Chaos in the Lorenz Equations: A Computer Assisted Proof; Part III: Classical Parameter Values

by

Konstantin Mischaikow[1]
Center for Dynamical Systems and Nonlinear Studies
School of Mathematics
Georgia Institute of Technology
Atlanta, GA 30030

Marian Mrozek[2]
Instytut Informmatyki
Uniwersytet Jagielloński
Krakow, Poland

and

Andrzej Szymczak
School of Mathematics
Georgia Institute of Technology
Atlanta, GA 30030

[1]Research supported in part by NSF 9805584
[2]Research supported by KBN, Grant 2 P03A 029 12.

1 Introduction

Proving that a given ordinary differential equation possesses chaotic dynamics is a difficult task for two reasons. First, such dynamics only occurs in nonlinear systems, and therefore, the necessary analysis is extremely difficult. Because of this, for most systems which are considered to be chaotic we have no proofs - only numerical evidence obtained by integrating the equations. At the same time however, it makes no sense to talk about chaotic trajectories - any accepted definition of chaos is, in fact, a statement about the existence of uncountably many orbits which together exhibit sensitive dependence on initial conditions.

In this paper we discuss a general computationally inexpensive technique for obtaining a computer assisted proof of the existence of chaos in the sense of symbolic dynamics. We use the Lorenz equations to give a concrete demonstration of this technique.

To be more precise, recall that the Lorenz equations are given by the following system of scalar ordinary differential equations,

$$\dot{x} = \sigma(y-x) \tag{1}$$
$$\dot{y} = Rx - y - xz \tag{2}$$
$$\dot{z} = xy - bz\ . \tag{3}$$

A description of the solutions to these equations will be given in terms of subshift dynamics on a finite set of symbols. In particular, let

$$\Pi_k := \prod_{n=0}^{\infty} \{1, 2, \ldots, k\}.$$

Π_k can be made into a compact metric space by means of the norm

$$||(\alpha_n)|| := \sum_{n=0}^{\infty} \frac{\alpha_n}{2^n}\ .$$

Given a $k \times k$ matrix $A = [a_{ij}]$ with integer entries, let

$$\Sigma(A) := \left\{ (\alpha_n) \,|\, n \in \mathbb{Z}^+,\ \alpha_n \in \{1, 2, \ldots, k\},\ \text{and}\ a_{\alpha_n \alpha_{n+1}} \neq 0 \right\} \subset \Pi_k.$$

The shift operator T defines a dynamical system on $\Sigma(A)$.

The theorem we will prove is the following.

Theorem 1.1 *Consider the Lorenz Equations with parameter values*

$$(\sigma, R, b) \in \{(10, 28, 8/3), (10, 60, 8/3), (10, 54, 45)\}$$

and the plane $P = \{(x, y, z) \mid z = R - 1\}$*. Set*

$$A_{(10,28,8/3)} := \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix},$$

$$A_{(10,60,8/3)} := \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad A_{(10,54,45)} := \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}.$$

Then, for all parameter values in a sufficiently small neighbourhood of (σ, R, b) *there exists a Poincare section* $N \subset P$ *such that the associated Poincare map* f *is Lipschitz and well defined. Furthermore, there is a continuous map* $\rho : \mathrm{Inv}(N, f) \to \Pi_k$*, where* $\mathrm{Inv}(N, f)$ *is the maximal invariant set in* N *under* f*, with the property that* $\Sigma(A_{(\sigma,R,b)}) \subset \rho(\mathrm{Inv}(N, f))$ *and*

$$\rho \circ f = T \circ \rho.$$

Moreover, for each periodic $\alpha \in \Sigma(A)$ *there exists an* $x \in \mathrm{Inv}(N, f)$ *that lies on a periodic trajectory of the same minimal period such that* $\rho(x) = \alpha$*.*

There are several ingredients required in the proof of this theorem. It is perhaps best to describe them in the reverse order from which they are actually used. This discussion will be done on a fairly general level to emphasize that the techniques being employed in this paper are not dependent on a particular structure of the Lorenz Equations.

We begin with some basic notions from dynamical systems. We are interested in understanding the dynamics generated by an ordinary differential equation $\dot{x} = f(x)$. In actuality we will reduce our study to that of the dynamics on a Poincaré section. Thus, we are in essence studying the dynamics generated by a homeomorphism $f : X \to X$, where X is a locally compact metric space. Let $N \subset X$. The *maximal invariant set* in N is defined by

$$\mathrm{Inv}(N, f) := \{x \in N \mid f^n(x) \in N \,\forall\, n \in \mathbb{Z}\}.$$

As can be seen in Theorem 1.1, we are interested in describing the dynamics in $\mathrm{Inv}(N, f)$ by means of symbolic dynamics. Observe that the assertions that ρ is continuous, onto $\Sigma(A)$, and that

$$\rho \circ f = T \circ \rho$$

implies that the symbolic dynamics of $T : \Sigma(A) \to \Sigma(A)$ is a lower bound on the complexity of the dynamics in $\mathrm{Inv}(N, f)$.

Ignoring for the moment how N and f are determined, let us assume that $N = \cup_{i=1}^{k} N_i$ where the N_i are mutually disjoint compact sets. Define the map $\rho : \mathrm{Inv}(N, f) \to \prod_{n=1}^{\infty}\{1, 2, \ldots, k\}$ by

$$\rho(x) = (\alpha_i) \Longleftrightarrow f^i(x) \in N_{b_i} \text{ for each } i \in \mathbb{Z}^+. \tag{4}$$

Since the N_i are disjoint it is easy to check that ρ is a continuous function.

To obtain a lower bound on the image of ρ requires some simple algebraic topology arising from the Conley index. The following concept is fundamental to this theory.

Definition 1.2 A pair $Q = (Q_1, Q_0)$ of compact subsets of X is called an *index pair* for f if the following conditions are satisfied.

(i) $Q_0 \subset Q_1 \subset U$,

(ii) $f(Q_1 \setminus Q_0) \cap Q_1 \setminus Q_0 \subset \mathrm{int}(Q_1 \setminus Q_0)$,

(iii) $f(Q_0) \cap Q_1 \subset \mathrm{int}_{Q_1}(Q_0)$.

The set Q_0 is referred to as the *exit set* for the pair.

A word of caution to the reader with some familiarity of the Conley index, this definition of an index pair is different from the standard definitions, e.g. those in [Mr1, A-J-M-R, R-S]. Its use is justified by [Sz1, Theorem 2.4] and convenient in the numerical context of this paper.

Example 1.3 The simplest nontrival example of an index pair arises in the case of a hyperbolic fixed point. So let $f : \mathbf{R}^2 \to \mathbf{R}^2$ be given by the linear map

$$f = \begin{bmatrix} 3 & 0 \\ 0 & \frac{1}{5} \end{bmatrix}.$$

Let $Q_1 = [-1, 1] \times [-1, 1]$ and let $Q_0 = [1/2, 1] \times [-1, 1] \cup [-1, -1/2] \times [-1, 1]$. The reader can easily check that $Q = (Q_1, Q_0)$ is an index pair.

The importance of an index pair comes from the fact that it can be used to transform the problem of describing the dynamics of the invariant set $\mathrm{Inv}(\mathrm{cl}(Q_1 \setminus Q_0), f)$ from a local question into a global one. More precisely, f induces a continuous function f_Q, called the *index map*, on the pointed compact space $(Q_1/Q_0, [Q_0])$ given by

$$f_Q([x]) = \begin{cases} [f(x)] & \text{if } x, f(x) \in Q_1 \setminus Q_0 \\ [Q_0] & \text{otherwise} \end{cases}$$

It is easy to see that $\mathrm{Inv}(Q_1/Q_0 \setminus \{[Q_0]\}, f_Q)$ is an exact copy of $\mathrm{Inv}(\mathrm{cl}(Q_1 \setminus Q_0), f)$.

In our approach $N := \mathrm{cl}(Q_1 \setminus Q_0)$ and the matrix A is obtained from the cohomology map of f_Q using rational coefficients, i.e.

$$f_Q^* : H^*(Q_1/Q_0, [Q_0]) \to H^*(Q_1/Q_0, [Q_0]).$$

The conclusion that the image of ρ contains $\Sigma(A)$ is discussed in Section 2. The observation that needs to be made at this point is that to obtain the surjectivity of ρ it is sufficient to know f_Q^*. As will be made clear in Section 6 cohomology is a combinatorial invariant, i.e. it can be computed from a finite amount of data. We use the computer to obtain these data points and as the reader will see most of this paper is spent discussing how to minimize the number of data points used and verifying that these data points give the correct results.

Determing the Poincaré map f and the index pair (Q_1, Q_0) are, of course, matters of analysis and as was just indicated this is a part of where the computer is employed. Ideally f would be the Poincaré map associated with the Lorenz equations. Of course, this is unknown. What we do know is a Runge-Kutta approximation of the map. Two issues have to be resolved. First, since we are using the computer we can only manipulate a finite amount of data. Second, we need to know that the index pair computed using the numerical approximation to the Lorenz equation provides us with the correct algebraic topological information.

To overcome these issues we first discretize the phase space using cubes; this is discussed in Section 3. Since we are after a rigorous proof, we need to keep track of error bounds. This is done by employing multivalued maps which are described in Section 4. The idea is that the images of the multivalued map contain the sets defined by the approximation plus the error bound. In particular, the error bounds that are ultimately used are bounds which are valid over the cubes used in the discretization. Of course to numerically integrate an ordinary differential equation and maintain reasonable bounds that are valid for all initial conditions in a cube requires that the cubes be extremely small. Thus, a straightforward application of these ideas (as was done in [M-M]) leads to very expensive computations. For this reason we employ a two step procedure.

The first step is based on the fact that while worst case error bounds typically grow exponentially fast, in reality errors are often reasonably small. Thus, using a coarse grid we obtain what appears to be a reasonable index pair with an appropriate Conley index. This is discussed in Section 7. We want to emphasize that the computations done in this section are in spirit the closest to standard numerical methods. We have faith in the Runge-Kutta scheme and so we compute with the belief that the results obtained will be correct. This of course is not a proof!

The second step is to rigorously verify that the previously mentioned computations do, in fact, give the correct results. Again, this is done in two parts. It needs to be rigorously shown that there is a well defined Poincaré map on what we believe to be a reasonable index pair. This is done first, using the algorithms from [M-M]. Now comes the expensive part, obtaining a multivalued map which captures the error bounds. However, as is shown in Section 5, because the Poincaré map is a homeomorphism one only needs to verify the conditions of the index pair at the cubes which define the boundary of the index pair. Thus, the expensive computations only need to be performed over a small region of the phase space. This in turn leads to a considerable savings in computational cost.

Before beginning with the details it should once again be emphasized that the primary point of this paper are the numerical techniques. The Lorenz Equations are used only as an example of how these ideas can be applied. In particular, for the classical parameter values (10,28,8/3) a much more complete description of the dynamics has been obtain by W. Tucker [T]. His approach is based on a different numerical approach combined with some detailed normal form analysis near the origin. In our approach the actual form of the equations plays no role. The results at the parameter values (10,60,8/3) and (10,54,45) appear to be new, but again, and this will become clear in Section 8, it should be emphasized the the computational proceedure is identical even though the dynamics at these values are quite different. Finally, we also report on a computation at the parameter value (10,490,1/4) where we have not been able to rigorously verify the computation - indicating room for improvement of these techniques.

2 The Lefschetz-Ważewski-Conley method

Our proof of chaos in the Lorenz Equations uses a very small portion of the Conley index theory for discrete dynamical systems. The purpose of this section is to describe the needed results in a way which avoids the categorical and algebraic details required for the full theory. The hope is that this approach will prove to be more accessible to readers not versed in the subject.

As in the introduction, X represents a locally compact metric space and $f : U \to X$ a continuous map defined on U an open subset of X. Though the results of this section are rather general in nature, the reader may wish to think of f as the Poincaré map of the Lorenz equation and X as the plane $P = \{(x, y, z) \mid z = R - 1\}$. Observe that in this special setting the stable manifold of the origin intersects P. Therefore, it is impossible to define a Poincaré map f whose domain is all of P. It is for this reason that we do not assume $U = X$.

Let $x \in U$. A *full trajectory* through x is a bi-infinite set $\{x_n\}_{n=-\infty}^{\infty} \subset U$ such that $x_0 = x$ and $x_{n+1} = f(x_n)$. A set $S \subset U$ is *invariant* under f if $f(S) = S$. For any set $K \subset U$ the invariant part of K, denoted by $\mathrm{Inv}(K, f)$, is defined as the *maximal invariant subset* of K. Alternatively, one can define it as the set of all $x \in X$ for which there exists a full trajectory through x contained entirely in K.

Let $Q = (Q_1, Q_0)$ be an index pair for f and assume that $\mathrm{cl}(Q_1 \setminus Q_0)$ decomposes into a finite number of compact sets $N_1, N_2, \ldots, N_k$ (where $k \in \mathbb{N}$). Let $\rho : \mathrm{Inv}(N, f) \to \prod_{n=1}^{\infty}\{1, 2, \ldots, k\}$ be defined by (4) and observe that on $\mathrm{Inv}(N, f)$

$$\rho \circ f = T \circ \rho, \tag{5}$$

where $T : \prod_{n=1}^{\infty}\{1, 2, \ldots, k\} \to \prod_{n=1}^{\infty}\{1, 2, \ldots, k\}$ is the shift map. Since the dynamics of the shift map is known, we obtain information about the dynamics on S by understanding the set $\rho(S)$. This last point is where the algebraic topology is used.

For each $i \in \{1, 2, \ldots, k\}$, define $r_i : (Q_1/Q_0, [Q_0]) \to (Q_1/Q_0, [Q_0])$ by

$$r_i([x]) = \begin{cases} [x] & \text{if } x \in N_i \\ [Q_0] & \text{otherwise.} \end{cases}$$

Let H^* be a cohomology functor with rational coefficients. Of importance to us is the fact that H^* takes us from the category of pairs of topological spaces and continuous maps to the category of finite dimensional vectors spaces and linear maps. Furthermore, given a continuous function f if the resulting linear map on cohomology $H^*(f)$ is nonzero, then this implies, in general, that f is nontrivial. With this as motivation define endomorphisms

$$\varphi_i^* : H^*(Q_1/Q_0, [Q_0]) \to H^*(Q_1/Q_0, [Q_0])$$

by

$$\varphi_i^* := H^*(f_Q \circ r_i) \quad \text{for} \quad i = 1, 2, \dots, k.$$

This provides an algebraic measurement of how elements of $N_i \setminus Q_0$ are mapped to $Q \setminus Q_0$. To generalize this define $\Pi_f^+ = \Pi_f^+(Q, \{N_i\})$ by

$$\Pi_f^+ = \left\{ (b_i)_{i \in \mathbb{Z}^+} \in \Pi : \varphi_{b_0}^* \circ \varphi_{b_1}^* \circ \dots \circ \varphi_{b_{n-1}}^* . \neq 0 \quad \text{for each } n \in \mathbb{N} \right\},$$

Notice that if $(b_i)_{i \in \mathbb{Z}^+}$, then given any $n \in \mathbb{Z}^+$ there exists a point $x \in Q$ such that the trajectory of x under f traverses through the sets N_{b_0}, N_{b_1}, ... , N_{b_n}. Let

$$\Pi_f = \Pi_f(Q, \{N_i\}) := \bigcap_{n \in \mathbb{Z}^+} T^n(\Pi_f^+).$$

Remark 2.1 As will be shown in the last section of this paper, the induced map on cohomology $\varphi_i^j = 0$ for all $j \neq 1$, i.e. only the first cohomology is non-trivial. In this case if we set $A = H^1(f_Q)$, then $\Sigma(A) = \Pi_f$.

To obtain stronger information concerning the types of orbits which exist we need to use more algebraic information. Assuming that $H^*(Q_1/Q_0, [Q_0])$ is of finite type,[3] define the set $P_{f,n} = P_{f,n}(Q, \{N_i\})$ as follows.

$$P_{f,n} = \left\{ (b_i)_{i \in \mathbb{Z}^+} \in \Pi(n) : \Lambda(\varphi_{b_0}^* \circ \varphi_{b_1}^* \circ \dots \circ \varphi_{b_{n-1}}^*) \neq 0 \right\}.$$

where $\Pi(n)$ denotes the subset of Π consisting of n-periodic sequences such that n is their least period and $\Lambda(\psi^*)$ denotes the Lefschetz number for the graded endomorphism ψ^*.

These ideas are summarized in the following theorem (for the proof, see [Sz2, theorems 4.4 and 4.5], which provides a description of the invariant set S in terms of these sets.

[3] $H^*(Q_1/Q_0, [Q_0])$ has *finite type* if $H^n(Q_1/Q_0, [Q_0])$ is finite dimensional for all $n \in \mathbb{Z}^+$ and $H^n(Q_1/Q_0, [Q_0]) = 0$ for all but finitely many values of n.

Theorem 2.2 **(i)** $\Pi_f \subset \rho(S)$

(ii) *If X is an ENR then the image under ρ of the set of periodic points of f in S whose least period is n contains $P_{f,n}$.*

Let us note that both the index pairs (in the sense of Definition 1.2) and the $P_{f,n}$ and Π_f sets are stable under small perturbations of the map f (under reasonable assumptions on X). Therefore, one does not need to possess precise information about the map f in order to come up with an index pair and compute these sets. Of course, this is a result of using the cohomology functor, which is a homotopy invariant. Let us stress again that this was made possible by globalizing the problem of describing the dynamics of f on S with the aid of an index pair Q. Indeed, in Theorem 2.2 we use the algebraic properties of the globally defined map f_Q rather than local properties of f near S.

3 Discrete geometrical structures

As was indicated in the introduction, to perform the numerical computations it is necessary to discretize the phase space of the Poincaré map. This section presents the notation used in this discretization. From a theoretical point of view our techniques are not limited by the dimension of the phase space, therefore we present a general version of the discretization with the expectation that it will prove useful for other applications. Obviously in practice dimension will have a large impact in the computational expense.

We will uniformly discretize $\mathbb{R}^s$ into s-dimensional cubes as follows. The first step is to determine the size of the cubes by choosing lengths in each direction. This is denoted by the vector

$$\xi = (\xi_1, \ldots, \xi_s) \in \mathbb{R}^s.$$

Define

$$\xi\mathbb{Z}^s := \{(\xi_1 n_1, \xi_2 n_2, \ldots, \xi_s n_s) \in \mathbb{R}^s \mid n_i \in \mathbb{Z}\}.$$

Obviously, there exists a bijection between $\xi\mathbb{Z}^s$ and $\mathbb{Z}^s$, and therefore, the entire presentation here could be done in terms of subsets of $\mathbb{Z}^s$. However, as will be made clear shortly, elements of $\xi\mathbb{Z}^s$ will be identified with cubes in $\mathbb{R}^s$. For the benefit of the reader we have chosen to make this identification as simple as possible.

Given $k = (k_1, k_2, \ldots, k_s) \in \xi\mathbb{Z}^s$ set

$$|k| = |k|_\xi = |(k_1, k_2, \ldots, k_s)|_\xi := \prod_{i=1}^{s} [k_i, k_i + \xi_i] \subset \mathbb{R}^s.$$

Thus we are assigning to each element of the lattice $\xi\mathbb{Z}^s$ an s-dimensional cube with sides of length ξ_i. Given $\mathbf{K} \subset \xi\mathbb{Z}^s$ define

$$|\mathbf{K}| = |\mathbf{K}|_\xi := \bigcup_{k \in \mathbf{K}} |k| \subset \mathbb{R}^s.$$

A set $V \subset \mathbb{R}^s$ is ξ-*representable* (or just *representable* whenever ξ is clear from the context) if there exists $\mathbf{K} \subset \xi\mathbb{Z}^s$ such that $V = |\mathbf{K}|$. To pass from ξ-representable sets to the lattice points we will use the notation

$$\xi\mathcal{R}(V) := \{k \in \xi\mathbb{Z}^s \mid |k| \subset V\}.$$

Observe that if V is ξ-representable, then $V = |\xi\mathcal{R}(V)|$.

Because we are restricted to using representable sets, having fixed a grid, neighborhoods of sets in $\mathbb{R}^s$ become quite restrictive in their form. To describe them we use the following notation. Given $\mathbf{K} \subset \xi\mathbb{Z}^s$:

$$\mathrm{o}(\mathbf{K}) = \{k \in \xi\mathbb{Z}^s \mid |k| \cap |\mathbf{K}| \neq \emptyset\}$$

which is the smallest neighborhood containing $\mathbf{K}$;

$$\mathrm{d}(\mathbf{K}) = \mathrm{o}(\mathbf{K}) \setminus \mathbf{K}$$

which can be thought of as the "external" boundary elements of $\mathbf{K}$; and

$$\tilde{\mathrm{d}}(\mathbf{K}) = \mathrm{d}(\xi\mathbb{Z}^s \setminus \mathbf{K})$$

which might be interpreted as the "internal" boundary elements of $\mathbf{K}$.

If $\mathbf{K} \subset \xi\mathbb{Z}^s$, then there exists an unbounded connected component U of $\mathbb{R}^s \setminus \mathrm{int}|\mathbf{K}|$. Let

$$b(\mathbf{K}) := \{k \in \xi\mathbb{Z}^s \mid |k| \not\subset U\}.$$

It is easy to see that for any $A \subset \mathrm{int}|\mathbf{K}|$, the union of all unbounded connected components of the complement of A and the set A itself is contained in $\mathrm{int}|b(\mathbf{K})|$.

The *center* of $|k|$ is the point of $\mathbb{R}^s$ defined by

$$C(k) = \Big(k_1 + \frac{1}{2}\xi_1, k_2 + \frac{1}{2}\xi_2, \dots, k_s + \frac{1}{2}\xi_s\Big).$$

In order to obtain the symbolic dynamics we need to have a decomposition of our index pair. On the combinatorial level this takes the following form.

Definition 3.1 Let $\mathbf{K}$ be a finite subset of $\xi\mathbb{Z}^s$. A family $\{\mathbf{K}_1, \mathbf{K}_2, \dots, \mathbf{K}_n\}$ of subsets of $\mathbf{K}$ is called a *decomposition* of $\mathbf{K}$ if and only if, for all $i \neq j$, $o(\mathbf{K}_i) \cap \mathbf{K}_j = \emptyset$ and $\mathbf{K} = \bigcup_{i=1}^n \mathbf{K}_i$.

Geometrically, a decompostion means that $|\mathbf{K}_1|, |\mathbf{K}_2|, \dots, |\mathbf{K}_n|$ are pairwise disjoint compact sets whose union is $|\mathbf{K}|$.

Two elements of the lattice, k and l, are *continguous* if there exists a unique $i_0 \in \{1, 2, \dots, s\}$ such that

$$|k_i - l_i| = \begin{cases} \xi_{i_0} & \text{if } i = i_0 \\ 0 & \text{otherwise.} \end{cases}$$

Observe that k and l contiguous implies that $|k|$ and $|l|$ share an $(s-1)$-dimensional face, i.e.

$$|k| \cap |l| = \prod_{i=1}^{s} J_i^{i_0}(k_i)$$

where

$$J_i^{i_0}(x_i) = \begin{cases} [x_i, x_i + \xi_i] & \text{if } i \neq i_0 \\ \{x_i\} & \text{if } i = i_0 \end{cases}.$$

Given a lattice point k by $\operatorname{cntg}(k)$ we denote the set of all lattice points l such that k and l are contiguous. For $\mathbf{K} \subset \xi\mathbb{Z}^s$ we put

$$\operatorname{cntg}(\mathbf{K}) = \bigcup_{k \in \mathbf{K}} \operatorname{cntg}(k) \setminus \mathbf{K}.$$

Roughly speaking, $\operatorname{cntg}(\mathbf{K})$ consists of the s-dimensional cubes whose intersection with the set $|\mathbf{K}|$ is $(s-1)$-dimensional. Let us note that, for each $\mathbf{K} \subset \xi\mathbb{Z}^s$, the boundary of $|\mathbf{K}|$ is contained in $|\operatorname{cntg}(\mathbf{K})|$. In fact, for any $x \in \operatorname{bd}|\mathbf{K}|$, there exist elements $k \in \mathbf{K}$ and $l \in \xi\mathbb{Z}^s \setminus \mathbf{K}$ which are contiguous and contain x.

The collection of all representable sets in $\mathbb{R}^s$ is too large and unwieldy for computational purposes. Thus, we shall focus on the special subcase of rectangular sets which are defined as follows. $\mathbf{K} \subset \xi\mathbb{Z}^s$ is *rectangular* if there exist two elements $k = (k_1, \ldots, k_s)$, $k' = (k'_1, \ldots, k'_s) \in \xi\mathbb{Z}^s$ such that

$$\mathbf{K} = \xi\mathrm{R}\textsc{ct}(k, k') := \{l \in \xi\mathbb{Z}^s \mid k_i \leq l_i \leq k'_i \text{ or } k'_i \leq l_i \leq k_i\}.$$

Observe that a rectangular set can be stored using only two data entries, and therefore, are convenient from the point of view of data structures.

Since we will often want to construct rectangular sets, it is convenient to define

$$\xi\mathcal{S}(k, r) := \xi\mathrm{R}\textsc{ct}((k_1 - r\xi_1, \ldots, k_s - r\xi_s), (k_1 + r\xi_1, \ldots, k_s + r\xi_s)) \subset \xi\mathbb{Z}^s.$$

for $k \in \xi\mathbb{Z}^s$ and $r \in \mathbb{Z}^+$. In order to simplify the notation, we define $\xi\mathcal{S}(k, -1) = \emptyset$. For a nonempty set $\mathbf{K} \subset \xi\mathbb{Z}^s$ and lattice point k the distance from k to $\mathbf{K}$ is defined by

$$\mathrm{dist}(k, \mathbf{K}) = \max\{r \in \{-1\} \cup \mathbb{Z} \mid \xi\mathcal{S}(k, r) \cap \mathbf{K} = \emptyset\}.$$

Notice that if $k \in \mathbf{K}$ then the distance from k to $\mathbf{K}$ is negative (equal to -1). Although this may seem rather unusual, it will turn out to be convenient later.

In what follows, we shall often use rectangular multivalued maps of $\xi\mathbb{Z}^s$ into itself, i.e. functions of the form $\Psi : \mathbf{K} \to 2^{\xi\mathbb{Z}^s}$, where $\mathbf{K}$ is some subset of $\xi\mathbb{Z}^s$ and $\Psi(k)$ is a rectangular set for every $k \in \mathbf{K}$. To simplify the notation we shall indicate multivalued maps by the symbol $\rightrightarrows$, e.g. $\Psi : \mathbf{K} \rightrightarrows \xi\mathbb{Z}^s$.

4 Enclosures

As will be clear at the end of the paper, in essence the final step in our proof of the existence of chaotic dynamics in the Lorenz equations is the application of Theorem 2.2. The essential input for this theorem is a continuous map and an index pair consisting of several disjoint sets. It was stated in Section 3 that our use of the computer involves the manipulation of a finite number of elements of the integer lattice $\xi\mathbb{Z}^s$. In this section we will present the framework by which we pass from the continuous topological setting to the finite combinatorial setting.

As with the previous sections, $f : U \to \mathbb{R}^s$ is a continuous map and U is an open subset of $\mathbb{R}^s$. For the moment we will be working with a fixed discretization of $\mathbb{R}^s$. Using the notation of Section 2 this corresponds to a particular choice of $\xi \in \mathbb{R}^s$.

Definition 4.1 A ξ-*enclosure* is a pair $(\mathbf{K}, \Phi)$ consisting of a finite set $\mathbf{K} \subset \xi\mathbb{Z}^s$ and a multivalued map with rectangular values

$$\Phi : \mathbf{K} \rightrightarrows \xi\mathbb{R}^s.$$

The function $f : U \to \mathbb{R}^s$ is *enclosed by* $(\mathbf{K}, \Phi)$ if $|\mathbf{K}| \subset U$ and for every $k \in \mathbf{K}$

$$f(|k|) \subset \mathrm{int}|\Phi(k)|.$$

$\mathrm{Encl}(\mathbf{K}, \Phi)$ denotes the set of all continuous functions enclosed by $(\mathbf{K}, \Phi)$.

Example 4.2 Recalling the linear map of Example 1.3, let $\xi = (1/2, 1/2)$. Let $\mathbf{K} = \xi\mathrm{R{\scriptsize CT}}((-1,-1),(1/2,1/2))$. Let $\Phi : \mathbf{K} \rightrightarrows \xi\mathbb{R}^s$ be given by $\Phi(k) = \xi\mathcal{S}(f(k), 4)$. Then, $(\mathbf{K}, \Phi)$ is a ξ-enclosure of f.

Observe that given an enclosure $(\mathbf{K}, \Phi)$ of f, $\mathbf{K}$ represents an "upper bound" on the domain of f while Φ serves as a "lower bound" on images of cubes under f.

To apply the results of the previous section we need a combinatorial representation of index pairs. This is provided for by the following definition.

Definition 4.3 Let $(\mathbf{K}, \Phi)$ be an enclosure. Given $\mathbf{B} \subset \xi\mathbb{Z}^s$ set

$$\mathbf{K}_0 := \mathrm{cntg}(\mathbf{B}) \cap \mathbf{K}.$$

$(\mathbf{K}, \Phi)$ is an *IP-enclosure* for $\mathbf{B}$ if the following conditions hold:

(i) $\mathbf{B} \subset \mathbf{K} \subset \mathbf{B} \cup \mathrm{cntg}(\mathbf{B})$,

(ii) for every $k \in \mathbf{K}_0$,

$$\Phi(k) \cap \mathbf{B} = \emptyset,$$

(iii) for every $k \in \mathbf{K} \setminus \mathbf{K}_0$,

$$\Phi(k) \cap \mathrm{cntg}(\mathbf{B}) \subset \mathbf{K}_0.$$

Example 4.4 Continuing with Example 1.3 and Example 4.2, Set $\mathbf{B} = \xi\mathrm{R{\scriptsize CT}}((-1/2,-1),(1/2,1))$. Then $(\mathbf{K}, \Phi)$ is an IP-enclosure for $\mathbf{B}$.

The reader should compare the definition of an IP-enclosure with that of an index pair. In analogy with this latter definition, $\mathbf{K}_0$ is referred to as the *exit set for* $(\mathbf{K}, \Phi)$. The following theorem justifies the definition of an IP-enclosure and in particular it implies that having an IP-enclosure provides one with an index pair for any dynamical system which it encloses.

Theorem 4.5 *Let $E = (\mathbf{K}, \Phi)$ be an IP-inclosure for $\mathbf{B}$ and $\mathbf{K}_0$ its exit set. Then, for any $f \in \mathrm{Encl}(E)$, the pair*

$$Q(E, \mathbf{B}) = (Q_1(E, \mathbf{B}), Q_0(E, \mathbf{B})) = (Q_1, Q_0) := (|\mathbf{K}|, |\mathbf{K}_0|)$$

is an index pair for f. Furthermore, the homotopy class of the index map $f_Q : (Q_1/Q_0, [Q_0]) \to (Q_1/Q_0, [Q_0])$ does not depend on the choice of an $f \in \mathrm{Encl}(E)$.

Proof. Notice that by Definition 4.3(ii),

$$\begin{aligned}
\mathrm{cl}(Q_1 \setminus Q_0) \cap f(Q_0) &= \mathrm{cl}(|\mathbf{K}| \setminus |\mathbf{K}_0|) \cap f(|\mathbf{K}_0|) \\
&\subset \bigcup_{k \in \mathbf{K}_0} \mathrm{int}|\Phi(k)| \cap |\mathbf{K} \setminus \mathbf{K}_0| \\
&\subset \bigcup_{k \in \mathbf{K}_0} \mathrm{int}|\Phi(k)| \cap |\mathbf{B}| \\
&= \emptyset.
\end{aligned}$$

It follows that

$$f(Q_0) \cap Q_1 \subset \mathrm{int}_{Q_1}(Q_0), \tag{6}$$

so Definition 1.2(ii) holds.

Furthermore,

$$\begin{aligned}
f(\mathrm{cl}(Q_1 \setminus Q_0)) \cap \mathrm{bd}(Q_1 \setminus Q_0) &\subset \bigcup_{k \in \mathbf{K} \setminus \mathbf{K}_0} f(k) \cap |\mathrm{cntg}(\mathbf{B})| \\
&\subset \bigcup_{k \in \mathbf{B}} \mathrm{int}|\Phi(k)| \cap |\mathrm{cntg}(\mathbf{B})|
\end{aligned}$$

The set on the right is contained in $Q_0 = |\mathbf{K}_0|$ by Definition 4.3(iii). Therefore,

$$f(\mathrm{cl}(Q_1 \setminus Q_0)) \cap Q_1 \setminus Q_0 \subset \mathrm{int}(Q_1 \setminus Q_0) \tag{7}$$

which proves that Definition 1.2(i) holds.

In order to prove the second statement, notice that if f^0 and f^1 are functions in $\mathrm{Encl}(E)$ then the function $f^t = tf^1 + (1-t)f^0$ is also in $\mathrm{Encl}(E)$ for each $t \in [0,1]$ and therefore Q is an index pair for f^t. Hence a homotopy connecting the corresponding index maps f_Q^0 and f_Q^1 can be defined by

$$h(p,t) = f_Q^t(p).$$

∎

At this point Example 4.4 may give the misleading impression that IP-enclosures are easily computable objects. To dispell this notion observe that $\mathbf{B}$ was given, in applications $\mathbf{B}$ needs to be computed. In fact, given the diameters of the values of Φ we cannot compute $\mathbf{B}$ (how $\mathbf{B}$ is found will be discussed in a later section). Unfortunately, if we make the diameters of the values of Φ much smaller then it will not enclose f, unless we simultaneously choose a finer grid which would rapidly increase the expense. On the other hand, we know that $(|\mathbf{K}|, |\mathbf{K}_0|)$ is a nice index pair even on this course grid.

To get around this dilemma, we make use of the fact that $f : U \to f(U)$ is a homeomorphism. The idea is that we use the coarse grid and a map Φ which does not satisfy the worst case error bounds, i.e. the diameters of its images are smaller than we can rigorously justify. With this small map, we are able to compute $\mathbf{B}$ and get the desired pair. Now, because f is a homeomorphism to rigorously verify that we have a correct index pair, it is sufficient to check for that enclose holds on the boundary of the index pair. For this reason we introduce the following definition.

Definition 4.6 Let $(\mathbf{K}, \Phi)$ be a ξ-enclosure and $\mathbf{B} \subset \xi\mathbb{Z}^s$ be a finite set. $(\mathbf{K}, \Phi)$ is a *BIP-enclosure* for $\mathbf{B}$ if and only if the following conditions hold:

(i) $\mathbf{K} \subset \mathbf{B} \cup \mathrm{cntg}(\mathbf{B})$

(ii) $\mathrm{bd}|\mathbf{B}| \subset |\mathbf{K}|$

(iii) for any $k \in \mathbf{K}_0$,

$$\Phi(k) \cap \mathbf{B} = \emptyset$$

(iv) There is a decomposition $\{\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_n\}$ of $\mathbf{B}$ with the following property.

$$\forall_{i\in\{1,2,\ldots,n\}} \quad b\big(\Phi(\mathbf{K} \cap \mathbf{L}_i)\big) \cap \mathrm{cntg}(\mathbf{B}) \subset \mathbf{K}_0,$$

where $\mathbf{L}_i = \mathbf{B}_i \cup \mathrm{cntg}(\mathbf{B}_i)$

If, in addition, there exists a set $F \subset |\mathbf{K}|$ such that the pair $(F, F \cap |\mathbf{K}_0|)$ is a strong deformation retract of $(|\mathbf{K} \cup \mathbf{B}|, |\mathbf{K}_0|)$, then the enclosure E is called a *sharp BIP-enclosure.*

As in Definition 4.3, $\mathbf{K}_0$ will be called the *exit set for* $(\mathbf{K}, \Phi)$.

The next theorem provides a justification for this definition.

Theorem 4.7 *Let $E = (\mathbf{K}, \Phi)$ be a BIP-inclosure for $\mathbf{B}$ and $\mathbf{K}_0$ its exit set. Then, for any homeomorphism $f \in \mathrm{Encl}(E)$ such that $|\mathbf{B}|$ is contained in the domain of f, the pair*

$$Q(E,\mathbf{B}) = (Q_1(E,\mathbf{B}), Q_0(E,\mathbf{B})) = (Q_1, Q_0) = (|\mathbf{K} \cup \mathbf{B}|, |\mathbf{K}_0|),$$

is an index pair for f.

If E is a sharp BIP-inclosure then the homotopy class of the index map $f_Q : Q_1/Q_0 \to Q_1/Q_0$ is independent of the choice of a map $f \in \mathrm{Encl}(E)$ such that $Q(E,\mathbf{B})$ is an index pair for f.

We shall refer to $Q(E,\mathbf{B})$ as the *pair associated with E*. Let us note that, both in the setting of the above Theorem 4.7 and that of Theorem 4.5,

$$Q(E,\mathbf{B}) = (|\mathbf{K} \cup \mathbf{B}|, |\mathrm{cntg}(\mathbf{B}) \cap \mathbf{K}|).$$

In this sense, the notation for $Q(E,\mathbf{B})$ is not ambiguous.

Proof. The requirement of Definition 1.2(ii) can be shown in the same way as in the previous proof.

Since f is a homeomorphism, $f(|\mathbf{B}_i|)$ is contained in the union of $f(\mathrm{bd}|\mathbf{B}_i|)$ and all bounded connected components of its complement. Making use of the inclusion (recall that $\mathbf{L}_i = \mathbf{B}_i \cup \mathrm{cntg}(\mathbf{B}_i)$)

$$f(\mathrm{bd}|\mathbf{B}_i|) \subset f(|\mathbf{K} \cap \mathbf{L}_i|) \subset \mathrm{int}|\Phi(\mathbf{K} \cap \mathbf{L}_i)|$$

one obtains

$$f(|\mathbf{B}_i|) \subset \bigcup_{i=1}^{n} \mathrm{int}|b(\Phi(\mathbf{K} \cap \mathbf{L}_i))|.$$

Together with the inclusion of Definition 4.6(iv), this gives

$$\begin{aligned} f(\mathrm{cl}(Q_1 \setminus Q_0)) \cap \mathrm{bd}(Q_1 \setminus Q_0) &\subset f(|\mathbf{B}|) \cap |\mathrm{cntg}(\mathbf{B})| \\ &\subset \bigcup_{i=1}^{n} \mathrm{int}|b(\Phi(\mathbf{K} \cap \mathbf{L}_i))| \cap |\mathrm{cntg}(\mathbf{B})| \\ &\subset |\mathbf{K}_0| = Q_0 \end{aligned}$$

so that the inclusion (7) holds and Definition 1.2(i) follows.

Let $A \subset |\mathbf{K}|$ be a set such that there exists a strong deformation retraction

$$r : (|\mathbf{K} \cup \mathbf{B}|, |\mathbf{K}_0|) \longrightarrow (A, A \cap |\mathbf{K}_0|).$$

Clearly, r induces the strong deformation retraction

$$\bar{r} : |\mathbf{K} \cup \mathbf{B}|/|\mathbf{K}_0| \longrightarrow i(A/(A \cap |\mathbf{K}_0|)),$$

where $i : A/(A \cap |\mathbf{K}_0|) \to |\mathbf{K} \cup \mathbf{B}|/|\mathbf{K}_0|$ is the inclusion-induced map.

Let $f^0, f^1 \in \mathrm{Encl}(E)$ be continuous maps such that Q is an index pair for each of them. As in the proof of the previous theorem, define $f^t = tf^1 + (1-t)f^0$ for each $t \in [0,1]$. Unlike the situation in Theorem 4.5, Q need not be an index pair for each of the maps f^t. However, each of these maps belongs to $\mathrm{Encl}(E)$ and therefore, since $A \subset |\mathbf{K}|$,

$$f^t(|\mathbf{K}_0|) \cap |\mathbf{K} \cup \mathbf{B}| \subset |\mathbf{K}_0|$$

and

$$\begin{aligned} f^t(A) \cap \mathrm{bd}|\mathbf{B}| &\subset \mathrm{int}|\Phi(\mathbf{K})| \cap |\mathrm{cntg}(\mathbf{B})| \\ &\subset \bigcup_{i=1}^{n} |\Phi(\mathbf{K} \cap \mathbf{L}_i)| \cap |\mathrm{cntg}(\mathbf{B})| \\ &\subset |\mathbf{K}_0|. \end{aligned}$$

Therefore, f^t induces a map of $i(A/(A \cap |\mathbf{K}_0|))$ into $|\mathbf{K} \cup \mathbf{B}|/|\mathbf{K}_0|$. Let us denote this map by $\bar{f}^t_Q$. We conclude that, for $p \in Q_1/Q_0$,

$$h(p,t) = \bar{f}^t_Q \circ \bar{r}(p)$$

is a homotopy connecting $\bar{f}^0_Q \circ \bar{r} = f^0_Q \circ i \circ \bar{r} \sim f^0_Q$ and $\bar{f}^1_Q \circ \bar{r} = f^1_Q \circ i \circ \bar{r} \sim f^1_Q$. ∎

5 Refinement

As has been indicated several times now, to decrease the computational costs we break the computation into several different steps using different grid sizes. In this section we will discuss how one moves from a coarse grid to a fine grid in an efficient manner.

The first step is to choose a coarse grid in $\mathbb{R}^s$, as was indicated in Section 3 this is done by choosing a vector $\xi \in \mathbb{R}^s$. Let $\psi : \xi\mathbb{Z}^s \to \xi\mathbb{Z}^s$ be any function. In practice ψ is generated numerically, e.g. by integrating the center of each cube in some ξ-representable set (outside of this set the values of ψ are unimportant). To obtain topological information we need to extend ψ from a map on the lattice to a map on $\mathbb{R}^s$. This is done via a rectangular map

$$\begin{array}{rcl} \Psi : \xi\mathbb{Z}^s & \rightrightarrows & \xi\mathbb{Z}^s \\ k & \mapsto & \xi S(\psi(k), m) \end{array} \tag{8}$$

where m is a positive integer representing an error estimate for the numerics. Observe that the word estimate, not bound, is used at this point. As has been mentioned before, the level of approximation used at this step is far too coarse to hope to obtain good error bounds. This level of approximation is used to identify the appropriate region of phase space in which we wish to do the careful numerical computations and to check that the Poincaré map is well defined. As will become clear later, this step greatly reduces the computational cost of our approach.

Let $\mathbf{B} \subset \xi\mathbb{Z}^s$ be a finite set which represents the region in phase space on which we think the interesting dynamics occurs. How $\mathbf{B}$ is chosen will be mentioned later, the important point for the moment is that it is selected in such a way that we expect $(|\mathbf{B} \cup \mathbf{K}_0|, |\mathbf{K}_0|)$ to be an index pair where $\mathbf{K}_0 := \mathrm{cntg}(\mathbf{B}) \cap \Psi(\mathbf{B})$.

Turning to the finer approximation, we need a simple way to refine our grid. Choose a positive integer q and let $\zeta = \frac{1}{q}\xi$. This gives rise to a new grid $\zeta\mathbb{Z}^s$. Observe that any ξ-representable set $\mathbf{A}$, is also ζ-representable. Therefore, the set $\zeta\mathcal{R}(\mathbf{A})$ is also well-defined. Furthermore, for any set $\mathbf{K} \subset \xi\mathbb{Z}^s$, $\mathbf{K}$ and $\zeta\mathcal{R}(|\mathbf{K}|)$ represent the same subset of $\mathbb{R}^s$. Therefore, we adopt the following convention. For a set $\mathbf{K} \subset \xi\mathbb{Z}^s$ and $k \in \zeta\mathbf{Z}^s$ by $\mathrm{dist}(k, \mathbf{K})$ we mean $\mathrm{dist}(k, \zeta\mathcal{R}(|\mathbf{K}|))$.

Let $\phi : \zeta\mathbb{Z}^s \to \zeta\mathbb{Z}^s$ be any function. In practice it will be closely correlated with ψ since it also is obtained via a numerical approximation to the Poincaré map. As before we are interested in extending ϕ. However, we shall extend it on a "small" set. Let

$$\mathbf{D}_0 = \mathrm{cntg}(\zeta\mathcal{R}(|\mathbf{B}|)) \cap \zeta\mathcal{R}(|\mathbf{K}_0|) \tag{9}$$

and let

$$\mathbf{D} = \mathbf{D}_0 \cup (\mathrm{cntg}(\zeta\mathbb{Z}^s \setminus (\zeta\mathcal{R}(|\mathbf{B}|) \cup \mathbf{D}_0)) \cap \zeta\mathcal{R}(|\mathbf{B}|)) \tag{10}$$

We extend ϕ on the set $\mathbf{D}$ by $\Phi : \mathbf{D} \rightrightarrows \zeta\mathbb{Z}^s$ where

$$\Phi(K) = \begin{cases} \zeta S\left(\phi(k), \mathrm{dist}(\phi(k), \mathbf{B})\right) & \text{if } k \in \mathbf{D}_0, \\ \zeta S\left(\phi(k), \mathrm{dist}(\phi(k), \mathrm{cntg}(\mathbf{B}) \setminus \mathbf{K}_0)\right) & \text{if } k \in \mathbf{D} \setminus \mathbf{D}_0. \end{cases}$$

We are now in a position to state an abstract result for index pairs involving symbolic dynamics. Up until this point we have been careful to distinguish between the lattice points $\zeta\mathbb{Z}^s$ which the computer manipulates and the elements of $\mathbb{R}^s$ which we think of as lying in the phase space of the continuous dynamical system. In the following theorem we will want to identify them so let $\iota : \zeta\mathbb{Z}^s \to \mathbb{R}^s$ be the obvious inclusion map.

Proposition 5.1 *Let ξ, ζ, Ψ, Φ, $\mathbf{B}$, $\mathbf{K}_0$, $\mathbf{D}_0$ and $\mathbf{D}$ be defined as above. Assume that there exists a decomposition $\{\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_n\}$ of $\mathbf{B}$ such that for all $i \in \{1, 2, \ldots, n\}$*

$$b\big(\Phi(\mathbf{D} \cap \mathbf{L}_i)\big) \cap \mathrm{cntg}(\mathbf{B}) \subset \mathbf{D}_0,$$

where $\mathbf{L}_i = \mathbf{B}_i \cup \mathrm{cntg}(\mathbf{B}_i)$. Then,

(i) *$E = (\mathbf{D}, \Phi)$ is a BIP-enclosure for $\zeta\mathcal{R}(|\mathbf{B}|)$ and $\mathbf{D}_0$ is its exit set.*

(ii) *Assume E is sharp, $E_0 = (\mathbf{B} \cup \mathbf{K}_0, \Psi_{|\mathbf{B} \cup \mathbf{K}_0})$ is an IP-enclosure for $\mathbf{B}$, and $\mathrm{Encl}(E_0) \cap \mathrm{Encl}(E) \neq \emptyset$. Then, for each homeomorphism $f \in \mathrm{Encl}(E)$ such that $|\mathbf{B}| \subset \mathrm{dom} f$ and each map $g \in \mathrm{Encl}(E_0)$ the index maps $f_{Q(E, \zeta\mathcal{R}(|\mathbf{B}|))}$ and $g_{Q(E_0, \mathbf{B})}$ are conjugate up to homotopy by a homeomorphism, i.e. there exists a homeomorphism*

$$h : \Big(Q_1(E, \zeta\mathcal{R}(|\mathbf{B}|))/Q_0(E, \zeta\mathcal{R}(|\mathbf{B}|)), [Q_0(E, \zeta\mathcal{R}(|\mathbf{B}|))]\Big) \longrightarrow \\ \longrightarrow \Big(Q_1(E_0, \mathbf{B})/Q_0(E_0, \mathbf{B}), [Q_0(E_0, \mathbf{B})]\Big)$$

such that $h \circ f_{Q(E, \zeta\mathcal{R}(|\mathbf{B}|))}$ is homotopic to $g_{Q(E_0, \mathbf{B})} \circ h$.

(iii) *Let $k \in \zeta\mathbb{Z}^s$. Assume that $\iota(k) \in |\mathbf{B} \cup \mathbf{K}_0|$ implies*

$$\bigcap_{l \in \mathbf{D} \,:\, \iota(k) \in |l|} \Phi(k) \cap \bigcap_{p \in \mathbf{B} \cup \mathbf{K}_0 \,:\, \iota(k) \in |p|} \zeta\mathcal{R}(|\Psi(p)|) \neq \emptyset. \tag{11}$$

Then, $\mathrm{Encl}(E_0) \cap \mathrm{Encl}(E) \neq \emptyset$.

Up until this point we have been carefull to distinguish between the lattice points $\zeta\mathbb{Z}^s$ which the computer manipulates and the elements of $\mathbb{R}^s$ which we think of as lying in the phase space of the continuous dynamical system. By making the statement $x \in \zeta\mathbb{Z}^s \subset \mathbb{R}^s$ we mean that we think of $x \in \mathbb{R}^s$, but haveing coordinate values which correspond to those used in the lattice grid.

Proof. (i) Since $\mathbf{D}_0 \subset \operatorname{cntg}(\zeta\mathcal{R}(|\mathbf{B}|))$ and $\mathbf{D} \setminus \mathbf{D}_0 \subset \zeta\mathcal{R}(|\mathbf{B}|)$, Definition 4.6(i) is satisfied for $E = (\mathbf{D}, \Phi)$.

Let $x \in \operatorname{bd}|\zeta\mathcal{R}(|\mathbf{B}|)| = \operatorname{bd}|\mathbf{B}|$. If there is a $k \in \mathbf{K}_0$ containing x then there is also an $l \in \zeta\mathcal{R}(\mathbf{K}_0)$ containing x. Clearly, such a l belongs to $\mathbf{D}_0$, so $x \in |\mathbf{D}_0|$.

Now, assume that there is no $k \in \mathbf{K}_0$ containing x. Take any $l \in \zeta\mathbb{Z}^s \setminus \zeta\mathcal{R}(|\mathbf{B}|)$ and $l' \in \zeta\mathcal{R}(|\mathbf{B}|)$ which are contiguous and contain x. Then, $l \notin \zeta\mathcal{R}(|\mathbf{K}_0|)$, so $l \notin \mathbf{D}_0$. Thus, $l \in \zeta\mathbb{Z}^s \setminus (\zeta\mathcal{R}(|\mathbf{B}|) \cup \mathbf{D}_0)$ and therefore, $x \in l' \in \operatorname{cntg}(l) \cap \zeta\mathcal{R}(|\mathbf{B}|) \subset \mathbf{D} \setminus \mathbf{D}_0$. This proves that $x \in |\mathbf{D}|$, so that Definition 4.6(ii) holds.

In order to prove Definition 4.6(iii) notice that, by the definition of Φ, for each $k \in \mathbf{D}_0 = \operatorname{cntg}(\zeta\mathcal{R}(|\mathbf{B}|)) \cap \mathbf{D}$, $\Phi(k) \cap \zeta\mathcal{R}(|\mathbf{B}|) = \emptyset$.

Definition 4.6(iv) follows immediately from the assumption of the decomposition.

Finally, it is easy to check that $\mathbf{D}_0$ is the exit set of $(\mathbf{D}, \Phi)$.

(ii) Take any $\bar{f} \in \operatorname{Encl}(E_0) \cap \operatorname{Encl}(E)$. One can easily check that, for $Q_i = Q_i(E_0, \mathbf{B})$ and $Q'_i = Q_i(E, \zeta\mathcal{R}(|\mathbf{B}|))$, $Q'_i \subset Q_i$ for $i \in \{0, 1\}$, $Q_1 \setminus Q_0 = Q'_1 \setminus Q'_0$ and $Q'_1 \cap Q_0 = Q'_0$. Therefore, the inclusion induced map $h : (Q'_1/Q'_0, [Q'_0]) \to (Q_1/Q_0, [Q_0])$ is a homeomorphism. Moreover, since the pair $Q = (Q_1, Q_0)$ is an index pair for $\bar{f}$ by Theorem 4.5, so is $Q' = (Q'_1, Q'_0)$ (note that we cannot use Theorem 4.7 here since $\bar{f}$ need not be a homeomorphism). Thus, the index maps $\bar{f}_Q$ and $\bar{f}_{Q'}$ are defined. Obviously, $\bar{f}_Q \circ h = h \circ \bar{f}_{Q'}$. Now, by Theorems 4.5 and 4.7, $\bar{f}_Q \sim g_Q$ and $\bar{f}_{Q'} \sim f_{Q'}$. We conclude that $g_Q \circ h \sim h \circ f_Q$.

(iii) For each $k \in \zeta\mathbb{Z}^s$, let $f_0(\iota(k))$ be an interior point of any of the cubes in the set on the left-hand side of (11). Let f_1 be a continuous map defined on $|\mathbf{B} \cup \mathbf{K}_0|$, extending f_0 with the property that

$$f_1(|k|) \subset \operatorname{conv}\{f_0(\iota(l)) \mid l \in o(k)\}$$

where conv means take the convex hull in $\mathbb{R}^s$. The f_1 map can be extended in a continuous manner to a map f defined on an open neighbourhood U of

$|\mathbf{B} \cup \mathbf{K}_0|$. Clearly, this map belongs to both $\mathrm{Encl}(E_0)$ and $\mathrm{Encl}(E)$. ∎

Since the BIP-enclosure defined in the above theorem will play an important role later, we are going to denote it by $E(\mathbf{B}, \xi, \zeta, \Phi, \Psi, m)$.

6 Cohomology computation

To apply the theoretical results of Section 2 in order to obtain the conclusion that $\Sigma(A) \subset \rho(\mathrm{Inv}(N, f))$, it is necessary to compute the cohomology of an index pair $Q = (Q_1, Q_0)$ and the cohomology of the associated index map f_Q. From the mathematical point of view it is a classical result that simplicial homology (and therefore cohomology) is computable [Mu]. However, from the point of view of optimal computation, many questions remain [D-E, K-M-S]. In this section a method for computing the first level cohomology for a pair of $\xi\mathbb{Z}^2$-representable spaces and for a continous map defined on that pair. For our application to the Lorenz equation this is sufficient. It is reasonably straight forward to generalize this approach to $\xi\mathbb{Z}^s$-representable sets, i.e. to higher dimensional sets [B]. However, this approach will not generalize to the higher cohomology groups (see [A-K, Pi, M-Sz] for work in this direction). It should be mentioned that the approach described here was first developed and applied for the index computation in the Henon map example discussed in [Sz1].

Throughout this section, we assume that the grid $\xi\mathbb{Z}^2$ is fixed and that $E = (\mathbf{K}, \Phi)$ is an IP-enclosure for a finite set $\mathbf{B} \subset \xi\mathbb{Z}^2$ such that $\mathrm{Encl}(E) \neq \emptyset$. By Theorem 4.5, the pair $Q = (Q_1, Q_0) = Q(E, \mathbf{B}) = (|\mathbf{K}|, |\mathbf{K}_0|)$ is an index pair for any $f \in \mathrm{Encl}(E)$ (recall that $\mathbf{K}_0 = \mathrm{cntg}(\mathbf{B}) \cap \mathbf{K}$ is the exit set of E and $\mathbf{B} \subset \mathbf{K} \subset \mathbf{B} \cup \mathrm{cntg}(\mathbf{B})$) and the homotopy class of the index map f_Q associated with that index pair does not depend on the choice of f.

Definition 6.1 The pair $(\mathbf{K}, \mathbf{K}_0)$ will be called *reducible* if and only if for each $k \in \mathbf{B}$ there exists a sequence $(k^0, k^1, \dots, k^m = k)$ of elements of $\mathbf{B}$ such that k^0 is contiguous to some element of $\xi\mathbb{Z}^2 \setminus (\mathbf{B} \cup \mathbf{K}_0)$ and k^i and k^{i+1} are contiguous for each $i \in \{0, 1, \dots, m-1\}$.

Using terminology from the game of chess, one can say that $(\mathbf{K}, \mathbf{K}_0)$ is reducible if and only if for every element $k \in \mathbf{B}$ a rook placed on some rectangle outside $\mathbf{B} \cup \mathbf{K}_0$ can reach k without stepping into $\mathbf{K}_0$.

Definition 6.2 A sequence $(k^0, k^1, \ldots, k^r)$ of elements of $\mathbf{B}$ is called a *reducing sequence* for $(\mathbf{K}, \mathbf{K}_0)$ if and only if, for each $i \in \{0, 1, \ldots, r\}$,

$$k^i \in \text{cntg}\Big(\{k^0, k^1, \ldots, k^{i-1}\} \cup (\xi\mathbb{Z}^2 \setminus (\mathbf{B} \cup \mathbf{K}_0))\Big). \tag{12}$$

A reducing sequence $(k^0, k^1, \ldots, k^r)$ is called *maximal* if and only if it cannot be extended to a longer reducing sequence, i.e. if there does not exist a reducing sequence $(k^{0'}, k^{1'}, \ldots, k^{r+1'})$ such that $k^i = k^{i'}$ for each $i = 0, 1, \ldots, r$.

We have the following simple proposition.

Proposition 6.3 $(\mathbf{K}, \mathbf{K}_0)$ *is reducible if and only if* $\mathbf{B} = \{k^0, k^1, \ldots, k^r\}$ *for any maximal reducing sequence* $\bar{K} = (k^0, k^1, \ldots, k^r)$.

Proof. $(\Rightarrow)$ Assume that $(\mathbf{K}, \mathbf{K}_0)$ is reducible. Let $\bar{K} = (k^0, k^1, \ldots, k^r)$ be a maximal reducing sequence for it. Assume that $\mathbf{B} \neq \{k^0, k^1, \ldots, k^r\}$. Consider any $k \in \mathbf{B} \setminus \{k^0, k^1, \ldots, k^r\}$. Let $l^0, l^1, \ldots, l^n = k$ be a sequence of elements of $\mathbf{B}$ such that l^i and l^{i+1} are contiguous for all i and l^0 is contiguous to some element of $\xi\mathbb{Z}^2 \setminus (\mathbf{B} \cup \mathbf{K}_0)$. Let i be the smallest number such that $l^i \notin \{k^0, k^1, \ldots, k^r\}$. Then, the sequence $(k^0, k^1, \ldots, k^r, l^i)$ can easily be shown to be a reducing sequence, which contradicts the maximality of $\bar{K}$.

$(\Leftarrow)$ Assume that $(k^0, k^1, \ldots, k^r)$ is a reducing sequence such that $\mathbf{B} = \{k^0, k^1, \ldots, k^r\}$. Take any $l \in \mathbf{B}$. There exists an i_0 such that $l = k^{i_0}$. Having defined i_{m-1}, we define i_m as follows. First of all, let

$$A_m = \Big\{ i \in \{0, 1, \ldots, i_{m-1} - 1\} \mid k^i \in \text{cntg}(k^{i_{m-1}}) \Big\}.$$

If $A_m \neq \emptyset$, we define i_m as any element of A_m. In this way, we obtain a decreasing sequence $i_0, i_1, \ldots, i_j$, where j is a natural number such that $A_{j+1} = \emptyset$. The corresponding sequence $(k^{i_j}, k^{i_{j-1}}, \ldots, k^{i_0} = l)$ has the property that each its consecutive elements are contiguous and the first one is contiguous to $\xi\mathbb{Z}^2 \setminus (\mathbf{B} \cup \mathbf{K}_0)$. Thus, we have proved that $(\mathbf{K}, \mathbf{K}_0)$ is reducible. ∎

Before proceeding further, let us introduce some new notation. The set of *edges* arising from the lattice $\xi\mathbb{Z}^2$ are the one-dimensional simplices

$$\mathcal{G} = \Big\{ |k| \cap |l| \subset \mathbf{R}^2 \;\mid\; k \in \xi\mathbb{Z}^2, l \in \text{cntg}(k) \Big\}.$$

For a set $A \subset \mathbf{R}^2$,
$$\mathcal{E}(A) := \{e \in \mathcal{G} \mid e \subset A\}.$$
For a subset $\mathcal{E} \subset \mathcal{G}$ by $|\mathcal{E}|$ we denote the union of all edges in $\mathcal{E}$.

Recall that $\iota : \xi\mathbb{Z}^2 \to \mathbf{R}^2$ is the natural inclusion map. The set of *vertices* arising from the lattice $\xi\mathbb{Z}^2$ is just the collection of lattice points viewed as elements of $\mathbf{R}^2$, i.e. $\iota(\xi\mathbb{Z}^2)$.

Observe that each edge $e \in \mathcal{G}$ is an interval connecting vertices $x = \iota(k)$ and $y = \iota(l)$ such that k and l are contiguous. We will let $\mathcal{V}(e)$ denote the set of endpoints of the edge e, i.e. $\mathcal{V}(e) = \{x, y\}$.

A *vertex path* is a sequence $V = (v^0, v^1, \ldots, v^j)$ of vertices with the property that any two consecutive vertices are distinct endpoints of a single edge. Let $I = [0,1]$ and $\delta I = \{0,1\}$. The *path* $|V| : I \to \mathbf{R}^2$ corresponding to the vertex path V is defined by

$$|V|(t) = (jt - n)v^{n+1} + (n + 1 - jt)v^n \quad \text{for } t \in [n/j, (n+1)/j].$$

The vertex path V is *inscribed* in a pair $P = (P_1, P_0)$ of subsets of the plane if and only if the map

$$|V|_P : (I, \delta I) \longrightarrow (P_1/P_0, [P_0])$$

induced by $|V|$, i.e. given by

$$|V|_P(t) = \begin{cases} [|V|(t)] & \text{if } |V|(t) \in P_1 \\ [P_0] & \text{otherwise,} \end{cases}$$

is well defined (i.e. maps δI into $[P_0]$) and continuous.

Definition 6.4 Let $K = (k^0, k^1, \ldots, k^r)$ be a reducing sequence. A sequence $(\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ of subsets of $\mathcal{G}$ is called a *retraction sequence* for K if and only if $|\mathcal{E}^i| \subset k^i$,

$$\mathcal{E}\left(|\mathbf{K}_0 \cup \mathbf{B} \setminus \{k^0, k^1, \ldots, k^i\}|\right) \cap \mathcal{E}^i = \emptyset \tag{13}$$

and

$$k^i \cap \left(|\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^i| \cup |\mathbf{K}_0 \cup \mathbf{B} \setminus \{k^0, k^1, \ldots, k^i\}|\right) \tag{14}$$

is a strong deformation retract of k^i.

Definition 6.5 Let $K = (k^0, k^1, \ldots, k^r)$ be a reducing sequence and $\bar{\mathcal{E}} = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ a retraction sequence for K. The *retract* of $Q = (|\mathbf{K}|, |\mathbf{K}_0|)$ defined by K and $\bar{\mathcal{E}}$ is the pair

$$R(K, \bar{\mathcal{E}}) = \Big(\; |\mathbf{K}_0 \cup \mathbf{B} \setminus \{k^0, k^1, \ldots, k^r\}| \cup |\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^r|, |\mathbf{K}_0| \; \Big)$$

We note that if $(\mathbf{K}, \mathbf{K}_0)$ is reducible and the reducing sequence K is maximal then

$$R(K, \bar{\mathcal{E}}) = \Big(\; |\mathbf{K}_0| \cup |\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^r|, |\mathbf{K}_0| \; \Big), \tag{15}$$

so that its quotient space is a one-dimensional complex. The following theorem shows that, in fact, this allows one to reduce the problem of homology computation to the one-dimensional case.

Theorem 6.6 *Let $K = (k^0, k^1, \ldots, k^r)$ be a reducing sequence and let $\bar{\mathcal{E}} = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ be a retraction sequence for K. Then, $R(K, \bar{\mathcal{E}})$ is a strong deformation retract of Q.*

Proof. The proof is inductive with respect to r. Clearly, the theorem holds for $r = -1$. Assume that it holds for some $r \in \mathbb{Z}^+$ and let $K = (k^0, k^1, \ldots, k^{r+1})$ be a reducing sequence and $\bar{\mathcal{E}} = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^{r+1})$ a retraction sequence for K. Then, $K' = (k^0, k^1, \ldots, k^r)$ is a reducing sequence and $\bar{\mathcal{E}}' = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ is a retraction sequence for K'. Therefore, by the inductive hypothesis, $P' = (P'_1, P'_0) = R(K', \bar{\mathcal{E}}')$ is a strong deformation retract of Q. Let $P = (P_1, P_0) = R(K, \bar{\mathcal{E}})$. It is not difficult to see that

$$P_1 \cap k^{r+1} = k^{r+1} \cap \Big(|\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^{r+1}| \cup |\mathbf{K}_0 \cup \mathbf{B} \setminus \{k^0, k^1, \ldots, k^{r+1}\}| \Big),$$

so that if $r_0 : k^{r+1} \to P_1 \cap k^{r+1}$ is a deformation retraction which exists by Definition 6.5 then a deformation retraction of P' to P can be defined by

$$r(x) = \begin{cases} r_0(x) & \text{if } x \in k^{r+1} \\ x & \text{otherwise.} \end{cases}$$

Since P' is a deformation retract of Q by the inductive hypothesis, so is P. ∎

In what follows, $K = (k^0, k^1, \ldots, k^r)$ and $\bar{\mathcal{E}} = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ denote a maximal reducing sequence for $(\mathbf{K}, \mathbf{K}_0)$ and a retraction sequence for K. We also assume that $(\mathbf{K}, \mathbf{K}_0)$ is reducible, which implies that $\mathbf{B} = \{k^0, k^1, \ldots, k^r\}$

and that $H_0(|\mathbf{K}|, |\mathbf{K}_0|) = 0$ (geometrically, this means that each connected component of $|\mathbf{B}|$ intersects $|\mathbf{K}_0|$).

The graph $\tilde{G} = (\tilde{V}, \tilde{E})$ is defined by

$$\tilde{V} = \bigcup_{e \in \mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^r} \mathcal{V}(e),$$

$$\tilde{E} = \Big\{ \mathcal{V}(e) : e \in \mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^r \Big\}.$$

Observe that the edges in this graph are being denoted by pairs of vertices.

Consider the graph $\bar{G} = (\bar{V}, \bar{E})$ is defined as follows

$$\bar{V} = \tilde{V} \cup \{*\}, \tag{16}$$

$$\bar{E} = \tilde{E} \cup \Big\{ \{*, v\} : v \in \tilde{V} \cap |\mathbf{K}_0| \Big\}. \tag{17}$$

Thus, $\bar{G}$ is obtained from $\tilde{G}$ by adding the vertex $*$ and all edges going from that vertex to any of the vertices in $\bar{V}_0 = \tilde{V} \cap |\mathbf{K}_0|$. Clearly, by reducibility of $(\mathbf{K}, \mathbf{K}_0)$, (15) holds. Furthermore, one can use (13) to show that

$$\bar{V}_0 = |\mathbf{K}_0| \cap |\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^r|. \tag{18}$$

Let T be the subtree of $\bar{G}$ with the set of edges $\{\{*, v\} : v \in \bar{V}_0\}$.

Clearly, (15) and (18) show that, in fact,

$$H_*(R(K, \bar{\mathcal{E}})) = H_*(|\bar{G}|, |T|),$$

where for a graph H by $|H|$ we denote the space of H, treated as a one-dimensional symplicial complex ([Sp, Section 3.1]). More precisely, $|\bar{G}|/|T|$ is homeomorphic to the quotient space $(|\mathbf{K}_0| \cup |\bigcup_{j=0}^r \mathcal{E}^j|)/|\mathbf{K}_0|$ of the pair $R(K, \bar{\mathcal{E}})$ in the natural way. In order to define the homeomorphism, one maps each vertex in $\tilde{V}$ into the corresponding point in $\mathbb{R}^2$ and extends this map to the realization of $\tilde{G}$ so that it is affine on each its simplex. It is easy to see that the induced map of the quotient spaces which sends $[|T|]$ into $[|\mathbf{K}_0|]$ is a homeomorphism.

In order to compute the homology of $(|\bar{G}|, |T|)$ we use a modification of the algorithm for the fundamental group [Sp, Section 3.6]. First of all, we compute a spanning tree $T_{\max} = (\bar{V}, E_{\max})$ for $\bar{G}$ containing T. There are efficient algorithms for a spanning tree - like Prim's or Kruskal's algrithms

[C-L-R, Section 24.2]. We used a suitable modification of the Prim's algorithm. Then, from [Sp, Section 3.7] it follows that one dimensional homology of the pair $(|\bar{G}|, |T|)$ with rational coefficients is a vector space over $\mathbb{Q}$ whose dimension is the same as the number of elements in $(\bar{E} \setminus E_{\max})$. Moreover, it is easy to compute a basis for that space. Namely, for each edge $e = \{v_e, w_e\} \in \bar{E} \setminus E_{\max}$ one can choose paths $(v_0, v_1, \ldots, v_n = v_e)$ and $(w_0, w_1, \ldots, w_m = w_e)$ in $T_{\max}$ such that they do not go through $*$ and such that $w_0, v_0 \in \bar{V}_0$. Now, define the path p_e in $\bar{G}$ (being a vertex path as well - that is why we required the paths to avoid $*$) by

$$p_e = (v_0, v_1, \ldots, v_{n-1}, v_n, w_m, w_{m-1}, \ldots, w_0)$$

and let $\sigma_e : (I, \delta I) \to R(K, \bar{\mathcal{E}})$ be the path corresponding to p_e, i.e. given by $\sigma_e(t) = |p_e|(t)$. It can be treated as a one-dimensional singular simplex in $R(K, \bar{\mathcal{E}})$. In fact, it is a cycle in $C_*(R(K, \bar{\mathcal{E}}))$. Hence it represents an element

$$[\sigma_e] \in H_1(R(K, \bar{\mathcal{E}})).$$

The set of all elements of the above form is a basis of $H_1(R(K, \bar{\mathcal{E}}))$ and hence also $H_1(Q)$ by Theorem 6.6.

Now, let $\bar{\sigma}_e : (I, \delta I) \to (Q_1/Q_0, [Q_0])$ be the path induced by σ_e (i.e. $\bar{\sigma}_e = |p_e|_Q$). Clearly, these paths define a basis of $H_1(Q_1/Q_0, [Q_0])$. Furthermore, if $N_1, N_2, \ldots, N_k$ is a decomposition of $\mathrm{cl}(Q_1 \setminus Q_0) = |\mathbf{B}|$ into pairwise disjoint compact sets then the corresponding $H_1(r_i)$ endomorphisms of $H_1(Q_1/Q_0, [Q_0])$ are the projections onto the space

$$V_i = \text{span } \{ \ [\bar{\sigma}_e] \ : \ e \subset N_i \ \},$$

which send $\oplus_{j \neq i} V_j$ into $\{0\}$. In order to compute the endomorphism

$$H_1(f_Q) : H_1(Q_1/Q_0, [Q_0]) \longrightarrow H_1(Q_1/Q_0, [Q_0])$$

we need to know homotopy classes of the paths $f_Q \circ \bar{\sigma}_e$ for each $e \in \bar{E} \setminus E_{\max}$. Suppose that $p_e = (u_0, u_1, \ldots, u_m)$, where $u_i \in \tilde{V}$. For each $i \in \{1, 2, \ldots, m\}$ let $\mathbf{C}_i$ be the set of all elements of $\mathbf{B} \cup \mathbf{K}_0$ containing u_i. Thus, $\mathbf{C}_i$ consists of at most 4 rectangles, meeting at u_i. Consider the intersection

$$\mathbf{D}_i = \bigcap_{k \in \mathbf{C}_i} \Phi(k).$$

Since $f(u_i) \in \operatorname{int}|\mathbf{D}_i|$ for any $f \in \operatorname{Encl}(E)$, $\mathbf{D}_i$ is nonempty. Thus, we can define u'_i as one of the vertices of any of the rectangles in $\mathbf{D}_i$. In this way, we obtain the sequence $(u'_0, u'_1, \ldots, u'_m)$. For each pair u'_i, u'_{i+1} of its consecutive vertices let $p'_i = (u_{i,0}, u_{i,1}, \ldots, u_{i,n_i})$ be a vertex path such that $u_{i,0} = u'_i$, $u_{i,n_i} = u'_{i+1}$, and all its entries are in the smallest rectangle with horizontal and vertical edges containing u'_i and u'_{i+1}. Let $p'_e = p'_0 \star p'_1 \star \ldots \star p'_{m-1}$, where $\star$ is the concatenation operation. More precisely, if $q_1 = (v_0, v_1, \ldots, v_l)$ and $q_2 = (w_0, w_1, \ldots, w_k)$ are sequences of vertices then $q_1 \star q_2$ is defined if $w_0 = v_l$ and

$$q_1 \star q_2 = (v_0, v_1, \ldots, v_l, w_1, w_2, \ldots, w_k).$$

Clearly, p'_e is a vertex path. Furthermore, the corresponding path $|p'_e|$ maps I into $|\Phi(\mathbf{B})|$ and δI into $|\Phi(\mathbf{B}) \setminus \mathbf{B}|$ (since $\mathbf{C}_0$ and $\mathbf{C}_m$ intersect $\mathbf{K}_0$, this follows from the condition (ii) in Definition 4.3) and hence p'_e is inscribed in Q. Therefore, it induces the path $|p'_e|_Q : (I, \delta I) \to (Q_1/Q_0, [Q_0])$, which can be shown to be homotopic to $f_Q \circ \bar{\sigma}_e$ for each $f \in \operatorname{Encl}(E)$. Since the proof is rather straighforward, we leave the details to the reader.

We need to express the element $[|p'_e|_Q] \in H_1(Q_1/Q_0, [Q_0])$ defined by the path $|p'_e|_Q$, treated as a relative cycle, in terms of the basis $\{[\bar{\sigma}_e] : e \in \bar{E} \setminus E_{\max}\}$ of $H_1(Q_1/Q_0, [Q_0])$. In order to do that, we apply to it the retraction defined in the proof of Theorem 6.6. Let us introduce some new notation first.

Assume that $\mathbf{A}, \mathbf{L} \subset \xi\mathbb{Z}^2$ are such that $\mathbf{L} \subset \mathbf{A}$, $\mathcal{E} \subset \mathcal{G}$ satisfies $\mathcal{E}(|\mathbf{A}|) \cap \mathcal{E} = \emptyset$, $k \in \operatorname{cntg}(\xi\mathbb{Z}^2 \setminus \mathbf{A}) \setminus \mathbf{L}$. Let $\mathbf{D} \subset \mathcal{E}(k)$ be such that

$$|\mathbf{D}| \cup \Big(k \cap (|\mathcal{E}| \cup |\mathbf{A} \setminus \{k\}|)\Big)$$

is a strong deformation retract of k, or, equivalently, is connected and not equal to the entire boundary of k. Let $\eta = (p_0, p_1, \ldots, p_k)$ be a vertex path inscribed in $(|\mathbf{A}| \cup |\mathcal{E}|, |\mathbf{L}|)$. Let $l \in \mathbb{Z}^+$ and $i_1, i_2, \ldots, i_l, j_1, j_2, \ldots, j_l \in \mathbb{Z}^+$ be such that

$$i_1 < j_1 + 1 < i_2 < j_2 + 1 < \ldots < i_l < j_l + 1 \leq k + 1$$

and $p_j \in k$ if and only if $i_m \leq j \leq j_m$ for some $m \in \{0, 1, \ldots, l\}$. For any $m \in \{1, 2, \ldots, l\}$ let $(p_{m,1}, p_{m,2}, \ldots, p_{m,c_m})$ be a sequence of pairwise distinct vertices of k such that $p_{m,1} = p_{i_m}$, $p_{m,c_m} = p_{j_m}$ and each of its consecutive vertices are endpoints of a single edge contained in $|\mathbf{D}| \cup (k \cap (|\mathcal{E}| \cup |\mathbf{A} \setminus \{k\}|))$.

Note that this can be done in the unique way since that set is connected and p_{i_m} and p_{j_m} can be shown to belong to $k \cap (|\mathcal{E}| \cup |\mathbf{A} \setminus \{k\}|)$. Now, let

$$\begin{aligned}
&\tau(\eta, \mathbf{A}, \mathbf{L}, \mathcal{E}, k, \mathbf{D}) = \\
&= (p_0, p_1, \ldots, p_{i_1} = p_{1,1}, p_{1,2}, \ldots, p_{1,c_1} = p_{j_1}, p_{j_1+1}, \ldots, p_{i_2} = p_{2,1} \\
&\quad p_{2,2}, \ldots, p_{2,c_2} = p_{j_2}, \ldots, \ldots, p_{i_l} = p_{l,1}, p_{l,2}, \ldots, p_{l,c_l} = p_{j_l}, p_{j_l+1}, \ldots, p_k).
\end{aligned}$$

Thus, $\tau(\eta, \mathbf{A}, \mathbf{L}, \mathcal{E}, k, \mathbf{D})$ can be obtained from η by substituting each portion with indices between i_m and j_m with the sequence $(p_{m,1}, p_{m,2}, \ldots, p_{m,c_m})$. It is easy to check that the path $|\tau(\eta, \mathbf{A}, \mathbf{L}, \mathcal{E}, k, \mathbf{D})|$ is homotopic to $|\eta|$ rel δI if both paths are treated as paths in $(|\mathbf{A}| \cup |\mathcal{E}|, |\mathbf{L}|)$ and, at the same time, inscribed in $(|\mathbf{A} \setminus \{k\}| \cup |\mathbf{D} \cup \mathcal{E}|, |\mathbf{L}|)$.

Now, let us define the sequence $(p'_{e,i})_{i=0}^{r+1}$ of vertex paths by

$$p'_{e,0} = p'_e, \tag{19}$$

$$p_{e,i+1} = \tau(p'_{e,i}, \mathbf{K}_0 \cup \mathbf{B} \setminus \{k^0, k^1, \ldots, k^{i-1}\}, \mathbf{K}_0, \mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^{i-1}, k^i, \mathcal{E}^i) \tag{20}$$

Using induction on i one can show that $p'_{e,i}$ is a vertex path, inscribed in $R((k^0, k^1, \ldots, k^{i-1}), (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^{i-1}))$ and hence (note that the endpoints of $p_{e,i}$ do not depend on i) also in Q. Furthermore, the paths $|p'_{e,i}|_Q$ are homotopic rel δI. Let $p'_{e,r+1} = (w'_{e,0}, w'_{e,1}, \ldots, w'_{e,n_e})$. Since $p'_{e,r+1}$ is inscribed in $(|\mathbf{K}_0| \cup |\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup |\mathcal{E}^r|, |\mathbf{K}_0|)$,

$$[|p'_e|_Q] = [|p'_{e,r+1}|_Q] = \sum_{f \in E \setminus E_{\max}} \alpha_{e,f} [\bar{\sigma}_f],$$

where

$$\begin{aligned}
\alpha_{e,f} = \#\Big\{ i \in \{0, 1, \ldots, n_e - 1\} : w_{e,i} = v_f \text{ and } w_{e,i+1} = w_f \Big\} - \\
\#\Big\{ i \in \{0, 1, \ldots, n_e - 1\} : w_{e,i} = w_f \text{ and } w_{e,i+1} = v_f \Big\}.
\end{aligned}$$

Clearly, the above formula describes the matrix of the $H_1(f_Q)$ endomorphism with respect the basis $\{[\bar{\sigma}_e] : e \in \bar{E} \setminus E_{\max}\}$.

Let us summarize the results of this section with the following algorithm.

1. Find a maximal reducing sequence $K = (k^0, k^1, \ldots, k^r)$. In order to do that, define the K_j's recursively in such a way that k^i is any rectangle satisfying (12) until it is possible, i.e. the set on the right-hand side of (12) is nonempty.

2. Find a retraction sequence $\bar{\mathcal{E}} = (\mathcal{E}^0, \mathcal{E}^1, \ldots, \mathcal{E}^r)$ for K. For example, one can put $\mathcal{E}^i = \emptyset$ if the set

$$A_i \;=\; k^i \cap (|\mathcal{E}^0 \cup \mathcal{E}^1 \cup \ldots \cup \mathcal{E}^{i-1}| \cup |\mathbf{K}_0 \cup \mathbf{B} \setminus \{K_0, K_1, \ldots, k^i\}|)$$

is a retract of k^i and $\mathcal{E}^i = \mathcal{E}(k^i) \setminus (\{e\} \cup \mathcal{E}(A_i))$ otherwise, where e is any edge not contained in $\mathcal{E}(A_i)$. It is easy to check that this indeed defines a retraction sequence.

3. Find a spanning tree $T_{\max} = (\bar{V}, E_{\max})$ for the graph $\bar{G} = (\bar{V}, \bar{E})$ defined by (16) and (17) containing the T tree.

4. For each edge $e = \{v_e, w_e\}$ compute the vertex path p_e. The basis of $H_1(Q_1/Q_0, [Q_0])$ is given by $\{[\bar{\sigma}_e] : e \in \bar{E} \setminus E_{\max}\}$, where the path $\bar{\sigma}_e : (I, \delta I) \to (Q_1/Q_0, [Q_0])$ is induced by p_e.

5. Compute the vertex paths p'_e, representing homotopy classes of $f_Q \circ \bar{\sigma}_e$ for any $f \in \mathrm{Encl}(E)$ and $e \in \bar{E} \setminus E_{\max}$.

6. Compute the $p'_{e,r+1}$ paths using the recursive formula (19) and (20).

7. Find the $\alpha_{e,f}$ coefficients for $e, f \in \bar{E} \setminus E_{\max}$. The matrix of $H_1(f_Q)$ in the ordered basis $B = ([\bar{\sigma}_{e_1}], [\bar{\sigma}_{e_2}], \ldots, [\bar{\sigma}_{e_q}])$ of $H_1(Q_1/Q_0, [Q_0])$, $q = \#(\bar{E} \setminus E_{\max})$, is given by $[\alpha_{e_j,e_i}]_{i,j=1,2,\ldots,q}$. In what follows, instead of writing α_{e_i,e_j} we shall simplify it to α_{ij}.

8. The matrix of $H^1(f_Q)$ is the transpose of α. If we assume that the ordered basis B is chosen in such a way that $e_{l_{i-1}+1}, e_{l_{i-1}+2}, \ldots, e_{l_i}$ are contained in N_i ($i = 1, 2, \ldots, k$, $0 = l_0 \leq l_1 \leq \ldots \leq l_k = q$) then the matrix of φ_i^1 (see Section 2) can be obtained by substituting all entries which are not in the part of the matrix on Figure 1 between the $(i-1)$-th and i-th horizontal lines (or, equivalently, all entries in the l_i-th row or above or in the $(l_{i+1}+1)$-th row or below) with zeroes.

7 The Lorenz Equations

As has been mentioned several times by now to reduce the computational cost we adopt a two step approach to the proof. Using a coarse approximation we obtain a reasonable choice for an index pair, then using a finer approximation

$$
\left[\begin{array}{ccccc}
\alpha_{11} & \alpha_{12} & \alpha_{13} & \cdots & \alpha_{1q} \\
\alpha_{21} & \alpha_{22} & \alpha_{23} & \cdots & \alpha_{2q} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_{l_1-1,1} & \alpha_{l_1-1,2} & \alpha_{l_1-1,3} & \cdots & \alpha_{l_1-1,d} \\
\hline
\alpha_{l_1 1} & \alpha_{l_1 2} & \alpha_{l_1 3} & \cdots & \alpha_{l_1 q} \\
\alpha_{l_1+1,1} & \alpha_{l_1+1,2} & \alpha_{l_1+1,3} & \cdots & \alpha_{l_1+1,q} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_{l_2-1,1} & \alpha_{l_2-1,2} & \alpha_{l_2-1,3} & \cdots & \alpha_{l_2-1,q} \\
\hline
\cdots & \cdots & \cdots & \cdots & \cdots \\
\hline
\alpha_{l_{k-1}1} & \alpha_{l_{k-1}2} & \alpha_{l_{k-1}3} & \cdots & \alpha_{l_{k-1}q} \\
\alpha_{l_{k-1}+1,1} & \alpha_{l_{k-1}+1,2} & \alpha_{l_{k-1}+1,3} & \cdots & \alpha_{l_{k-1}+1,q} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_{q1} & \alpha_{q2} & \alpha_{q3} & \cdots & \alpha_{qq}
\end{array}\right]
$$

Figure 1: The representation of φ_i^1 endomorphisms

we prove that we have in fact obtained an index pair with interesting index information. In this section we describe the first step. Referring back to Proposition 5.1 this means that we are going to compute $E(\mathbf{B}, \xi, \zeta, \Phi, \Psi, m)$.

In what follows, we shall consider the return map $f = f_{\sigma,R,b}$ defined by the Lorenz system for the plane $P = \{(x, y, z) \in \mathbb{R}^3 \mid z = R - 1\}$. Since z is constant we will use the x and y coordinates to represent points on this plane. f describes how the trajectory of a point on P comes back to the plane after some positive time intersecting it in the same direction (see [MiMr] for a precise definition of the Poincare map we use). Note that f is at a best a partial map. In particular, the local stable manifold of the origin intersects this plane and a thus every point in this intersection never returns to P.

What needs to be done is to obtain an approximation of f and use this approximation to determine $E(\mathbf{B}, \xi, \zeta, \Phi, \Psi, m)$. To do this we need to establish appropriate data structures, tools for computing the return map, including the domain of f, and finally methods for computing the invariant set and index pair.

Let us fix a grid size ξ as was done in the preceding sections. In order to compute the return map, we integrate the Lorenz system using the the fourth order Runge-Kutta method. In what follows, we use the following record structure to represent cubes, i.e. elements of $\xi\mathbb{Z}^2$, in the Poincare plane

$$\text{rect} = \quad \textbf{record} \quad \text{x, y : integer;} \quad \textbf{end};$$

Points (vectors) of $\mathbb{R}^3$ are recorded as

$$\text{point3D} = \quad \textbf{record} \quad \text{x, y, z : real;} \quad \textbf{end};$$

Variables v of type rect represent the element $((\text{v.x})\xi_1, (\text{v.y})\xi_2) \in \xi\mathbb{Z}^2$ and the variables p of type point3D represent the element $(\text{p.x}, \text{p.y}, \text{p.z}) \in \mathbb{R}^3$.

To compute the vector field at given point of $\mathbb{R}^3$ represented by the value of its argument we use the function vector_fld given by

```
function vector_fld ( p : point3D ) : point3D;
begin
  return (σ * (p.y − p.x), R*p.x − p.y − p.x * p.z, p.x * p.y−b*p.z);
end;
```

As was mentioned earlier the fourth order Runge-Kutta method is used to approximate trajectories. The function RK1step performs a single Runge-Kutta step with a fixed step size h for a given point of $\mathbb{R}^3$ represented by the value of their arguments.

```
function RK1step ( p : point3D ) : point3D;
var
    p0, p1, p2, p3 : point3D;
begin
    p0 := vector_fld(p);
    p1 := vector_fld(p+h/2 * p0);
    p2 := vector_fld(p+h/2 * p1);
    p3 := vector_fld(p+h*p2);
    return p+h/6 * (p0 + 2 * p1 + 2 * p2 + p3);
end;
```

The next function, next_int, measures (in terms of numbers of iterates of the Runge-Kutta method) the time needed for the approximate trajectory of a point of $\mathbb{R}^3$ represented by its argument of type point3D to cross the Poincare plane in the direction of decreasing z. It also sets the value of the argument variable so that after a call to this function it represents the approximation of the intersection point. Clearly, using a fixed step size Runge-Kutta approximation to the trajectory, one cannot expect that a numerically computed point will land exactly on a section. Instead we use linear interpolation to approximate the trajectory of the ODE between numerically computed points that precede and follow the intersection with the section.

```
function next_int ( var p : point3D ) : integer;
var
    q : point3D;
    i : integer;
begin
    q := RK1step(p);
    i := 0;
    while  p.z−R+1 ≤ 0 or (q.z−R+1) ∗ (p.z−R+1) > 0  do
    begin
        p := q;
        q := RK1step(p);
        i := i + 1;
    end;
    p := (R−1 − p.z)/(q.z − p.z) ∗ q + (q.z−R+1)/(q.z − p.z) ∗ p;
    return i;
end;
```

The pseudocode for the function $\psi : \xi\mathbb{Z}^2 \to \xi\mathbb{Z}^2$ which, for any $k \in \xi\mathbb{Z}^2$ in the Poincare plane, returns a cube $\psi(k) \in \xi\mathbb{Z}^2$ which contains the point where the Runge-Kutta approximation of the forward trajectory of the center of k intersects it (cf remarks at the end of Section 4).

```
function ψ ( k : rect ) : rect;
var
    p : point3D;
begin
    p := ((k.x + 0.5)∗ξ1, (k.y + 0.5)∗ξ2, R − 1);
    next_int(p);
    return ([p.x/ξ1], [p.y/ξ2]);
end;
```

In order to define the BIP-inclosure $E(\mathbf{B}, \xi, \zeta, \Phi, \Psi, m)$ introduced in Proposition 5.1 ξ, $\mathbf{B}$,ζ and m have to be specified. Unfortunately, as of yet, there is no general algorithmic approach for determining them. Thus, we are forced to experiment with arbitrary values of ξ, ζ and m until we obtain an inclosure which suggests the existence of a chaotic invariant set.

Finding the set $\mathbf{B}$ also requires experimental work, but in this case we have at our disposal a procedure for computing isolating neighbourhoods defined in [Sz1]. One begins with an initial guess, $\mathbf{B}_0$, within which the isolating neighborhood is to be found. Our experience indicates that this initial guess need not be very precise. In the case of the Poincare map for the Lorenz Equations, $\mathbf{B}_0$ was chosen as follows.

Consider a rectangle $[-a, a] \times [-b, b] \subset P$ in the Poincare plane. Clearly, the local stable manifold to the orgin cannot be part of the domain of f and so it needs to be excised. Recall [Spa] that this stable manifold is two dimensional, and thus, one should expect it to intersect the plane $z = R - 1$ in a line which passes through the point $(0, 0, R - 1)$, i.e. the origin in the Poincare plane. Of course, this set is not representable and it is impossible to compute it precisely, so we have to use a representable approximation.

Let $a = r_1\xi_1$ and $b = r_2\xi_2$, where $r_1, r_2 \in \mathbb{N}$. We shall use the following array structure to represent the approximation of the local unstable manifold:

$$\text{graph} = \textbf{array } [-r_1 - 1, -r_1, \ldots, r_1] \ \textbf{ of } \text{integer;}$$

In particular, if sm is a variable of this type storing the information about the unstable manifold, then the manifold is suppose to pass through to each of the cubes of the form $(x_1\xi_1, \mathrm{sm}[x_1]\xi_2) \in \xi\mathbb{Z}^2$ in the Poincare plane for each $x_1 \in \{-r_1 - 1, -r_1, \ldots, r_1\}$.

If a point lies on the stable manifold, then it cannot return to the Poincaré section. With this in mind we compute sm by maximizing the return time. A pseudocode for the function unstable_manifold which we used for this task is as follows.

```
function unstable_manifold : graph;
var
    m, m0, i, j, j0, t : integer;
    sm : graph;
begin
    m0 := −1;
    for j := − r₂ − 1 to r₂ do
    begin
        m := next_int((−r₁ − 0.5) ∗ ξ₁, (j + 0.5) ∗ ξ₂, R − 1);
        if m > m0 then begin
            j0 := j;  m0 := m;
        end;
    end;
    sm[−r₁ − 1]:= j0;
    sm[r₁]:= −j0 − 1;
    for i := − r₁ to  − 1 do
    begin
        t := next_int((i + 0.5)∗ξ₁, (sm[i − 1] + 0.5)∗ξ₂, R − 1);
        sm[i] := sm[i − 1];
        if next_int((i + 0.5)∗ξ₁, (sm[i − 1] + 1.5)∗ξ₂, R − 1) > t then
            sm[i] := sm[i − 1] + 1;
        if next_int((i + 0.5)∗ξ₁, (sm[i − 1] − 0.5)∗ξ₂, R − 1) > t then
            sm[i] := sm[i − 1] − 1;
        sm[−i − 1] := −sm[i] − 1;
    end;
    return sm;
end;
```

The idea of the above procedure is as follows. Consider the cubes of the form $((-r_1-1)\xi_1, x_2\xi_2) \in \xi\mathbb{Z}^2$ in the Poincare plane and define sm$[-r_1-1]$ to be the value of x_2 for which the return time for the center of such a cube is maximal. Having defined sm$[i]$ (let it be s_i) we look at the cubes $((i+1)\xi_1, (s_i \pm 1)\xi_2)$. If the return time for the center of one of these is bigger than the return time for the center of the cube between them, we choose sm$[i+1]$ in such a way that $((i+1)\xi_1, (\mathrm{sm}[i+1])\xi_2)$ is that cube. If not, we let sm$[i+1]$ be the same as sm$[i]$. Each time we give a value to sm$[i]$, we also set the right value for sm$[-i-1]$ by using the symmetry in the

Lorenz system (for the map f, this symmetry means that $f(-x) = -f(x)$ whenever $f(x)$ is defined).

Let the function $\Psi : \xi\mathbb{Z}^2 \rightrightarrows \xi\mathbb{Z}^2$ be defined by

$$\Psi(k) = \xi\mathcal{S}(\psi(k), m)$$

(cf Equation (8)). This can be viewed as a dynamical system. In particular, analogous to the definition in Section 2 a *trajectory* of Ψ through k is a double sided sequence $\{k^i\}_{i\in\mathbb{Z}}$ of elements of $\xi\mathbb{Z}^2$ such that $k^0 = k$ and $k^{i+1} \in \Psi(k^i)$ for each $i \in \mathbb{Z}$. The invariant part of a set $\mathbf{B} \subset \xi\mathbb{Z}^2$ with respect to Ψ is similarly defined by the set of all cubes k in $\mathbf{B}$ such that there exists a trajectory for Ψ through k contained entirely in $\mathbf{B}$. The function inv whose pseudocode is given below, when called with its argument representing a finite subset of $\xi\mathbb{Z}^2$, returns its invariant part with respect to Ψ (cf [Sz1, Theorem 2.1]). One can also use the modification of this procedure described in [Sz1, Theorem 4.1].

```
function inv(B : set of rect) : set of rect;
var
    A: set of rect;
begin
    do
        A:=B;
        B:=A ∩ Ψ(A) ∩ Ψ^{-1}(A);
    while A ≠ B;
    return A;
end;
```

The next function, isolating_neighbourhood returns a representation of an isolating neighbourhood for f under the assumption that it satisfies the condition $f(k) \subset |\Psi(k)|$ (cf [Sz1, Theorem 4.2]). Its argument of type **set of** rect plays the role of an initial guess. For a finite set $\mathbf{A} \subset \xi\mathbb{Z}^2$ let min $\mathbf{A}$ and max $\mathbf{A}$ denote the minimal and the maximal element of $\mathbf{A}$ with respect to the lexicographical order on $\xi\mathbb{Z}^2$, i.e. the order $\preceq$ defined by

$$(x_1, y_1) \preceq (x_2, y_2) \Longleftrightarrow x_1 < x_2 \quad \text{or} \quad (x_1 = x_2 \quad \text{and} \quad y_1 \leq y_2),$$

for $(x_1, y_1), (x_2, y_2) \in \xi\mathbb{Z}^2$. For $k \in \mathbf{B} \subset \xi\mathbb{Z}^2$, let $\mathcal{C}(\mathbf{B}, k)$ be the set representing the connected component of $|\mathbf{B}|$ containing k.

```
procedure isolating_neighbourhood(B_0 : set of rect) : set of rect;
var
    D, B : set of rect;
    i : integer;
begin
     i := 0;
     B := B_0;
     D:=d̃(B);
     while D ∩ B ≠ ∅ do
     begin
          B:= inv(B)
          if D ∩ B ≠ ∅ and i mod 2 = 0 then
               B := B \ C(B, max B ∩ D);
          if D ∩ B ≠ ∅ and i mod 2 ≠ 0 then
               B := B \ C(B, min B ∩ D);
          i := i + 1;
     end;
     return inv(B);
end;
```

The following function inclosure_set returns the $\mathbf{B}$ set which is used in the definition of the BIP-inclosure (the validity of $\mathbf{B}$ will be rigorously verified later). Its argument w represents the width of the strip around the unstable manifold which is to be removed from the rectangle $[-a,a]\times[-b,b]$ in order to get the argument for a call to the isolating_neighbourhood function.

```
function inclosure_set(w : integer) : set of rect;
var
    A : set of rect;
    sm : graph;
begin
     sm := unstable_manifold;
     A := {(iξ_1, jξ_2) ∈ ξR([-a, a] × [-b, b]) : |j - sm[i]| > w};
     return isolating_neighbourhood(A);
end;
```

8 Proof of Theorem 1.1

As has been indicated earlier and will be made clear in this section, the proof of Theorem 1.1 involves two major computational parts. The first part concerns the verification that an a priori enclosure for the Poincaré map (obtained via a combination of guessing and traditional, non-rigorous numerical computations) gives rise to an isolating neighborhood for the Poincaré map with an appropriate Conley index. The machinery necessary to complete this part of the proof was introduced in the preceding chapters. The second part consists of showing that the Poincaré map is well defined in the domain of the *a priori* enclosure and that the Poincaré map is actually enclosed by this enclosure. To carry out this part we basically use the approach developed in [MiMr]. The algorithm FINDIMVPOINC presented in that paper (see [MiMr], Algorithm 8.7 and Theorem 8.8) enables one to check if the Poincaré map is well defined in a given region and to find its multivalued enclosure. To save computational time we introduce one essential modification. As we have shown in Proposition 5.1, once it is known that the Poincaré map is well defined in the region which is a candidate for the isolating neighborhood, it is sufficient to verify the enclosure only in a certain subset covering the boundary of the isolating neighborhood. This can save considerable computational time, since the verification that the Poincaré map is well defined is much cheaper than the verification together with finding a good enclosure. For this end we need the following simplification of the Algorithm 8.7 in [MiMr] (in what follows we assume that the reader is familiar with the terminology and notation introduced in [MiMr]).

Algorithm 8.1 *:*

```
procedure CHECKPOINC(n : INTEGER, N : set of SBALL2D,
        Δ : array[1 : n] of IMVMDATA, γ, h_max : REAL)
begin
   var i : INTEGER; b : SBALL2D; c : SBALL3D;
      F : IMVMAP; A_0 : set of SBALL3D;
   A_0 := ∅;
   for every b ∈ N do
   begin
      c.x[1] := b.x[1]; c.x[2] := b.x[2]; c.x[3] := R − 1;
      c.r := b.r; A_0 := A_0 ∪ { c };
   end ;
    (* Find the enclosure of the first partial Poincaré map *)
   FINDIMVMAP(A_0, Δ[1], F);
    (* Step by step compute the following enclosures *)
   for i := 2 to n do
```

begin
$\textit{FINDIMVMAP}(\Delta[i-1].\mathbf{A}, \Delta[i], \mathcal{F})$;
end ;
end ;

Theorem 8.2 *Assume Algorithm 8.1 is called with its arguments satisfying the following two conditions*

$$|\mathbf{N}| \subset |\Theta| \subset |\Delta[n].\eta| \text{ and } |\Delta[n].\eta| \text{ is a local section in } |\Delta[1].\nu| \tag{21}$$

$$|\Delta[i].\nu| \cap \Theta = \emptyset \text{ for } i = 2, \dots n-1, \tag{22}$$

where Θ *is a given compact set. If the algorithm stops and does not fail then* $N := |\mathbf{N}| \subset \mathrm{dom}\varphi^{\Theta}$ *and* $\varphi^{\Theta}|_N$ *is continuous.*

Proof: For $i = 1, 2, \dots n$, let $\mathbf{A}_{i-1}$ denote the value of the first argument in the i-th call to FINDIMVMAP . The construction of Algorithm 8.1, Theorem 8.4 in [MiMr] and conditions (21),(22) imply that the sets $A_i := |\mathbf{A}_i|$ and $\Xi := |\eta|$ satisfy the assumptions of Lemma 5.2 in [MiMr]. Thus $N \subset \mathrm{dom}\varphi^{\Theta}$ and $\mathrm{dom}\varphi^{\Theta}_{|N}$ is continuous. ∎

Proof of Theorem 1.1

Let $(\sigma, R, b) \in \{ (10, 28, 8/3), (10, 60, 8/3), (10, 54, 45) \}$. Let $f = f_{\sigma,R,b}$ be the Poincaré map associated with the Lorenz system on the Poincaré plane $\{ (x, y, z) \mid z = R - 1 \}$.

Let $E = E(\mathbf{B}, \xi, \zeta, \Phi, \Psi, m) =: (\mathbf{D}, \Psi)$ be the BIP-inclosure (cf Proposition 5.1 and remarks following its proof), where $\mathbf{B}$ is the set returned by the function *inclosure_set* run with variables $r_1, r_2, \xi, k, m, w, h$ fixed for the selected parameter values as in Table 1. In all cases, $\xi_1 = \xi_2$, so we give only the ξ_1 value. Let $B := |\mathbf{B}|$ and $D := |\mathbf{D}|$.

Let us define the enclosure E_0 as in Proposition 5.1, i.e. by

$$E_0 = (\mathbf{B} \cup \mathbf{K}_0, \Psi_{|\mathbf{B}\cup\mathbf{K}_0}), \quad \mathbf{K}_0 = \mathrm{cntg}(\mathbf{B}) \cap \Psi(\mathbf{B}).$$

Notice that E_0 is an IP-inclosure. This follows directly from the construction of $\mathbf{B}$ (in fact, the proof of Theorem 2.4 in [Sz1] shows that $\Psi(k) \cap \mathbf{B} = \emptyset$ for each $k \in \mathbf{K}_0$). Using a computer we showed that for any $x, y \in \mathbb{Z}$ such that

$$((x-1)\xi_1, (x+1)\xi_1; (y-1)\xi_2, (y+1)\xi_2) \cap (\mathbf{B} \cup \mathbf{K}_0) \neq \emptyset$$

(σ, R, b)	r_1	r_2	ξ_1	k	m	h	w
$(10, 28, 8/3)$	150	150	30/1024	10	8	0.005	12
$(10, 60, 8/3)$	150	150	100/1024	10	8	0.005	5
$(10, 54, 45)$	275	85	21/1024	10	12	0.0025	3
$(10, 490, 1/4)$	150	150	100/1024	10	10	0.005	37

Table 1: xi_1,r_1,r_2,k,m,h and w values for different parameters. Recall that $a = r_1\xi_1$, $b = r_2\xi_2$, $\zeta = \frac{1}{k}\xi$, h is the Runge-Kutta step size, and w is the width of the strip around the stable manifold in P.

the intersection

$$\bigcap_{k\in\xi\mathcal{R}(|((x-1)\xi_1,(x+1)\xi_1;(y-1)\xi_2,(y+1)\xi_2)|)} \zeta\mathcal{R}(|\Psi(k)|)\cap \bigcap_{l\in\zeta\mathcal{R}(|((x-1)\xi_1,(x+1)\xi_1;(y-1)\xi_2,(y+1)\xi_2)|)} \Phi(l)$$

is nonempty. We used a straighforward algorithm (which just checked the nonemptiness of that intersection for all possible values of x and y), and therefore, omit the details. Since the above condition is stronger than the assumption of Proposition 5.1 (iii), $\mathrm{Encl}(E) \cap \mathrm{Encl}(E_0) \neq \emptyset$.

Next, we proved that E is sharp. Clearly, this is a consequence of the following statement.

There is a decomposition $\{\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_i\}$ of $\mathbf{B}$ (recall that this means that $|\mathbf{B}_\alpha| \cap |\mathbf{B}_\beta| = \emptyset$ for $\alpha \neq \beta$) such that, for each $j = 1, 2, \ldots, i$, $|\mathbf{B}_j|$ is homeomorphic to a 2-dimensional disc and $|\mathbf{B}_j| \cap |\mathbf{K}_0|$ is nonempty and is not equal to the whole boundary of $\mathbf{B}_j$.

We proved the above statement using a computer in the following way. First, we found the decomposition $\{\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_i\}$ of $\mathbf{B}$ such that $|\mathbf{B}_j|$ is connected for each $j = 1, 2, \ldots, i$. Then, we checked if the edges contained in the boundary of $|\mathbf{B}_j|$ can be arranged in a cycle in such a way that only pairs of neighboring ones intersect. Again, the algorithm is quite obvious and we shall not discuss its details.

An application of the procedure for cohomology computation described in Section 6 yields the results shown in Figure 2. The matrices shown there describe the φ_i^1 endomorphisms for any map $g \in \mathrm{Encl}(E_0)$. By Proposition 5.1 (ii), these results are valid for any homeomorphism $\bar{g} \in \mathrm{Encl}(E)$ such that $|\mathbf{B}| \subset \mathrm{dom}\ \bar{g}$. Hence, by Theorem 2.2, what remains to be proved in order to show Theorem 1.1 is that these two conditions are satisfied for the return map f defined by the Lorenz Equations.

$$\left[\begin{array}{cccccc} 0&1&1&0&0&0\\ \hline 0&0&0&1&1&0\\ \hline 0&0&0&0&0&1\\ \hline 1&0&0&0&0&0\\ \hline 0&1&1&0&0&0\\ \hline 0&0&0&1&1&0 \end{array}\right] \qquad \left[\begin{array}{cccc} 0&0&1&0\\ \hline 0&0&0&1\\ \hline 1&1&0&0\\ \hline 0&0&1&0 \end{array}\right]$$

$$\left[\begin{array}{cccc} 1&1&0&0\\ \hline 0&0&1&1\\ \hline 1&1&0&0\\ \hline 0&0&1&1 \end{array}\right] \qquad \left[\begin{array}{cccccc} 0&0&1&0&1&0\\ \hline 1&0&0&0&0&0\\ \hline 0&1&0&1&0&0\\ \hline 0&0&1&0&1&0\\ \hline 0&0&0&0&0&1\\ \hline 0&1&0&1&0&0 \end{array}\right]$$

Figure 2: Representations of φ_i^1 for parameter values (10,28,8/3), (10,60,8/3), (10,54,45) and (10,490,1/4)

In other words we have to check that

$$\mathbf{B} \subset \mathrm{dom} f \tag{23}$$

$$\forall_{k\in\mathbf{D}}\ f(k) \subset \mathrm{int}|\Phi(k)| \tag{24}$$

To achieve this we used the technique of intermediate sections developed in [MiMr]. Let Φ be the classic 4-th order Runge-Kutta method for (1). Let $n = 20, 17$ and 26 respectively for $(\sigma, R, b) = (10, 54, 45), (10, 28, 8/3)$ and $(10, 60, 8/3)$. To verify (23) and (24) we take an arithmetic complying with the 64-bit IEEE standard (see [ieee]) and for $i = 1, 2, \ldots n$ we initialize the variables $\Delta[i].\zeta, \Delta[i].\xi, \Delta[i].\mu, \Delta[i].\nu$ as in the tables which may be fetched from http://www.ii.uj.edu.pl/~mrozek/lorenz.html. We take $\mathbf{N}$, the minimal cover of B with elements of $\mathcal{G}^3 := \mathcal{G}^3_{\frac{300}{2^{20}}}$ and start Algorithm 8.1. It stops and does not fail. This shows that condition (23) is satisfied. To prove (24) we take $\mathbf{N}$ to be the minimal cover of $\mathbf{D}$ with elements of $\mathcal{G}^3$ and start Algorithm 8.7 in [MiMr]. It stops and does not fail. Let Π be the multivalued map returned by this algorithm. A straightforward to implement algorithm verifies that this multivalued map is a submap of Φ which implies condition (24). This completes the proof.

∎

Figure 3 shows the **B** sets (marked black), their images under the Ψ map (black and grey parts) and the boundary of the initial guess (thin black lines). One can see that the index pairs are symmetric except for the case of $(\sigma, R, b) = (10, 60, 8/3)$. It is possible to obtain a symmetric **B** in this case using the method described in this section, but since the distance between such a set and the unstable manifold is very small, the rigorous check for the E_0 inclosure for such a **B** would be much harder (if possible at all).

Let us note that the total computational time for the combinatorial part of the proof was about 5-6 minutes on a SUN SPARCstation 5. Clearly, we used the symmetry in the Lorenz Equations whenever we could. This computation time includes the calculation of the E_0 inclosure. The verification that the Poincaré map is well defined in the required region and that the E_0 enclosure actually encloses the map took (on an IBM compatible machine with PENTIUM II 300MHz processor) respectively 8 min, 40 min and 110 min for parameter values $(\sigma, R, b) = (10, 54, 45), (10, 28, 8/3)$ and $(10, 60, 8/3)$. Let us recall that the proof of chaos for parameter values $(\sigma, R, b) = (10, 54, 45)$ presented in [M-M, MiMr] took about 33 hours. So far, we were not able to complete this part of computations for the last set of parameter values (i.e. $(\sigma, R, b) = (10, 490, 1/4)$).

References

[A-K] M. Allili, T. Kaczynski, An Algorithmic Approach to the Construction of Homomorphisms induced by Maps in Homology, preprint.

[A-J-M-R] L. Arnold, C. Jones, K. Mischaikow, and G. Raugel, *Dynamical Systems*, Lect. Notes in Math. **1609**, Springer-Verlag 1995.

[B] A. Baker, in progress.

[C-L-R] T.H.Cormen, C.E.Leiserson, R.L.Rivest, Introduction to Algorithms, The MIT Press & McGraw Hill Book Company 1989.

[D-E] Cecil Jose A. Delfinado and Herbert Edelsbrunner, An Incremental Algorithm for Betti Numbers of Simplicial Complexes on the 3-sphere, *CAGD*, **12** (1995) 771–784.

[K-M-S] Tomasz Kaczyński, Marian Mrozek and Maciej Ślusarek, *Homology Computation by Reduction of Chain Complexes*, *Computers & Mathematics*, 35(1998), no. 4, 59–70.

[M-Sz] M. Mazur and J. Szybowski, in progress.

[M-M] K. Mischaikow and M.Mrozek, *Chaos in the Lorenz Equations: a Computer Assisted Proof* , Bull.AMS **32** (1995), 66-72.

[MiMr] K.Mischaikow and M.Mrozek, *Chaos in the Lorenz Equations: a Computer Assisted Proof. Part II: Details* , *Math. Computation*, **67**(1998), 1023-1046.

[Mr1] M.Mrozek, *Leray functor and cohomological Conley index for discrete dynamical systems* , Trans.Am.Math.Soc. **318** (1990), 149-178.

[Mu] J. Munkres, *Elements of Algebraic Topology*, Addison Wesley, 1984.

[Pi] P. Pilarczyk, work in progress.

[R-S] J.W.Robbin and D.Salamon, *Dynamical systems, shape theory and the Conley index* , Ergodic Th.Dyn.Sys. $\mathbf{8}^*$ (1988), 375-393.

[Sp] E.Spanier, Algebraic Topology, McGraw Hill Book Company, New York 1966.

[Spa] C.Sparrow, The Lorenz Equations: Bifurcations, Chaos and Strange Attractors, Springer-Verlag NY Inc 1982.

[Sz1] A.Szymczak *A combinatorial procedure for finding isolating neighbourhoods and index pairs* , Proc.Royal Soc.Edinburgh, to appear.

[Sz2] A.Szymczak *The Conley Index for Decompositions of Isolated Invariant Sets* , Fund.Math. **148** (1995), 71-90.

[T] W. Tucker, The Lorenz Attractor Exists, preprint 1998.

[ieee] *The IEEE Standard for Binary Floating-Point Arithmetic*, ANSI/IEEE Std 754,1985.

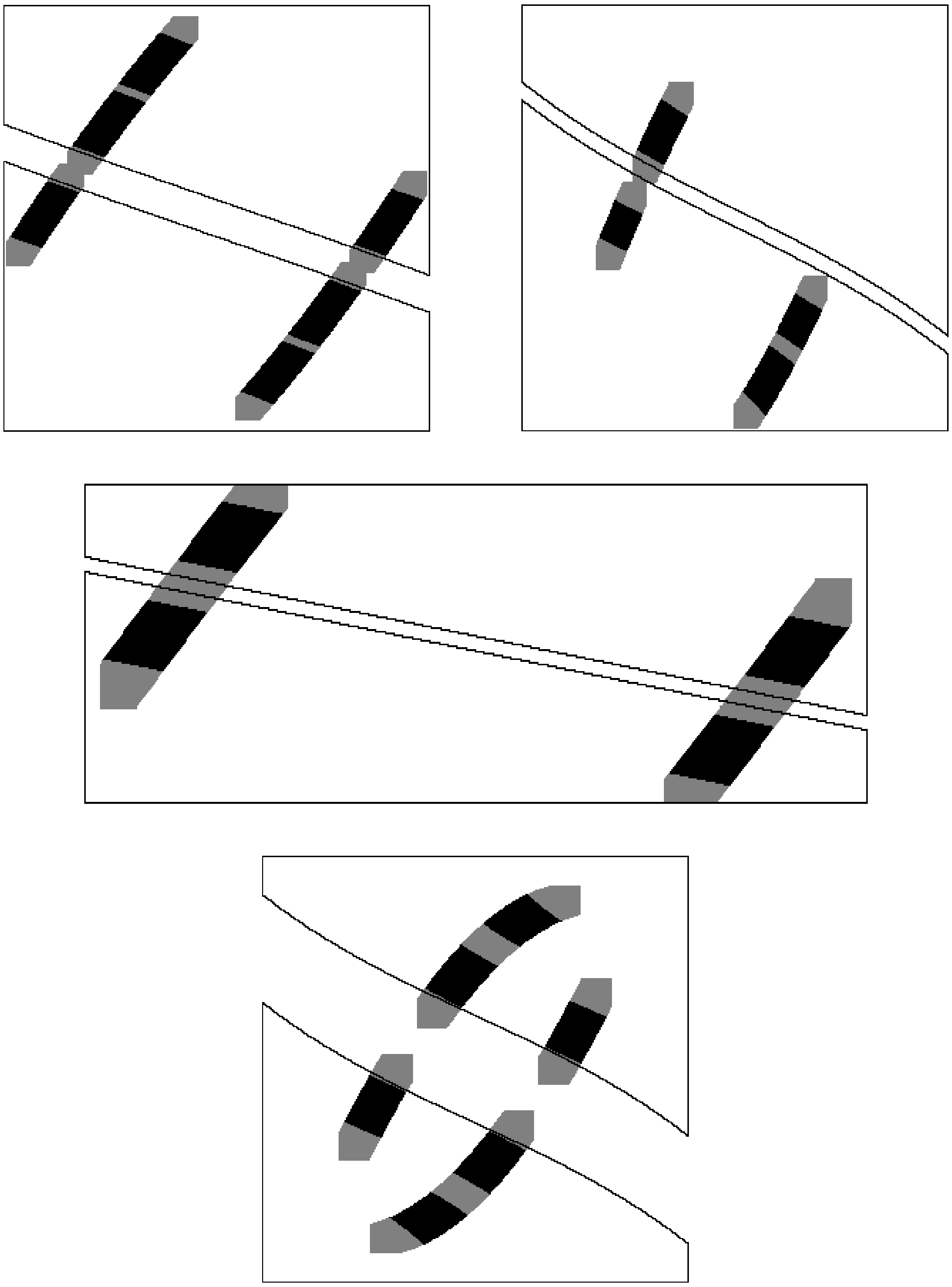

Figure 3: Index pairs and initial guesses for parameter values (10,28,8/3), (10,60,8/3), (10,54,45) and (10,490,1/4)