

Computing periodic orbits with arbitrary precision

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This paper deals with the computation of periodic orbits of dynamical systems up to any arbitrary precision. These very high requirements are useful, for example, in the studies of complex pole location in many physical systems. The algorithm is based on an optimized shooting method combined with a numerical ordinary differential equation (ODE) solver, TIDES, that uses a Taylor-series method. Nowadays, this methodology is the only one capable of reaching precision up to thousands of digits for ODEs. The method is shown to be quadratically convergent. Some numerical tests for the paradigmatic Lorenz model and the Hénon-Heiles Hamiltonian are presented, giving periodic orbits up to 1000 digits.

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I. INTRODUCTION

An important topic in physics is the study of dynamical systems, where the location and the study of the periodic orbits (POs) of the systems give relevant information. Poincaré [1] pointed out that the skeleton of a dynamical system is formed by the families of POs depending on the parameters of the system [2,3]. The nature of such POs, in particular the unstable periodic orbits (UPOs), gives us a good knowledge of the system and provides critical information in chaotic regions. The position and stability of the POs [4,5] determine the long behavior of the system. Thus, the POs are the main kernel of several important physical applications, as in the “scar” theory in quantum mechanics [6], in the analysis and control of chaotic dynamical systems [7,8], in the study of open Hamiltonian systems in several fields [9], and so on. The location of POs has been a well-studied problem by physicists [10–13] and mathematicians using several numerical algorithms, but the procedures to compute them numerically are not exact, in general.

The goal of this paper is to obtain a fast and accurate algorithm for computing periodic orbits up to any arbitrary precision for low-dimensional problems. This study has been motivated by the problem of complex pole location in physics [14–16] and, in particular, by the work of D. Viswanath [17], where very high precision in POs has become essential. Viswanath developed a method [18] to compute high-precision POs and applied it to the Hill’s problem [19] that describes the motion of the Moon around the Earth. Later, regarding his method [20] he computed very high precision (500 digits) POs in the Lorenz problem and used them to study the fractal structure of the Lorenz attractor and the pole location. Nowadays, his algorithm is the unique algorithm in literature capable of computing high-precision POs. To reach this goal he has used very clever algorithms in order to avoid numerical ordinary differential equation

(ODE) integration methods because a standard method cannot integrate up to such a high precision level, but it is quite difficult to use in a general setting. So, in this paper we are going to develop a new method to compute POs with arbitrary precision, which combines three important themes: an optimized shooting method with the Newton-Raphson method, the Taylor-series method (implemented by means of the software TIDES [21]), and the singular value decomposition (SVD) [22,23].

The equations of the proposed method differ when we study a dissipative case or a conservative one, like a Hamiltonian system. To check the method with both models, we choose two classical and well-known problems: the Lorenz model and the Hénon-Heiles problem. The Lorenz system of differential equations arises from the work of E. N. Lorenz [24], who was studying thermal variations in an air cell underneath a thunderhead. He noticed that initial conditions with small differences eventually produced vastly different solutions. The Lorenz system has become one of the most widely studied systems of ODEs because of its wide range of behaviors. The classical Hénon-Heiles Hamiltonian [25] was posed to the study of galactic dynamics to describe the motion of stars around a galactic center. It was one of the first models of Hamiltonian chaos and this model has several applications in theoretical chemistry.

The organization of the paper is as follows. In Sec. II, we show our corrector algorithm. We present the equations for both the dissipative and the Hamiltonian cases. In Sec. III, we explain the necessity of the use of an accurate numerical ODE integrator like TIDES (Taylor integrator for differential equations) [21]. This freeware library computes, simultaneously, both the solution and the partial derivatives in any arbitrary precision. Another important point that we deal with in Sec. IV is to solve the above linear systems where the matrix of the system is not necessarily a square matrix. So, we use the SVD to find the least-norm solution that will be the solution if the matrix of the system is a nonsingular square matrix. In Sec. V we show the results of some numerical tests that prove the good behavior of the method for both cases, the dissipative case and the Hamiltonian case, respectively. Finally, in Sec. VI we present the conclusions of this work.

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II. THE CORRECTOR ALGORITHM

Let

$$\mathbf{x} = \mathbf{x}(t; \mathbf{y}), \quad t \in \mathbb{R}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^n, \quad (1)$$

be the solution of the autonomous differential system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}); \quad \mathbf{x}(0) = \mathbf{y}, \quad \mathbf{x} \in \mathbb{R}^n, \quad (2)$$

where \mathbf{y} represents the initial conditions.

A periodic orbit of the system (2) is characterized by a vector \mathbf{y} of initial conditions and a period T such that the periodicity condition

$$\mathbf{x}(T; \mathbf{y}) - \mathbf{y} = \mathbf{0} \quad (3)$$

is fulfilled.

To find the roots of Eq. (3), that is, to find the initial conditions of the periodic orbit, we will use a method [26,27] based on the Newton-Raphson method. This is an iterative scheme that begins with a set, (\mathbf{y}_0, T_0) , of approximate initial conditions $[\mathbf{x}(T_0; \mathbf{y}_0) - \mathbf{y}_0 \approx \mathbf{0}]$. These approximated initial conditions may be obtained, for instance, by use of the grid-search method [28,29] or the Schmelcher and Diakonou method [10,30], which are often used in the physics community.

Let us suppose that at step i we have a set of corrected initial conditions (\mathbf{y}_i, T_i) . Now, we improve these initial conditions by adding the corrections $(\Delta \mathbf{y}_i, \Delta T_i)$ in such a way that

$$\|\mathbf{x}(T_i + \Delta T_i; \mathbf{y}_i + \Delta \mathbf{y}_i) - (\mathbf{y}_i + \Delta \mathbf{y}_i)\| < \|\mathbf{x}(T_i; \mathbf{y}_i) - \mathbf{y}_i\|. \quad (4)$$

Approximate corrections $(\Delta \mathbf{y}_i, \Delta T_i)$ are obtained by expanding

$$\mathbf{x}(T_i + \Delta T_i; \mathbf{y}_i + \Delta \mathbf{y}_i) - (\mathbf{y}_i + \Delta \mathbf{y}_i) = \mathbf{0}$$

in a multivariable Taylor series up to the first order

$$\mathbf{x}(T_i; \mathbf{y}_i) - \mathbf{y}_i + \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}} - I \right) \Delta \mathbf{y}_i + \frac{\partial \mathbf{x}}{\partial t} \Delta T_i = \mathbf{0}, \quad (5)$$

where I is the identity matrix of order n and the partial derivatives of the solution with respect to the initial conditions and with respect to the time must be evaluated at (\mathbf{y}_i, T_i) .

The $n \times n$ matrix $\partial \mathbf{x} / \partial \mathbf{y}$ is the solution of the variational equations. This matrix evaluated at (\mathbf{y}_i, T_i) is an approximation of the monodromy matrix M of the PO. The column vector $\partial \mathbf{x} / \partial t$ represents the derivative of the solution with respect to the time, i.e., $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. This vector, evaluated at (\mathbf{y}_i, T_i) , corresponds to the expression $\mathbf{f}(\mathbf{y}_{T_i})$, where $\mathbf{y}_{T_i} = \mathbf{x}(T_i, \mathbf{y}_i)$. Then we write

$$(M - I) \Delta \mathbf{y}_i + \mathbf{f}(\mathbf{y}_{T_i}) \Delta T_i = -(\mathbf{y}_{T_i} - \mathbf{y}_i), \quad (6)$$

or, in matrix formulation,

$$\left((M - I) \quad \mathbf{f}(\mathbf{y}_{T_i}) \right) \begin{pmatrix} \Delta \mathbf{y}_i \\ \Delta T_i \end{pmatrix} = (\mathbf{y}_i - \mathbf{y}_{T_i}), \quad (7)$$

that represents a linear system with n equations and $n + 1$ unknowns.

To solve the linear system (7) we have several options. We may reduce the number of unknowns by looking for periodic orbits with the same period ($\Delta T_i = 0$), but the existence of these orbits is not warranted. Another possibility is to take into

account that a tangent displacement is a translation along the initial solution. Such displacement is avoided by constraining the variation of the initial conditions to an n -dimensional plane that is not tangent to the solution, in particular, an orthogonal displacement,

$$(\mathbf{f}(\mathbf{y}_i))^T \Delta \mathbf{y}_i = 0, \quad (8)$$

is considered.

Adding the condition (8) to the system (7), we have the $(n + 1) \times (n + 1)$ linear system

$$\begin{pmatrix} M - I & \mathbf{f}(\mathbf{y}_{T_i}) \\ (\mathbf{f}(\mathbf{y}_i))^T & 0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{y}_i \\ \Delta T_i \end{pmatrix} = \begin{pmatrix} \mathbf{y}_i - \mathbf{y}_{T_i} \\ 0 \end{pmatrix}. \quad (9)$$

When the differential system (2) admits one or more integrals, a new constrain or vector of constrains, respectively, $\mathbf{G}(t; \mathbf{x}) = \mathbf{g}$, must be added to the periodicity condition (3). To maintain the new constrain we impose the condition

$$\begin{aligned} & \mathbf{G}(T_i + \Delta T_i; \mathbf{y}_i + \Delta \mathbf{y}_i) - \mathbf{g} \\ & \approx \mathbf{G}(T_i; \mathbf{y}_i) - \mathbf{g} + \frac{\partial \mathbf{G}}{\partial \mathbf{x}} \Big|_{(T_i, \mathbf{y}_i)} \Delta \mathbf{y}_i + \frac{\partial \mathbf{G}}{\partial t} \Big|_{(T_i, \mathbf{y}_i)} \Delta T_i = 0. \end{aligned}$$

In an autonomous Hamiltonian problem we have the integral of the energy $\mathcal{H}(\mathbf{x}) = h$. Then, taking into account that the Hamiltonian does not depend on the time, the constraint condition has the form

$$(\nabla_{\mathbf{x}} \mathcal{H}) \Big|_{(T_i, \mathbf{y}_i)} \Delta \mathbf{y}_i = h - h_{T_i}. \quad (10)$$

So, in a Hamiltonian system, (9) must be completed with the condition (10), and we have

$$\begin{pmatrix} M - I & \mathbf{f}(\mathbf{y}_{T_i}) \\ (\mathbf{f}(\mathbf{y}_i))^T & 0 \\ (\nabla_{\mathbf{x}} \mathcal{H}) \Big|_{(T_i, \mathbf{y}_i)} & 0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{y}_i \\ \Delta T_i \end{pmatrix} = \begin{pmatrix} \mathbf{y}_i - \mathbf{y}_{T_i} \\ 0 \\ h - h_{T_i} \end{pmatrix}, \quad (11)$$

that is, a linear system with $n + 2$ equations and $n + 1$ unknowns.

III. SOLVING ODE'S AND VARIATIONAL EQUATIONS WITH ARBITRARY PRECISION ARITHMETIC

In our algorithm there are two key points to compute the correction: computing the left matrix of the linear system (7), (9) or (11) and then solving them. To compute the matrix we need to integrate the ODE (2) and to compute the partial derivatives of its solution (1) with respect to the initial conditions \mathbf{y} . To do that, we use the software TIDES, which computes simultaneously both the solution and the partial derivatives of the solution of (2) in double or multiple precision (using TIDES together with the multiple precision libraries MPFR and GMP), by using the Taylor-series method (TSM) [21,31].

Let us suppose that the Taylor-series expansion of (1) is given by the expression

$$\mathbf{x}(t) = \sum_i \mathbf{x}^{[i]} h^i, \quad h = t - t_0, \quad \mathbf{x}^{[i]} = \frac{1}{i!} \frac{d\mathbf{x}^{(i)}(t_0)}{dt^i}. \quad (12)$$

Then, substituting \mathbf{x} by its power series expansion in (1), expanding the function $\mathbf{f}(\sum_i \mathbf{x}^{[i]} h^i) = \sum_i \mathbf{f}^{[i]}(\mathbf{x}^{[0]}, \dots, \mathbf{x}^{[i]}) h^i$, and equating the coefficients of the

series, we eventually have the main relation of the TSM:

$$\mathbf{x}^{[i+1]} = \frac{\mathbf{f}^{[i]}(\mathbf{x}^{[0]}, \dots, \mathbf{x}^{[i]})}{(i+1)}, \quad (13)$$

which gives, in an iterative way, beginning from the initial condition $\mathbf{x}^{[0]} = \mathbf{y}$, a method of finding the coefficients $\mathbf{x}^{[i+1]}$ of the Taylor expansion of the solution of the system. This procedure is based on automatic differentiation techniques [32]. Finally, we use this Taylor series to compute the numerical value of the solution if the integration point is inside the convergence radius of the series or we recompute the expansion until this condition is fulfilled.

Usually, the matrix of partial derivatives $\Phi = \partial \mathbf{x} / \partial \mathbf{y}$ of the solution with respect to the initial conditions is computed by using the variational equations $\dot{\Phi} = (\partial \mathbf{f} / \partial \mathbf{x}) \cdot \Phi$, which differ for each problem and are sometimes very difficult to formulate. In TIDES, instead of formulating the variational equations, we use the relations (12) to create iterative formulas (see Ref. [33]) and to compute simultaneously the solution and the partial derivatives in an automatic way. This simplifies the process and permits us to extend it to any differential equation and to work with any precision without difficulties.

IV. LINEAR SYSTEMS AND SINGULAR VALUE DECOMPOSITION

Finally, to find the correction we need to solve a linear system $A\mathbf{x} = \mathbf{b}$, where the matrix A is not necessarily a square matrix. Instead, to solve the system, we will use the least-norm method. This method tries to find a vector \mathbf{x} that minimizes the residual $d = \|A\mathbf{x} - \mathbf{b}\|$. When A is a nonsingular square matrix, the minimum of the residual is zero and the least-norm solution coincides with the solution of the linear system $A\mathbf{x} = \mathbf{b}$. Then, we will try to obtain the least-norm solution to ensure a correction when we do not have an exact solution. To find the least-norm solution we will use the SVD [22,23].

Apart from the SVD method we may use the QR decomposition. Although the QR method has lower computational cost [$2n^2m - 2n^3/3 + \mathcal{O}(n^2)$ for an $m \times n$ matrix] than the SVD method [$4n^2m - 4n^3/3 + \mathcal{O}(n^2)$] we have chosen SVD because it is specially well adapted for rank-deficient problems and we want to develop a general algorithm useful also in these situations. In fact, a periodic orbit presents a rank-deficient matrix when its family of POs crosses a bifurcation point or when the system has some extra unknown integrals. In any case, the most expensive part of the algorithm is the numerical solution of the ODE system with high precision, and so the global complexity is similar, using both SVD and QR algorithms.

A *singular value decomposition* of a $m \times n$ matrix A is a (nonunique) factorization

$$A = U \Sigma V^T, \quad (14)$$

where U is a $m \times m$ orthogonal matrix, V is a $n \times n$ orthogonal matrix, and Σ is a $m \times n$ matrix whose elements are all zero except the elements, $\sigma_{ii} = s_i \geq 0$, $i \leq \min(n,m)$, of the diagonal. The numbers s_i are the *singular values* of the matrix A , and the number $r \leq \min(n,m)$ of singular values different from zero is the rank of the matrix A .

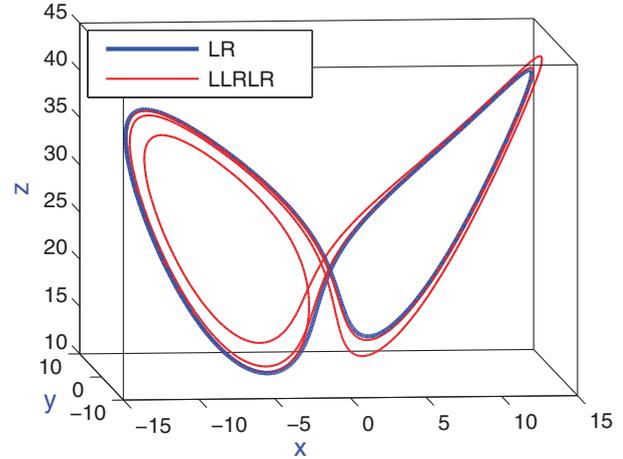


FIG. 1. (Color online) The periodic orbits LR and LLRLR of the Lorenz model.

By multiplying the system $A\mathbf{x} - \mathbf{b} = U \Sigma V^T \mathbf{x} - \mathbf{b}$, by U^T , it is transformed into the system $\Sigma \mathbf{x}^* - \mathbf{b}^*$, where $\mathbf{x}^* = V^T \mathbf{x}$ and $\mathbf{b}^* = U^T \mathbf{b}$. Since orthogonal matrices preserve norm $d = \|A\mathbf{x} - \mathbf{b}\| = \|\Sigma \mathbf{x}^* - \mathbf{b}^*\|$. As Σ is a diagonal matrix, we may find easily the vector \mathbf{x}^* that minimize d . This solution is given by taking $x_i^* = b_i^*/s_i$ if $s_i \neq 0$, and x_i^* any value in other case. Then $\mathbf{x} = V \mathbf{x}^*$ is the least-norm solution of the linear system with a residual $d = (\sum (b_i^*)^2)^{1/2}$, where the sum is over all index i corresponding with a singular value equal to zero. If there is no singular value equal to zero, then least-norm solution is the exact solution of the linear system.

V. TESTS

In order to show the performance of this method we present in this section some tests on two classical models: the Lorenz model, as an example of chaotic dissipative systems, and the Hénon-Heiles model, as an example of Hamiltonian systems. All the tests have been done on a personal computer PC Intel Core i7 CPU 860, 2.80 GHz under a 2.6.32-29-generic SMP x86_64 GNU/Linux system. The files with the initial conditions, with 1000 precision digits, of the four examples in this paper, and the programs to check that the initial conditions correspond to a periodic orbit of such precision, are presented online [http://gme.unizar.es/pages/fourpoLHH.html].

A. The Lorenz model

The Lorenz model is given by [24]

$$\dot{x} = \sigma(y - x), \dot{y} = -x z + r x - y, \dot{z} = x y - b z, \quad (15)$$

where $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ and $b, \sigma, r \in \mathbb{R}$ are the parameters. In this case we will take the classical Saltzman's values of the parameters $b = 8/3$, $\sigma = 10$, and $r = 28$.

It is well known that the chaotic attractor of the Lorenz model presents the shape of the wings of a butterfly. This system has three equilibrium points, one at the origin and two symmetric ones on the center of the wings, one of them P^R with $x > 0$ and another one P^L with $x < 0$. To classify the orbits foliated to the chaotic attractor, we may use symbolic notation [20]. Every time a trajectory passes through the left

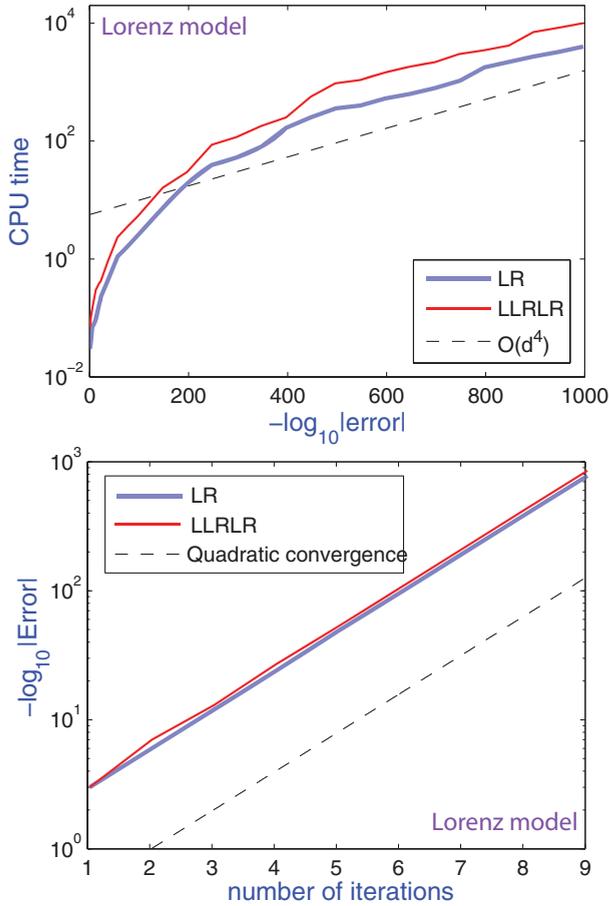


FIG. 2. (Color online) Computational relative error vs. CPU time and number of iterations.

side of the butterfly the letter L is assigned to the trajectory. If the trajectory passes through the right side of the butterfly the letter R is assigned. Then, an infinite chain of symbols characterizes each trajectory. Periodic orbits repeat indefinitely the finite sequence of symbols of its period, and then they can be characterized by a finite number of symbols.

To check the method proposed in this paper we have taken two sets of approximate initial conditions (with just five correct digits) of two different periodic orbits with symbolic sequences LR and LLRLR (see Fig. 1). The LR orbit has the initial values for our algorithm:

$$(x, y, z) = (-13.764, -19.579, 27),$$

and a period $T = 1.5586$. The LLRLR orbit has the initial values for our algorithm:

$$(x, y, z) = (-12.699, -17.197, 27),$$

and a period $T = 3.8695$.

On the top of Fig. 2, we show the CPU time in seconds versus the number of digits for obtaining periodic orbits for the Lorenz model up to 1000 digits of precision. We observe that the behavior is quite similar for both periodic orbits, LR and LLRLR, of the Lorenz model and the computational complexity of our numerical algorithm is $\mathcal{O}(d^4)$ being $d = -\log_{10}(\text{TOL})$ the requested number of digits.

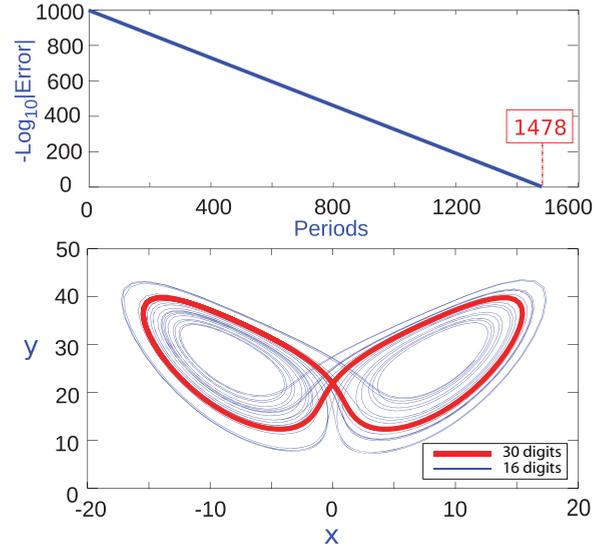


FIG. 3. (Color online) (Top) Number of exact digits depending on the number of time periods in the numerical integration of an unstable periodic orbit for the Lorenz model using 1000 digits. (Bottom) Forty time periods using multiple precision and standard double precision.

It is well known that the Newton method has quadratic convergence, so our algorithm is quadratically convergent, too, as we see on the bottom picture of the Fig. 2. We obtain our goal of 1000 digits of precision in just 10 iterations and, as shown on the two periodic orbits, the number of digits of precision is doubled at each iteration.

Once we have our POs with any precision, we are able to obtain high-precision estimates of the orbit. For example, the Lyapunov exponent λ of a periodic orbit is defined as $\log m_1/T$, where m_1 is the magnitude of its leading characteristic multiplier and T is its period. For instance, we show the value of λ up to 40 digits for the orbit LR,

$$\lambda \simeq 0.9946500250305010060026396388385871828508,$$

that is, we correct the values given in Ref. [20]. So, with this value, we may estimate the number of periods that we may follow the periodic orbit with some precision. This total time is of the order of $e^{\lambda T_{\text{total}}} \simeq 1/u$, with u being the round-off unit of the computations. If we take as example the LR orbit with 1000 digits ($u \approx 3.8055 \times 10^{-1000}$), we obtain $T_{\text{total}} = -\log u/\lambda \approx 2313.74$, that is, we can follow 1484 orbits approximately.

The picture on the top of Fig. 3 shows that with real simulations we can go up to 1478 orbits, that is, quite close to the theoretical estimate. In the bottom picture we observe the evolution of 40 periods using double precision (in thin blue line) and 30 digits of precision (in thick red line). We observe that to maintain the precision we need initial conditions with high precision, as the ones given by our algorithm.

We remark that our algorithm computes POs with very high precision in a quite reasonable time, less than 3 h, for orbits with 1000 precision digits. This means that nowadays it is able to make high-precision studies when needed.

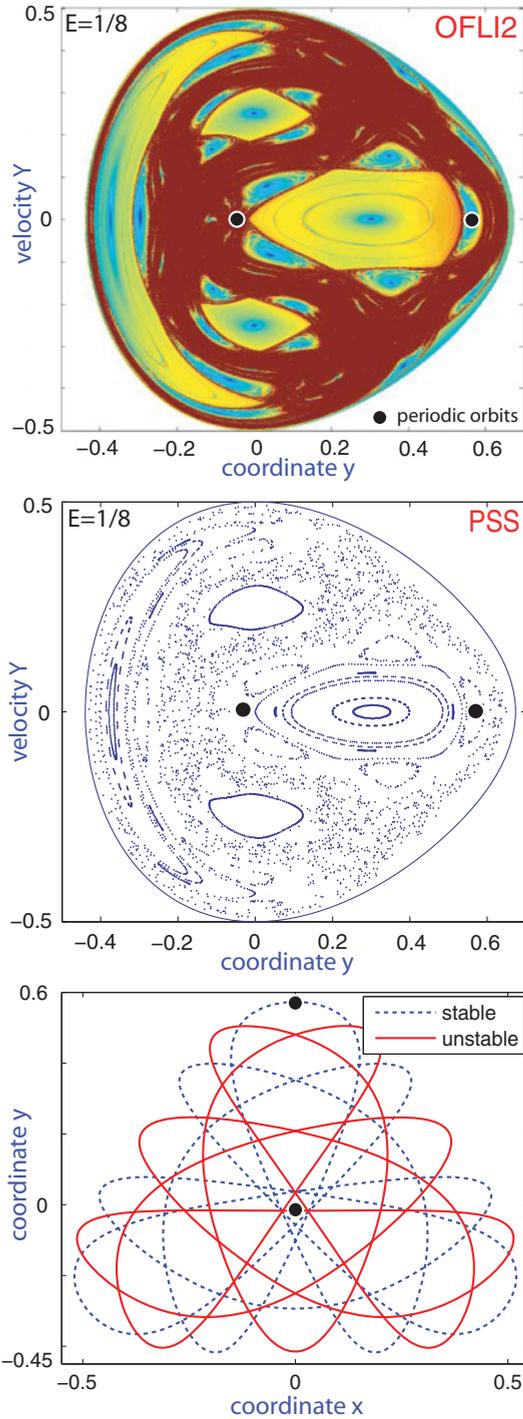


FIG. 4. (Color online) OFLI2 and PSS sections and two periodic orbits of the Hénon-Heiles problem for $\mathcal{H} = E = 1/8$.

B. Hamiltonian case: Hénon-Heiles

The Hénon-Heiles system is given by the Hamiltonian:

$$\mathcal{H} = \frac{1}{2}(X^2 + Y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3, \quad (16)$$

where (x, y) represents the position vector and (X, Y) represents the velocity.

The Poincaré surfaces of section (PSS) and more recent techniques like the chaos indicator OFLI2 [34] give a good

way to distinguish regular from chaotic orbits in Hamiltonian systems with two degrees of freedom. On the top of the Fig. 4 we can see the OFLI2 section $x = 0$ of the Hénon-Heiles problem at the energy level $\mathcal{H} = 1/8$ [red (dark) color is associated with chaotic motion, whereas blue (light gray) color with regular region]. The plot is very similar to the PSS of the Hénon-Heiles problem at the same energy level, but in this figure we see more details about the islands of periodic orbits inside the chaotic sea. In this figure, we have taken the two periodic orbits pointed out with a black circle. The left point corresponds to an unstable periodic orbit with initial conditions (with just five correct digits):

$$(x, y, X, Y) = (0, -0.0170, 0.4997, 0),$$

of period $T = 32.040$. The right point corresponds to a stable periodic orbit with initial conditions:

$$(x, y, X, Y) = (0, 0.5729, 0.2170, 0),$$

with period $T = 32.377$. At the bottom picture of Fig. 4, we show our orbits, the stable one in the dashed blue line and the unstable one in a continuous red line (the dots are the values of the initial conditions).

If we want to follow the unstable periodic orbit for a long time we may use high-precision initial conditions to propagate them without falling into the chaotic region. On the top of Fig. 5, we show the CPU time in seconds versus the number of

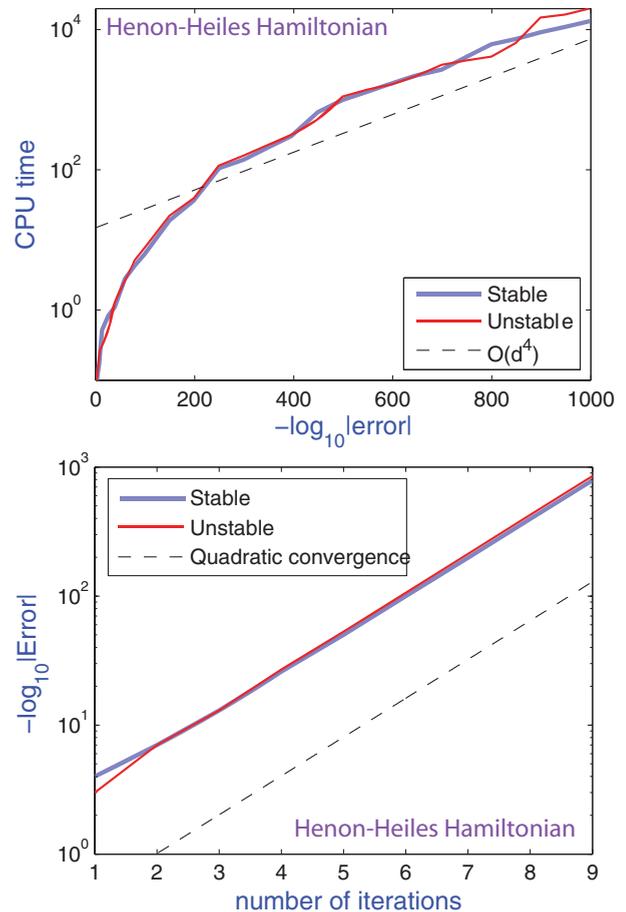


FIG. 5. (Color online) Computational relative error vs. CPU time and number of iterations.

digits for obtaining periodic orbits for the Hénon-Heiles model up to 1000 digits of precision. We observe that the behavior is quite similar for the two orbits, the stable and the unstable, of the Hénon-Heiles Hamiltonian and the computational complexity behaves like $\mathcal{O}(d^4)$ as in the Lorenz model. As before, the algorithm presents a quadratic convergence as shown in Fig. 5. We remark that in this test we have to use the extended linear system (11) to be able to obtain the periodic orbits for the Hamiltonian case.

VI. CONCLUSIONS

In this paper we extend classical algorithms to compute periodic orbits in dynamical systems in order to be able to obtain high-precision periodic orbits. This method may be used in the studies of dynamical systems where high precision is demanded. The method combines the use of an optimized shoot-

ing method, the singular value decomposition, and recent techniques of a high-precision solution of ODEs. Moreover, it can be applied to any dynamical system, dissipative or Hamiltonian, just by using the correct system of equations. The method has proved its applicability with two paradigmatic examples, the Lorenz model and the Hénon-Heiles Hamiltonian, obtaining orbits with 1000 precision digits. Besides, we show that the computer time is reasonable since the complexity is polynomial in the number of digits. Therefore, with this technique it is possible to give, in an easy way, periodic orbits with an arbitrary number of precision digits for any dynamical system.

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