A FAST AND RELIABLE METHOD FOR DISTINGUISHING REGULAR FROM CHAOTIC MOTION IN HAMILTONIAN SYSTEMS

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Abstract: *We describe the recently introduced method of the Smaller Alignment Index (SALI) for distinguishing ordered from chaotic motion in conservative dynamical systems and apply it to Hamiltonian systems of* 2 *degrees of freedom. We show the effectiveness and the speed of the method in the determination of the dynamical nature of orbits of Hamiltonian systems that possess a very rich structure on a Poincaré surface of section. Of particular interest is the fact that the SALI method applies equally well to the case of many degrees of freedom, where it is expected to prove most useful, since very few similar tools are available. This paper is dedicated to Professor Constantine L. Goudas, on his retirement, as a tribute and a complement to his approach of using periodic orbits to separate order from chaos in Hamiltonian systems.*

Keywords: SALI method, Lyapunov exponents, ordered and chaotic behavior, Hamiltonian systems.

1 INTRODUCTION

1.1 Other methods for distinguishing order from chaos in conservative dynamical systems

In the theory of dynamical systems the distinction between regular and chaotic motion is of great importance, since in ordered domains we have predictability while in chaotic regions we are unable to predict the time evolution of the dynamical system after a short time period. This is fundamental in many applied sciences, such as physics, chemistry, biology and engineering where the dynamics is often dissipative and the motion occurs on a strange attractor [12], [6]. However, the ability to distinguish between order and chaos becomes much more subtle when the motion is conservative and the number of degrees of freedom of the system is large, since in that case we can not even visualize their dynamics. So, it is evident that we need methods that will help us decide accurately and efficiently about the chaotic or ordered character of an orbit especially in systems with many degrees of freedom.

Many methods have been developed over the years to solve the problem of distinguishing ordered from chaotic motion in dynamical systems. One of the first was the well known method of the Poincaré surfaces of section (PSS). This method has to do with the successive intersections of an orbit with an $(n-1)$–dimensional surface (n is the number of phase space dimensions) and has been used mainly in conservative dynamical systems with a small number of degrees of freedom. For example in 2 degrees of freedom (2D) Hamiltonian systems where the phase space is 4 dimensional, the energy integral can be used to lower the dimension to 3, thus rendering the PSS 2 dimensional. The results of this method however are difficult to interpret in systems with more than 2 degrees of freedom.

More recently, Ch. Skokos [7] introduced a new, accurate and easy to compute method to distinguish regular from chaotic motion in conservative dynamical systems: the Smaller Alignment Index method (SALI). In this paper, we recall the definition of the SALI and show its effectiveness in distinguishing regular from chaotic motion in Hamiltonian systems of 2 degrees of freedom.

1.2 Definition of the Smaller Alignment Index (SALI)

Let us consider the $2n$–dimensional phase space of an arbitrary autonomous Hamiltonian dynamical system

$$H \equiv H(q_1(t), \ldots, q_n(t), p_1(t), \ldots, p_n(t)) = E \tag{1}$$

where $q_i(t),\ i = 1, \ldots, n$ are the canonical coordinates, $p_i(t),\ i = 1, \ldots, n$ are the corresponding canonical conjugate momenta and E is the total energy of the system. The time evolution of an orbit of the above dynamical system associated with the initial condition

$$\vec{x}(t_0) = (q_1(t_0), \ldots, q_n(t_0), p_1(t_0), \ldots, p_n(t_0))$$

at initial time t_0 is defined as the solution of the system of $2n$ first order differential equations

$$\frac{dq_i(t)}{dt} = \frac{\partial H}{\partial p_i(t)}, \quad \frac{dp_i(t)}{dt} = -\frac{\partial H}{\partial q_i(t)}, \quad i = 1, \ldots, n \tag{2}$$

which are known as Hamilton's equations of motion and the solution is refereed to as the orbit which passes by the above initial condition $\vec{x}(t_0)$.

In order to define the Smaller Alignment Index (SALI) we need to introduce the notion of the variational equations. These equations are the corresponding linearized equations of the system of ODEs (2), about a reference orbit $\vec{x}(t) = (q_1(t), \ldots, q_n(t), p_1(t), \ldots, p_n(t))$ and are defined by the relation

$$\frac{d\vec{v_i}(t)}{dt} = \mathcal{J}(\vec{x}(t)) \cdot \vec{v_i}(t), \quad i = 1, \ldots, 2n \tag{3}$$

where $\mathcal{J}(\vec{x}(t))$ is the Jacobian of the RHS of the system of ODEs (2). The vectors $\vec{v_i}(t) = (v_{i,1}(t), \ldots, v_{i,2n}(t))$, $i = 1, \ldots, 2n$ are known as deviation vectors of the above orbit. This is because they describe small deviations of neighboring orbits from the reference orbit. Then, we choose arbitrarily two linearly independent such deviation vectors, $\vec{v_1}(t)$ and $\vec{v_2}(t)$ and define the two Alignment Indices (ALI) $\forall t \geq t_0$ as

$$\mathrm{ALI}_-(t) = \left\| \frac{\vec{v_1}(t)}{\|\vec{v_1}(t)\|} - \frac{\vec{v_2}(t)}{\|\vec{v_2}(t)\|} \right\|, \ \mathrm{ALI}_+(t) = \left\| \frac{\vec{v_1}(t)}{\|\vec{v_1}(t)\|} + \frac{\vec{v_2}(t)}{\|\vec{v_2}(t)\|} \right\| \tag{4}$$

where $\| \cdot \|$ denotes the usual Euclidean norm in $\mathbb{R}^{2n}$.

The Smaller Alignment Index (SALI) is now defined as

$$\mathrm{SALI}(t) \equiv \min \left\{ \mathrm{ALI}_-(t), \mathrm{ALI}_+(t) \right\}, \quad \forall t \geq t_0 \tag{5}$$

where t_0 is the initial time of the evolution [7], [8], [9]. From the definition of the two ALIs and the SALI quantity, it follows that we can normalize the length of the deviation vectors at each integration time step without affecting their inner angle.

When $\mathrm{ALI}_-(t) \to 0$ from (4) the two deviation vectors, $\vec{v_1}(t)$ and $\vec{v_2}(t)$, tend to become collinear and with the same sense because their inner angle tends to 0 and so $\mathrm{ALI}_+(t) \to 2$, while when $\mathrm{ALI}_+(t) \to 0$ the two deviation vectors tend to become collinear and with opposite sense because their angle tends to π and so $\mathrm{ALI}_-(t) \to 2$.

If the orbit under consideration $\vec{x}(t) = (q_1(t), \ldots, q_n(t), p_1(t), \ldots, p_n(t))$ is chaotic then it follows from (5) that

$$\lim_{t \to \infty} \mathrm{SALI}(t) = \min\{0, 2\} = 0 \tag{6}$$

because in this case both deviation vectors $\vec{v_1}(t)$ and $\vec{v_2}(t)$ tend to coincide with the direction of the most unstable manifold of the variational equations as $t \to \infty$ [13].

In the case where the reference orbit is regular then the SALI is always seen to oscillate about a positive number $\alpha \in (0, \sqrt{2}]$. To explain this, note first that both deviation vectors eventually become tangential to the torus on which the orbit is confined. Since they generally have components evolving along the torus in directions given by the n independent vector fields (the Hamiltonian and $(n-1)$ quasi–integrals of the motion) their angle never becomes zero and oscillates about some arbitrarily constant [11].

On the contrary, if the reference orbit is chaotic, it can be shown that the evolution of the SALI after long enough times is given by an expression of the form $\exp^{-(\lambda_1-\lambda_2)t}$ where λ_1 and λ_2 are the two largest Lyapunov exponents of the motion [10]. Since $\lambda_1 > 0$ and $\lambda_2 \geq 0$ this clearly implies that the SALI converges to zero exponentially and thus allows us to decide rapidly and unambiguously about the chaotic nature of the reference orbit.

This totally different behavior of the SALI for regular and chaotic orbits makes it a very easy and reliable way to distinguish between chaos and order in Hamiltonian dynamical systems. It is evident that the choice of the initial deviation vectors $\vec{v_1}(t_0)$ and $\vec{v_2}(t_0)$ is arbitrary and does not affect the correctness of the method. This is also ensured by the results found in other papers [7], [8], [9], [11], [10].

2 BEHAVIOR OF THE SALI IN 2D HAMILTONIAN SYSTEMS

2.1 Illustration of the behavior of the SALI in 2D Hamiltonian systems

We apply the SALI method presented above to some examples of 2 degrees of freedom Hamiltonian systems. The first one, due to Hénon and Heiles [5] is described by

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(Ax^2 + By^2) + x^2 y - \frac{C}{3} - E \equiv 0 \tag{7}$$

where x, y are the generalized coordinates and p_x, p_y are the generalized conjugate momenta. We consider the case where $A = B = C = 1$ and take as the total energy of the system $E = \frac{1}{8}$. For this choice of parameters, the PSS $(y, p_y), x = 0, p_x > 0$ reveals a very rich structure with regions containing chaotic motion as well as islands of stability and regular motion confined on 2–dimensional surfaces topologically equivalent to 2–dimensional tori (see figure 1(a)). The final integration time used for the computation of the above PSS, for every orbit, is $t_f = 4000$. 120 orbits where integrated with initial conditions suitably distributed on the PSS.

In order to examine the effectiveness and speed of the SALI method let us consider two characteristic initial conditions of the system (7): The first one with coordinates $(x = 0, y = 0.55, p_x \simeq 0.24170, p_y = 0)$ (black color) corresponding to a regular orbit and the second one with coordinates $(x = 0, y = -0.016, p_x \simeq 0.49974, p_y = 0)$ (gray color) corresponding to a chaotic orbit as can be seen in figure 1(b). The positions of these two initial conditions belongs to the PSS of figure 1(a) and are marked by a black and a gray circle respectively in figure 1(b), together with their successive intersections on the PSS.

As we can see in figure 2(a) the SALI of the ordered orbit (black color) remains almost constant and has a positive non–zero value about 0.61367 for final integration time of $1 \cdot 10^5$ time units. On the other hand, the SALI of the chaotic orbit (gray color) initially remains almost constant but after a small transient period it quickly reaches the value $1 \cdot 10^{-16}$, which is the limit accuracy of the computer, for an integration time of 1758 time units. This means that both deviation vectors used for the computation of the SALI have the same or opposite sign coordinates in the computer representation. The initial deviation vectors used for the computation of the SALI are $\vec{v_1}(0) = (1, 0, 0, 0)$ and $\vec{v_2}(0) = (0, 0, 1, 0)$.

In figure 2(b) we can see the time evolution of the maximum Lyapunov Characteristic Numbers (maximum LCNs) of the same two orbits. The maximum LCN of the ordered orbit (black color) after an initial period of fluctuations about a constant value starts to decrease linearly on the average (in the $\log_{10} - \log_{10}$ plane) reaching the value $1.7 \cdot 10^{-6}$ at final integration time $t_f \simeq 1 \cdot 10^5$. On the other hand, the maximum LCN of the chaotic orbit (gray color) exhibits fluctuations and tends to a small positive value of about $0.42 \cdot 10^{-1}$.

We underline at this point that in the chaotic case we are able to decide about the character of the orbit already at integration time $t \simeq 500$ at which the SALI has become practically zero while it remains nearly

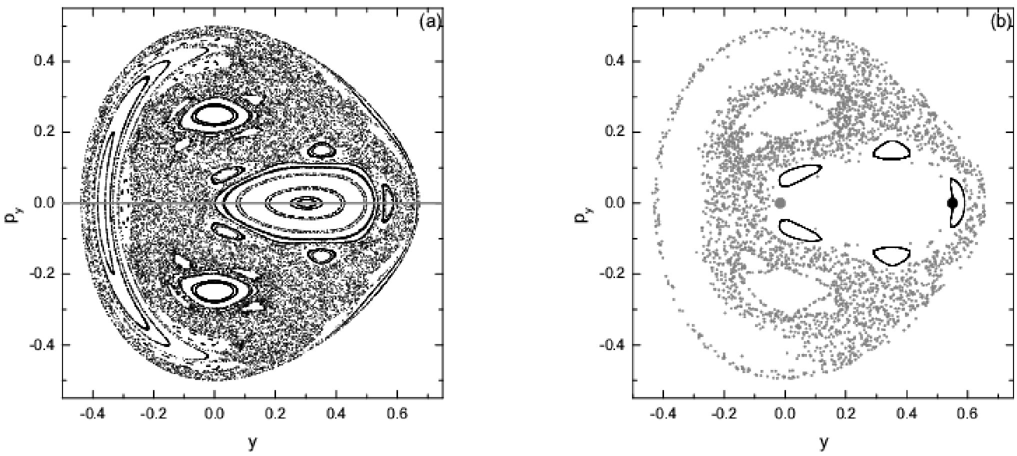

Figure 1: Panel (a): The Poincaré surface of section $(y, p_y), x = 0, p_x > 0$ of the 2 degrees of freedom Hénon and Heiles Hamiltonian (7) with $E = \frac{1}{8}$. The axis $p_y = 0$ is also plotted. Panel (b): Successive intersections for the ordered orbit with initial condition $(x = 0, y = 0.55, p_x \simeq 0.24170, p_y = 0)$ (black points) and for the chaotic orbit with initial condition $(x = 0, y = -0.016, p_x \simeq 0.49974, p_y = 0)$ (gray points). The initial conditions of the two orbits are marked by big black and gray filled circles respectively.

constant for the ordered trajectory. On the other hand, the behavior of the maximal LCN, shown in figure 2(b), after a similar interval has certainly not converged to zero for the ordered orbit, while for the chaotic one it still has not completely settled down to its limiting non–zero value.

2.2 Scanning the PSS of 2D Hamiltonian systems: A global picture of the dynamics

As we can see in figure 1(a), the Poincaré surface of section of the Hénon and Heiles Hamiltonian (7) with $E = \frac{1}{8}$ exhibits a very rich dynamical structure. There are islands of stability represented by smooth invariant closed curves as well as large regions filled with scattered points representing chaotic motion. Since the SALI tends to completely different values for ordered and chaotic orbits, we can compute it for a sample of initial conditions in order to distinguish clearly the regions where regular and chaotic motion occurs and compare the result with that of the PSS of figure 1(a).

As a first step, we consider orbits with initial conditions that lie on the $p_y = 0$ axis on the PSS of figure 1(a), with $x = 0$ and p_x defined by the Hamiltonian (7) solved for $p_x > 0$. The values of the SALI for all these initial conditions at time $t = 4000$ are plotted in figure 3(a) as a function of y and are represented by black colored dots, connected through gray colored lines as an interpolation for the SALI of the non–computed initial conditions.

We can distinguish clearly intervals of regular motion where the SALI has values within $[1 \cdot 10^{-4}, \sqrt{2}]$. These initial conditions (y, p_y) correspond to invariant smooth closed curves (islands of stability) of figure 1(a). We can also see intervals of strong chaotic motion with corresponding SALI values between $[0, 1 \cdot 10^{-12})$.

Although, most of the SALI values are greater or equal than $1 \cdot 10^{-4}$ or smaller than $1 \cdot 10^{-12}$, there are also some initial conditions y on the line $p_y = 0$ that their corresponding SALI values lie in the intermediate interval $[1 \cdot 10^{-12}, 1 \cdot 10^{-4})$. The SALI for all these initial conditions indicates that these orbits are sticky and wander for very long times near the borders of islands of regular motion.

We have chosen one characteristic point with initial condition $(0, -0.2088, 0.44759, 0)$, indicated by an arrow in the figure 3(a), which has a SALI value around 0.53954 at final integration time $t_f = 4000$, and

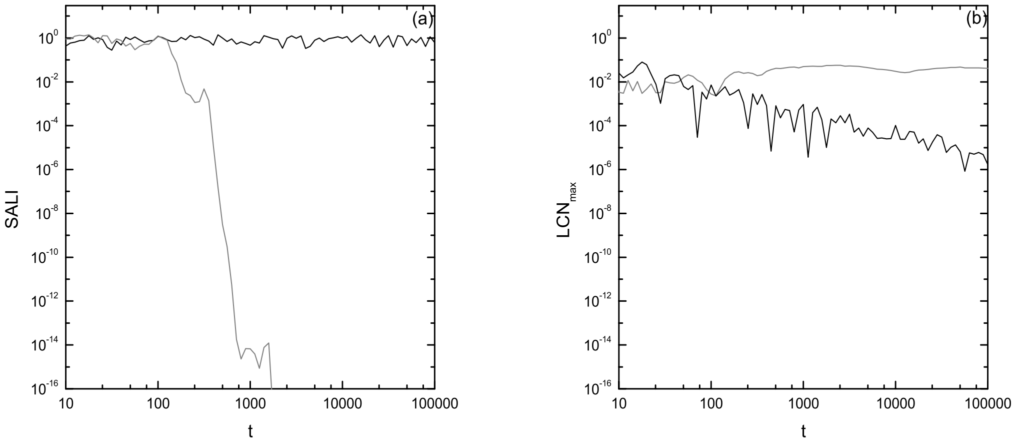

Figure 2: Panel (a): The time evolution in the $\log_{10} - \log_{10}$ plane of the SALI, for the Hénon and Heiles Hamiltonian (7) with $E = \frac{1}{8}$, for the ordered orbit with initial condition $(x = 0, y = 0.55, p_x \simeq 0.24170, p_y = 0)$ (black color) and for the chaotic orbit with initial condition $(x = 0, y = -0.016, p_x \simeq 0.49974, p_y = 0)$ (gray color). Panel (b): The maximum Lyapunov Characteristic Number (LCN) as a function of the integration time t in the $\log_{10} - \log_{10}$ plane, for the Hénon and Heiles Hamiltonian (7) with $E = \frac{1}{8}$, for the same two initial conditions.

corresponds to an orbit which is regular. The dynamical nature of this initial condition is not at all obvious looking at the corresponding PSS of figure 1(a) but becomes clear when we consider its SALI value. Indeed, this initial condition lies within a chain of 35 very small islands inside a big chaotic sea as shown in figure 3(b) which are so small as to be invisible in the corresponding PSS of panel of figure 1(a). In figure 3(b) we have calculated their successive intersections of this regular orbit on the PSS $(y, p_y), x = 0, p_x > 0$.

Next we apply the above analysis to the whole PSS and plot in figure 4(a) with different shades of gray initial conditions that give SALI values in different intervals. In this way, we obtain a global picture of the PSS plane, with light gray in regions where regular motion occurs, for example in islands of stability, and black in regions where the motion is chaotic.

The picture of figure 4(a) strongly reminds us of the PSS of figure 1(a). We expect of course that as the orbits are integrated for longer times the size of the regular regions of figure 4(a) will diminish and resemble even more the PSS of figure 1(a). Still, it is obvious that the SALI gives us a clear view of the global dynamics of the system and helps us identify small size regions of regular behavior which are deeply embedded in the chaotic sea. This becomes even more evident in figure 4(b), where the SALI provides a very detailed picture of the small scale dynamics when it is used to investigate a blow up of a part of the PSS at the center of figure 4(a).

For comparison purposes, we have estimated the real CPU time needed for the calculation of the PSS of figure 1(a) and for the calculation of figure 4(a). Using an AMD ATHLON XP+ 2000 it takes approximately 200 sec for the computation of the PSS, using 120 initial conditions each integrated up to 4000 time steps, while the SALI method takes about 26000 sec to complete the scanning of the PSS image using 225×100 initial conditions each integrated up to 1000 time steps and exploiting the symmetry of the figure.

2.3 The SALI for thin chaotic regions

In order to demonstrate the strength of the SALI method as an indicator of chaos in Hamiltonian systems let us consider an example of a Hamiltonian for which regular behavior is dominant and the size of the chaotic regions is so small that they can easily be overlooked by a first straightforward calculation of the PSS.

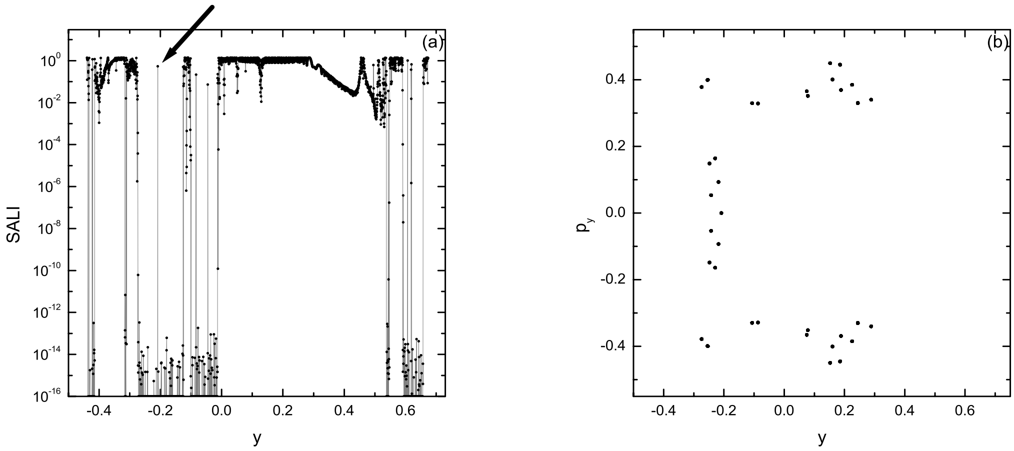

Figure 3: Panel (a): The SALI values up to final integration time $t_f = 4000$ for orbits with initial conditions on the $p_y = 0$ axis for the PSS shown in figure 1(a), plotted as a function of the initial condition y. The SALI values are plotted as black points and are connected through gray lines. Panel (b): The PSS $(y, p_y), x = 0, p_x > 0$ of the orbit with initial condition $(0, -0.2088, 0.44759, 0)$ of panel (a) which is indicating by a black arrow.

In particular, let us consider the two degrees of freedom Hamiltonian

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{4}(x^4 + y^4 + \eta(x - y)^4) - E \equiv 0 \qquad (8)$$

where x, y are the generalized coordinates, p_x, p_y are the generalized conjugate momenta and $\eta \in \mathbb{R}$ is a constant parameter, whose dynamics was first investigated from the point of view of singularity analysis in the complex time domain in [4]. It was observed that for η near 0.25 practically all of phase space is filled with invariant tori and only few chains of islands are visible around which one expects to find chaotic behavior (see figure 5(a)).

Taking $\eta = 0.24$ we decided to use the SALI method to study one such chaotic orbit starting with the initial condition $(x = 0, y = 0, p_x = 0.77, p_y \simeq 44.71473)$ corresponding to the gray dot at the center of figure 5(b).

Interestingly enough, the SALI started to converge exponentially to zero after only about 100 time units (see figure 6(a) demonstrating thus clearly the chaotic nature of the orbit. Computing also the maximum LCN for this case we found that it does converge to a small non–zero positive value but takes somewhat longer to settle down to its final limit value (see figure 6(b)).

3 CONCLUSIONS

In this paper, we have first described a novel accurate and efficient method based on the computation of the so called Smaller Alignment Index (SALI) for multidimensional Hamiltonian dynamical systems. We then applied the SALI method to the well known Hénon and Heiles Hamiltonian and another example of a 2 degree of freedom Hamiltonian system and showed that the computation of the SALI allows us to distinguish in a cost effective and reliable way between ordered and chaotic orbits.

We have found that the SALI tends to zero exponentially for chaotic orbits, while in general, it fluctuates around positive non–zero values for ordered orbits. This approach, in fact, begins to be truly valuable for Hamiltonian systems of 2 degrees of freedom (where detailed surface of section plots are often computationally

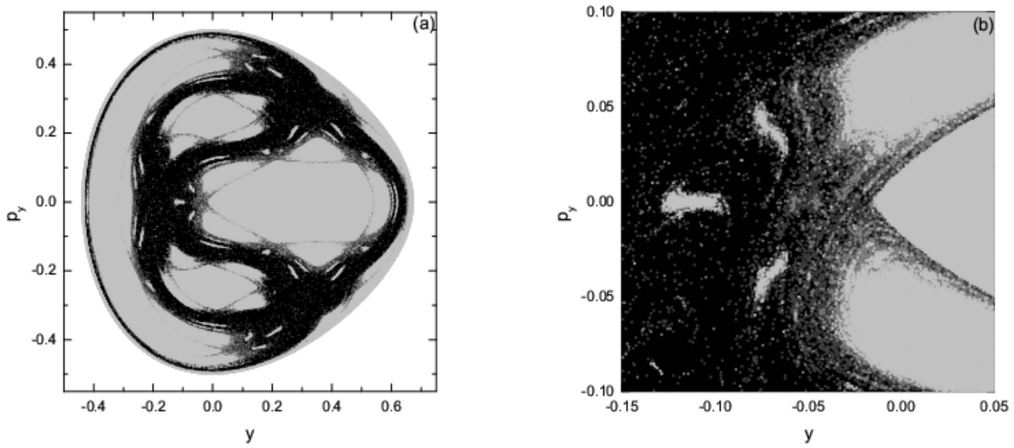

Figure 4: Panel (a): Regions of different SALI values on the PSS $(y, p_y), x = 0, p_x > 0$ up to final integration time $t_f = 1000$. Panel (b): A blow up of part of the PSS at the center of figure 4(a) shows interesting small size regions of stability not visible on the PSS of figure 1(a). In both panels initial conditions that give SALI $< 1 \cdot 10^{-12}$ are marked by black points, initial conditions that give $1 \cdot 10^{-12} \leq$ SALI $< 1 \cdot 10^{-8}$ are marked by dark gray points, initial conditions that give $1 \cdot 10^{-8} \leq$ SALI $< 1 \cdot 10^{-4}$ are marked by gray points, while initial conditions that give $1 \cdot 10^{-4} \leq$ SALI $\leq \sqrt{2}$ are marked by light gray points.

costly) and promises to become very useful for higher than 2 degree of freedom Hamiltonian systems where the PSS have little meaning because they are difficult to interpret.

Finally, exploiting the fact that the SALI gives useful information over short time intervals, we have computed it for a suitably fine grid of initial conditions, thus delineating regions of phase space which contain regular and chaotic behavior. In fact, we have observed that the SALI is accurate enough to make this distinction even if a chaotic layer is very thin or a chain of "islands" is too small to be visible in a standard PSS plot.

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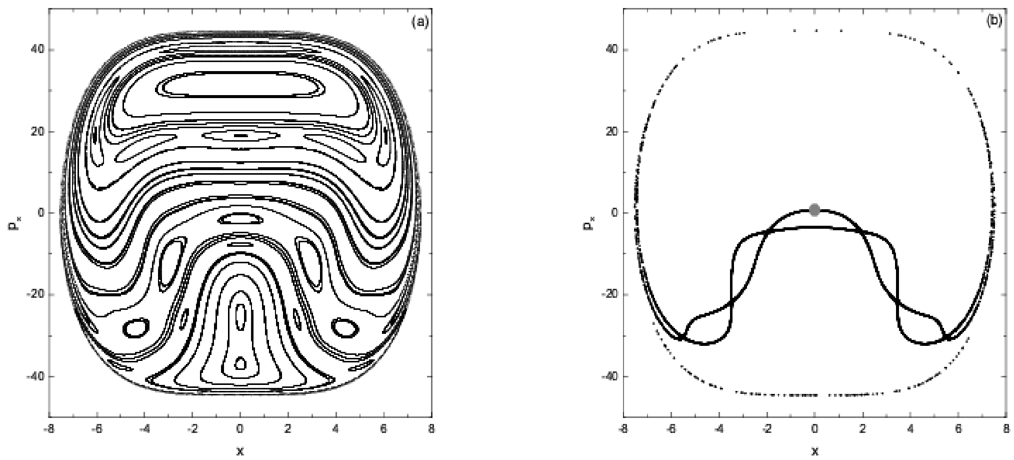

Figure 5: Panel (a): The Poincaré surface of section $(x, p_x), y = 0, p_y > 0$ of the 2 degrees of freedom Hamiltonian (8) with $\eta = 0.24$ and $E = 1000$. Panel (b): A very thin chaotic region between chains of islands on the PSS $(x, p_x), y = 0, p_y > 0$ of figure 5(a) for the initial condition $(x = 0, y = 0, p_x = 0.77, p_y \simeq 44.71473)$ which is shown by a gray colored filled circle.

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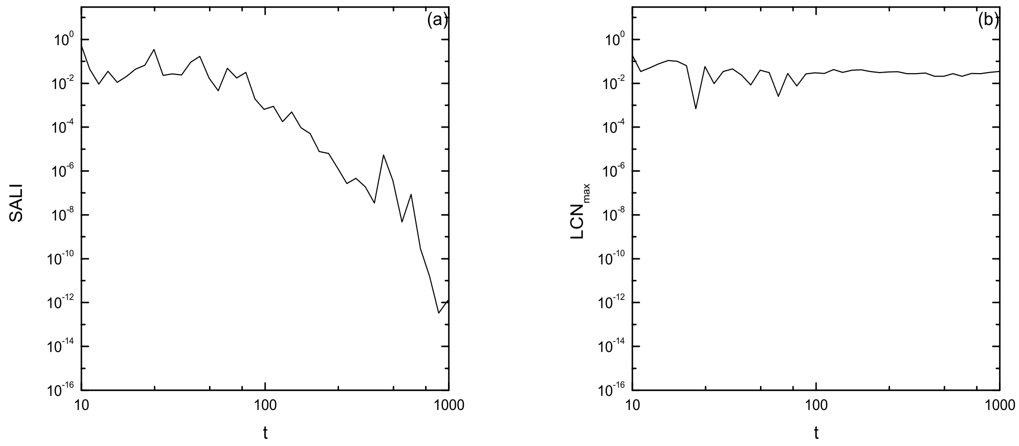

Figure 6: Panel (a): The time evolution in the $\log_{10}-\log_{10}$ plane of the SALI, for the Hamiltonian (8) with $\eta = 0.24$ and $E = 1000$, for the initial condition ($x = 0, y = 0, p_x = 0.77, p_y \simeq 44.71473$). Panel (b): The corresponding maximum Lyapunov Characteristic Number (LCN) as a function of the integration time t in the $\log_{10}-\log_{10}$ plane.

Περίληψη: *Στο άρθρο αυτό περιγράφουμε την πρόσφατα εισαχθείσα μέθοδο του Μικρότερου Δείκτη Ευθυγράμμισης (SALI) για τον διαχωρισμό μεταξύ οργανωμένης και χαοτικής κίνησης σε διατηρητικά δυναμικά συστήματα και την εφαρμόζουμε σε Χαμιλτώνια συστήματα 2 βαθμών ελευθερίας. Δείχνουμε την αποτελεσματικότητα και ταχύτητα της μεθόδου ως προς τον προσδιορισμό της δυναμικής τροχιών Χαμιλτώνιων συστημάτων τα οποία παρουσιάζουν πλούσια δομή σε κατάλληλες τομές επιφανειών Poincaré. Ιδιαίτερο ενδιαφέρον παρουσιάζει το γεγονός ότι η μέθοδος του SALI μπορεί να εφαρμοσθεί με επιτυχία και στην περίπτωση πολλών βαθμών ελευθερίας, όπου αναμένεται να αποδειχθεί εξαιρετικά χρήσιμη, αφού πολύ λίγα παρόμοια εργαλεία είναι διαθέσιμα. Το άρθρο μας είναι αφιερωμένο στον Καθηγητή κ. Κωνσταντίνο Λ. Γούδα, ως φόρος τιμής αλλά και ως συμπλήρωμα της δικής του προσέγγισης διαχωρισμού τάξης και χάους σε Χαμιλτώνια συστήματα μέσω περιοδικών τροχιών.*

Keywords: Μέθοδος SALI, εκθέτες Lyapunov, οργανωμένη και χαοτική συμπεριφορά, Χαμιλτώνια συστήματα.