \sum_{s=1}^p D_b x^{(i)}(x, \operatorname{Id}) \frac{h^s}{s!},$$

where δ_{ij} is a Kronecker symbol: $\delta_{ij} = 1$ if i = j and $\delta_{ij} = 0$ otherwise.

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