On the use of the MEGNO indicator with the Global Symplectic Integrator

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To distinguish between regular and chaotic orbits in Hamiltonian systems, the Global Symplectic Integrator (GSI) has been introduced [Libert et al., 2010], based on the symplectic integration of both Hamiltonian equations of motion and variational equations. In the present contribution, we show how to compute efficiently the MEGNO indicator jointly with the GSI. Moreover, we discuss the choice of symplectic integrator, in fact we point out that a particular attention has to be paid to the structure of the Hamiltonian system associated to the variational equations. The performances of our method is illustrated through the study of the Arnold diffusion problem.

Keywords: Symplectic integration, chaos, variational equations, MEGNO, Arnold diffusion.

1. Introduction

Several detection techniques exist in order to study the regular or chaotic behavior of orbits of Hamiltonian systems. All Lyapunov-like methods are based on the resolution of the so-called variational equations giving the evolution of deviation vectors associated to a given orbit. These are essentially the FLI [Froeschl´e et al., 1997], MEGNO [Cincotta et al., 2003], SALI [Skokos, 2001] and GALI [Skokos et al., 2007] methods. In [Libert et al., 2010], we have introduced the Global Symplectic Integrator (for short the GSI), a method allowing to solve both Hamiltonian equations of motion and variational equations using a totally symplectic integration scheme. Based on a comparison of the GSI with non-symplectic integration schemes, it was clearly shown that the GSI was more accurate in the detection of regular and chaotic orbits, using the SALI chaos indicator, and less time-consuming than non-symplectic methods. Such a kind of symplectic integration scheme for the variational equations has also been recently and independently proposed in [Skokos et al., 2010].

The purpose of this work is to show that other chaos detection techniques, for instance the MEGNO, can be used jointly with the GSI and their efficiency thus improved. The computation of the MEGNO needs to study the time evolution of a single deviation vector. This advantage, with respect to the SALI that needs the knowledge of the evolution of two deviation vectors, becomes critical when considering...
a large amount of orbits on long time spans. Moreover, the use of the GSI does not rely on the use of a specific symplectic integrator scheme. Hence, our second aim is to discuss and compare different symplectic integrators. It turns out that methods adapted to the structure of the Hamiltonian equations of motion are not necessarily suited for the associated variational equations.

While the study of the dynamics of two well-known Hamiltonian systems, Hénon-Heiles and the restricted three-body problem, have been addressed in [Libert et al., 2010], we hereby propose to use the GSI to improve the detection of slow diffusion in Hamiltonian systems, the so-called Arnold diffusion, analyzed according to the model proposed in [Lega et al., 2003].

The organization of the paper is as follows. In Section 2, we briefly summarize the GSI method, and we review two classes of symplectic integrators. Section 3 is devoted to the definition of the MEGNO indicator and the algorithm used to compute it. An application to the Arnold diffusion problem is then presented in Section 4, for which the the GSI method is compared to a non-symplectic scheme. Finally, in Section 5 we sum up and draw our conclusions.

2. Global Symplectic Integrator

2.1. Method

Let us consider an autonomous Hamiltonian system with $N$ degrees of freedom $H(p, q)$ where $p, q \in \mathbb{R}^N$ are the momenta and variables vectors. The Hamiltonian vector field may be written as

$$\dot{x} = J \nabla_x H = W(x),$$

where $x = \left( \begin{array}{c} p \\ q \end{array} \right) \in \mathbb{R}^{2N}$ and

$$J = \left( \begin{array}{cc} 0_N & -1_N \\ 1_N & 0_N \end{array} \right)$$

is the standard symplectic matrix, being $1_N$ the $N \times N$ identity matrix and $0_N$ the $N \times N$ matrix whose entries are all zero.

Many chaos indicators like the FLI [Froeschlé et al., 1997], the MEGNO [Cincotta et al., 2003], the SALI [Skokos, 2001] and more recently the GALI [Skokos et al., 2007] require the time evolution of deviation vectors to be computed. These vectors, $\delta(t)$, satisfy the variational equations given by

$$\dot{\delta}(t) = D_x W \delta(t) = J \nabla^2_x H \delta(t)$$

where $D_x W$ is the Jacobian matrix of the vector field $W$ and $\nabla^2_x H$ is the Hessian matrix of $H$.

In [Libert et al., 2010], the GSI has been introduced to simultaneously integrate both systems of equations (1) and (3) by means of a symplectic integrator. This method assumes that $H$ may be split into two separately integrable parts. For instance when

$$H(p, q) = A(p) + B(q),$$

the variational equations (3) can be written as

$$\begin{pmatrix} \dot{\delta}_p \\ \dot{\delta}_q \end{pmatrix} = \begin{pmatrix} 0 & -\nabla^2_{q^2} B \\ \nabla^2_{p^2} A & 0 \end{pmatrix} \begin{pmatrix} \delta_p \\ \delta_q \end{pmatrix} = \begin{pmatrix} -\nabla^2_{q^2} B \delta_q \\ \nabla^2_{p^2} A \delta_p \end{pmatrix} = \begin{pmatrix} -\nabla_{q^2} B \\ \nabla_{p^2} A \end{pmatrix},$$

while the associated Hamiltonian $K$ is expressed as

$$K(p, q, \delta_p, \delta_q) = \frac{1}{2} \delta_p^T \nabla^2_{p^2} A \delta_p + \frac{1}{2} \delta_q^T \nabla^2_{q^2} B \delta_q = A(p, \delta_p) + B(q, \delta_q).$$

The above introduced notations will be use throughout the paper.
2.2. Integrator

In the present work, two symplectic integrators have been tested. Both are based on the Campbell-Baker-Hausdorff (CBH) [Bourbaki, 1972] formula which ensures that one can find a general explicit integrator with \( n \) steps of the form

\[
S_n(\tau) = e^{c_1 \tau L_A} e^{d_1 \tau L_B} \ldots e^{c_n \tau L_A} e^{d_n \tau L_B} = e^{\tau G},
\]

whose coefficients \( c_i \) and \( d_i \) have to be carefully chosen to get the required precision, i.e. reach the integrator order \( m \). Integrating \( \mathcal{H} \) at order \( m \) means that we exactly evaluate \( e^{\tau G} \) where

\[
G = A + B + O(\tau^m).
\]

In [Laskar et al., 2001], four classes of symmetric symplectic integrators have been presented:

- **SABA\(_{2n}\)(\( \tau \))** = \( e^{c_1 \tau L_A} e^{d_1 \tau L_B} \ldots e^{c_{n-1} \tau L_A} e^{d_{n-1} \tau L_B} e^{c_n \tau L_A} \ldots e^{d_{n-1} \tau L_B} e^{c_1 \tau L_A} \)
- **SABA\(_{2n+1}\)(\( \tau \))** = \( e^{c_1 \tau L_A} e^{d_1 \tau L_B} \ldots e^{c_{n+1} \tau L_A} e^{d_{n+1} \tau L_B} e^{c_n \tau L_A} \ldots e^{d_{n+1} \tau L_B} e^{c_1 \tau L_A} \)
- **SBAB\(_{2n}\)(\( \tau \))** = \( e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_2 \tau L_B} \ldots e^{c_{n+1} \tau L_A} e^{d_{n+1} \tau L_B} e^{c_n \tau L_A} \ldots e^{d_{n+1} \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} \)
- **SBAB\(_{2n+1}\)(\( \tau \))** = \( e^{d_1 \tau L_B} e^{c_2 \tau L_A} e^{d_2 \tau L_B} \ldots e^{c_{n+2} \tau L_A} e^{d_{n+2} \tau L_B} e^{c_n \tau L_A} \ldots e^{d_{n+2} \tau L_B} e^{c_2 \tau L_A} e^{d_1 \tau L_B} \).

If \( \varepsilon := |B|/|A| \) is small enough, it is shown that one can find specific coefficients such that

\[
G = A + B + O(\tau^{2n+\varepsilon + \tau^2}).
\]

Obviously, since the approximation error depends on the weight \( \varepsilon \) of the perturbation, these classes of integrators are not well suited for Hamiltonian systems that are not perturbations of integrable ones.

In general, for the Hamiltonian \( \mathcal{K} \) associated to variational equations, the ratio \( |B|/|A| \) is not necessarily small. Hence, the method presented in [Laskar et al., 2001] is not suitable. To tackle this problem, we have chosen to use another class of symmetric and explicit symplectic integrators presented in [Yoshida, 1990]. The latter does not take into account the importance of the perturbation and can be defined starting from the basic bloc given by the second order Störmer-Verlet/Leap Frog scheme, \( T_{\text{2nd}}(\tau) = e^{\frac{1}{2} \tau L_A} e^{\tau L_B} e^{\frac{1}{2} \tau L_A} \), as follows:

\[
T_{\text{4th}}(\tau) = T_{\text{2nd}} \left( \frac{1}{2 - 2^{1/3}} \right) T_{\text{2nd}} \left( \frac{-2^{1/3}}{2 - 2^{1/3}} \right) T_{\text{2nd}} \left( \frac{1}{2 - 2^{1/3}} \right)
\]

\[
T_{\text{6th}}(\tau) = T_{\text{4th}} \left( \frac{1}{2 - 2^{1/5}} \right) T_{\text{4th}} \left( \frac{-2^{1/5}}{2 - 2^{1/5}} \right) T_{\text{4th}} \left( \frac{1}{2 - 2^{1/5}} \right).
\]

In this case, the error depends only on the time step \( \tau \), as in Eq. (8). While this method turns out to be very efficient for the variational Hamiltonian \( \mathcal{K} \), it does not take advantage of the structure of \( \mathcal{H} \) as a perturbation of an integrable system.

3. MEGNO

3.1. Definition

According to [Cincotta et al., 2003], the Mean Exponential Growth factor of Nearby Orbits is defined as

\[
Y(t) = \frac{2}{t} \int_0^t \frac{\delta(s)}{\delta(s)} ds
\]

where \( \delta(s) \) denotes the Euclidean norm of \( \delta(s) \). A more useful and stable indicator is given by the mean MEGNO, namely the time-average:

\[
\overline{Y}(t) = \frac{1}{t} \int_0^t Y(s) ds.
\]

While \( Y(t) \) may not converge nor admit a limit for \( t \to \infty \), it has been proven by [Cincotta et al., 2003] that the asymptotic value of \( \overline{Y} \) provides a good characterization of the regular or chaotic nature of
orbits. Basically, \( \lim_{t \to \infty} \bar{Y}(t) = 2 \) for quasi-periodic orbits on an irrational torus for a non-isochronous system and for orbits close to stable periodic ones. In the limit case where the orbit coincides with a stable periodic orbit, \( \bar{Y}(t) \) asymptotically reaches zero. Considering irregular orbits, \( \bar{Y}(t) \) increases linearly with time, being the slope half of the first Lyapunov exponent.

### 3.2. Computation

The computation of the MEGNO and its time-average requires both integrals \( 13 \) and \( 14 \) to be solved accurately. Different methods are available.

A straightforward approach is based on the introduction of two auxiliary functions \( v \) and \( w \) such that

\[
v(t) = t \bar{Y}(t) \quad \text{and} \quad w(t) = t \bar{Y}(t),
\]

whose time evolution is directly given by the following differential equations:

\[
\dot{v}(t) = 2 \frac{\delta(t)}{\delta(t)} t = 2 \frac{\delta \cdot \delta}{\delta^2} t \quad \text{and} \quad \dot{w}(t) = Y(t) = \frac{v(t)}{t}.
\]

Obviously, \( 3 \) and \( 16 \) have to be computed with the same integrator (see e.g. Goździewski et al. 2001, Valk et al. 2009, Hinse et al. 2010). In this case, the time step used to integrate Eq. \( 3 \) is fixed by the integration of Eq. \( 16 \). However, the use of auxiliary functions is less efficient within a symplectic integration scheme (in fact, \( 16 \) are not generally Hamiltonian equations). Indeed, it is well-known that symplectic integrators show very good energy conservation properties, allowing us to consider larger step sizes and limit energy loss. In light of these considerations, other alternatives have been studied.

In particular, using the definition of the MEGNO for discrete time dynamical systems (i.e. maps) given by Cincotta et al. 2003, it has been proposed in Breiter et al. 2005 to compute \( Y(t) \) and \( \bar{Y}(t) \) by observing that a fixed step size integrator can be considered as equivalent to a discrete time map. Hence

\[
Y_{\text{Breiter et al., 2005}}(t + h) = \frac{t}{t + h} Y_{\text{Breiter et al., 2005}}(t) + 2 \ln \frac{\delta(t + h)}{\delta(t)} \quad \text{and} \quad \bar{Y}_{\text{Breiter et al., 2005}}(t + h) = \frac{t \bar{Y}_{\text{Breiter et al., 2005}}(t) + h Y_{\text{Breiter et al., 2005}}(t + h)}{t + h},
\]

\( h \) being the integration step size. Let us note that these formulas can be obtained by using a simple rectangular quadrature method to solve both integrals \( 13 \) and \( 14 \). On the other hand, a mixed scheme has been proposed in Goździewski, 2003, that relies on the computation of the MEGNO by using the so-called trapezoidal rule \( 1 \) to compute the integral in the definition \( 13 \) and then the discrete time approximation for the mean MEGNO.

In the present work, we develop further this idea: we propose to use the trapezoidal rule to compute both integrals \( 13 \) and \( 14 \). First, we rewrite \( 13 \) as

\[
Y(t) = 2 \log \delta(t) - \frac{2}{t} \int_0^t \log \delta(s) ds,
\]

then using the trapezoidal rule we get

\[
Y(t + h) = \frac{t}{t + h} Y(t) + \frac{2t + h}{t + h} \ln \frac{\delta(t + h)}{\delta(t)} + O(h^3)
\]

and

\[
\bar{Y}(t + h) = \frac{1}{t + h} \int_0^{t + h} Y(s) ds = \frac{1}{t + h} \left[ t \bar{Y}(t) + 0.5h(Y(t) + Y(t + h)) \right] + O(h^3).
\]

\( ^1 \)Given a real-valued function \( f \) and an interval \([a, b]\), one has Press et al. 2007

\[
\int_a^b f(x) dx = 0.5(b-a)[f(a) + f(b)] + O((b-a)^3 f'').
\]

the second derivative being estimated on the interval \([a, b]\).
Fig. 1. Arnold web. Two-dimensional phase plane \((I_1, I_2)\) represented using mean MEGNO values at \(t = 10^7\) time units (the values greater than three have been fixed to three). A set of 600 \(\times\) 600 uniformly distributed initial conditions has been integrated with \(T_{4th}\) (with time steps equal to 0.01). Other initial conditions are fixed to \(I_3 = 1, \phi_1 = \phi_2 = \phi_3 = 0\) and \(\nu = 0.007\). The dashed line represents the \(I_1 = 2I_2\) resonance. The box encloses a part of it and is analyzed in more detail in Fig. 2.

Let us observe that the above formulas (19) and (20) improve the aforementioned ones corresponding to lower order approximations of the integrals defining MEGNO and mean MEGNO.

In the following, Eq. (19) and (20) will be used to compute the MEGNO whenever we use a symplectic scheme, whereas Eq. (16) will be used with RK4. Let us note that in the rest of the paper we will be interested in asymptotic values of mean MEGNO i.e. mean MEGNO values at the end of the integration process. In order not to introduce any bias in the computation of the MEGNO and mean MEGNO, initial deviation vectors \(\delta(0)\) will always be randomly chosen with uniform probability in the appropriate hypersphere.

4. Arnold Diffusion

4.1. Model

As shown in [Libert et al., 2010], the GSI proves to be more efficient than non-symplectic schemes to correctly identify the behavior of a given orbit especially on dynamics acting on long time scales. In this section, we will show that this is particularly relevant in case of slow chaotic diffusion. To that purpose, we decided to consider the following Hamiltonian system described in [Lega et al., 2003]:

\[
H_{\text{Arnold}}(I_1, I_2, I_3, \phi_1, \phi_2, \phi_3) = \frac{1}{2}(I_1^2 + I_2^2) + I_3 + \nu \frac{1}{\cos(\phi_1) + \cos(\phi_2) + \cos(\phi_3) + 4},
\]

\[\text{Eq. (21)}\]
where actions $I_1, I_2, I_3 \in \mathbb{R}$ and angles $\phi_1, \phi_2, \phi_3 \in \mathbb{T}$ are canonically conjugate variables and $\nu$ is assumed to be a small parameter.

Given the structure of (21), $\dot{\phi}_1 = I_1$, $\dot{\phi}_2 = I_2$ and $\dot{\phi}_3 = 1$. Hence, each straight line
\[
  k_1 I_1 + k_2 I_2 + k_3 = 0, \quad (k_1, k_2, k_3) \in \mathbb{Z}^3 \setminus \{0\}
\]
on the two-dimensional plane $(I_1, I_2)$ represents a resonance.

As illustrated in Fig. 1, most relevant resonances are clearly visible on the plane $(I_1, I_2)$, to form the so-called *Arnold Web*. Mean MEGNO values are shown for a grid of $600 \times 600$ equally spaced initial conditions in this plane. Other initial conditions are $I_3 = 1$ and $\phi_1 = \phi_2 = \phi_3 = 0$, and the parameter $\nu$ has been fixed to 0.007, as in the rest of this work. This value needs to be small in order to avoid resonances overlap. Besides, as pointed out in [Lega et al., 2003], the smaller the perturbation, the slower the diffusion. The GSI has been used with $T_{4th}$ integrator with a fixed time step $\tau = 0.01$ and an integration time of $10^7$. The dashed line highlights the $I_1 = 2I_2$ resonance. This web of resonances is of particular interest. Indeed, it has been proven (see [Arnold, 1963]) that Arnold diffusion exists along resonances. Moreover, in [Lega et al., 2003], a numerical proof of diffusion along resonances for this model is given.

The analysis presented in Section 4.2 will be performed in the region delimited by $0.29 \leq I_1 \leq 0.33$ and $0.14 \leq I_2 \leq 0.18$, centered on the $I_1 = 2I_2$ resonance. This small region is enclosed in the box shown in Fig. 1. An enlargement of this box is presented in Fig. 2. Again, a grid of $600 \times 600$ equally spaced initial conditions has been numerically integrated using the GSI with $T_{4th}$ integrator up to $10^7$ time units. Other initial conditions and parameters are the same as the ones used to produce Fig. 1. In the following analysis,
we will consider several orbits around the top hyperbolic border (in brown in Fig. 2) of the resonance where diffusion is actually confined.

4.2. Analysis

In this section, we will compare the results on the correct determination of regular or chaotic orbits behavior obtained with the GSI and a non-symplectic scheme. Through an analysis of the maximum relative errors on the energy, percentage of correctly identified orbits and CPU time, we will show that our symplectic scheme outperforms the non-symplectic one in the determination of the behavior of orbits.

As it is necessary to consider long integration times and a lot of different initial conditions, it has been decided to use and compare fourth-order integrators. In fact, this turns out to be a good compromise between reliability of the numerical results, as measured in term of relative energy loss, and number of evaluations of the vector fields, translated easily into required CPU time. On the one hand, we considered the well-known non-symplectic fourth-order Runge Kutta (RK4) integrator. While it is simple to implement, it is also robust and efficient. On the other hand, both symplectic integrators presented in Section 2.2 have been tested. As far as only the Hamiltonian system (21) is concerned, SABA and SBAB integrator classes outperform Yoshida integrator. Indeed, given that $\nu$ is small, this system can be seen as a perturbation of an integrable system. Hence, the error (10) is smaller than Yoshida’s one (8). However, SABA and SBAB classes performances become rapidly poor for the Hamiltonian system $K_{\text{Arnold}}$ associated to the variational equations. It is mainly due to the structure of $K_{\text{Arnold}}$. As time increases, the weight of the $B$ part, say the perturbation, of the Hamiltonian $K_{\text{Arnold}}$ may become larger than the $A$ part, or vice versa without any possible control, see Fig. 3. This implies that the error on the energy increases too. Fortunately, Yoshida integrators do not depend on this kind of consideration and are then more suited for this application. As already stated in Section 2.2 Yoshida integrators do not take advantage of the structure of $H_{\text{Arnold}}$ but it is conversely useful for the integration of variational equations. Hence, for the purpose of the present study, it has been decided to compare RK4 integrator to $T_{2\text{nd}}$ and $T_{4\text{th}}$.

The comparison has been performed considering 100 orbits whose initial conditions $(I_1(0), I_2(0))$ are uniformly distributed around the top hyperbolic border of the resonance (the parallelogram in Fig. 2). First, for each one of these orbits, a reference value of the mean MEGNO has been computed with $T_{4\text{th}}$, a time step equal to $\tau = 0.01$ and an integration time of $2.5 \times 10^6$. Afterwards, for time steps between 0.01 and 1, the same orbits have been numerically integrated with both methods (the GSI and the non-symplectic scheme) in order to obtain the corresponding MEGNO values. Eventually, a comparison with the reference MEGNO values has been done, enabling us to classify orbits as correctly identified or not. At the same time, CPU times and maximum relative errors in energy have been stored. In order to reduce
numerical truncation errors, it has been decided to achieve this study using quadruple precision.

A relevant indicator to test the goodness of the numerical integration, is to compare the maximum relative errors in energy

$$\frac{\Delta E}{E} = \max_{0 \leq t \leq 2.5 \times 10^6} \frac{|E_i(t) - E_i(0)|}{|E_i(0)|},$$

(22)

where $E_i(t)$ is the energy, i.e. the value of the Hamilton function, at time $t$ on the $i$–th orbit.

A second important indicator, related to the speed of the integration algorithm, is the CPU time

$$T_{CPU} = \sum_{i=1}^{100} T^i_{CPU},$$

(23)

$T^i_{CPU}$ being the CPU time needed to integrate the $i$–th orbit and the associated deviation vector on the defined time span.

Both indicators are reported in Fig. 4 as functions of the time step for the different integrators. It appears that $T_{4th}$ shows always smaller energy loss than RK4 integrator. Moreover, as time step increases, this difference becomes larger too. Also note that the maximum error becomes larger with RK4 than with $T_{2nd}$ beyond $\tau \simeq 0.25$. That means that, even if $T_{2nd}$ is only a second order integrator, it is more reliable than RK4 when using big time steps. Another advantage of the GSI is the relatively low required CPU time ($T_{CPU}$) in comparison to RK4. This is particularly important as we are considering lots of different initial conditions and long integration times. Obviously, the lower-order $T_{2nd}$ asks less CPU time than $T_{4th}$.

Moreover, the GSI correctly identifies more orbits than RK4 as time steps increase (see Fig. 5). Indeed, mean MEGNO values computed by means of RK4 are wrong for regular orbits when the time step is greater than 0.1. The percentage of well identified regular orbits even reaches zero while, at the same time, $T_{4th}$ is still beyond 50%. This difference is less discernible for chaotic orbits, since a small drift from the orbit and/or tangent direction does not lead to completely different behaviors. However, in the following, we will use the total percentage, $p$, that presents a summary of both results. Eventually, let us point out that the lower-order $T_{2nd}$ integrator manages to identify correctly approximately the same percentage of orbits as $T_{4th}$.

![Fig. 4. Maximum relative errors in energy $\Delta E/E$ (left panel) and CPU time $T_{CPU}$ (right panel) as a function of the time step, in logarithmic scale. The integration time for this analysis has been set to $2.5 \times 10^6$ time units. The comparison involved 100 orbits whose initial conditions $(I_1(0), I_2(0))$ have been taken around the top hyperbolic border of the $I_1 = 2I_2$ resonance (see Fig. 2). Symbols are : (red) * RK4 integrator, (blue) ○ the 4th order Yoshida integrator and (black) □ the 2nd order Yoshida integrator. Straight lines denote best linear fits (left panel).](image-url)
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Fig. 5. Percentages of correctly identified orbits with respect to time step in logarithmic scale. The comparison involve 100 orbits whose initial conditions \((I_1(0), I_2(0))\) have been taken around the top hyperbolic border of the \(I_1 = 2I_2\) resonance (see Fig. 2). Solid lines and dashed lines represent respectively the identification of regular orbits and chaotic orbits.

Fig. 6. Efficiency index \(\phi\) with respect to time step. The comparison involved 100 orbits whose initial conditions \((I_1(0), I_2(0))\) have been taken around the top hyperbolic border of the \(I_1 = 2I_2\) resonance.

Eventually, all these observations can be recombined into a single efficiency index. As introduced in Libert et al., 2010,

\[
\phi = p \left| \log_{10}(\Delta E/E) \right| \left| \log_{10}(T_{CPU}) \right|^{-1}
\]

enables us to quantify the efficiency of each method. The larger \(\phi\), the better the method. On the one hand, the percentage of correctly identified orbits must be as big as possible. On the other hand, relative error in energy \((\in [0, 1])\) and CPU time must remain low. The evolution of \(\phi\) with respect to time step is shown in Fig. 6. It turns out that this index presents larger values for computations realized with the GSI, coupled to \(T_{4th}\). It results obviously from previous considerations. For relatively small times steps \((\tau < 0.02)\), the non-symplectic scheme (RK4) behaves similarly to the GSI. After that, this method is quickly penalized by its energy loss and lower percentage of well identified orbits. Eventually, efficiency index for the GSI used with \(T_{2nd}\) presents similar behavior to the ones of \(T_{4th}\) but on a lower level. It comes directly from its larger maximum relative error in energy. However, at time step \(\tau \simeq 0.2\), the GSI with \(T_{2nd}\) becomes more efficient than the non-symplectic method, due to the joint effect of better energy conservation and number of correctly estimated orbits.

Let us observe that the same analysis has been performed in double precision. Results concerning the percentage of correctly identified orbits are exactly the same. Obviously, CPU times are proportionally smaller than the present ones. The main difference occurs with the evolution of maximum relative energy errors with respect to time step which are not perfect straight lines anymore. In particular, numerical
truncation errors appear for too small relative errors in energy. This leads to an inaccurate efficiency index.

5. Conclusion

In this work, we have shown that the GSI is a powerful tool to characterize the regular or chaotic behavior of orbits in Hamiltonian systems. It proves to be especially efficient for dynamics acting on long time scales like the Arnold diffusion problem analyzed here, as energy conservation properties of symplectic integration schemes are fully pointed up.

As it only asks for the knowledge of a single deviation vector, the MEGNO indicator is less time consuming than other chaos indicators and should be used jointly with the GSI. To numerically compute both MEGNO and mean MEGNO, we have introduced a quadrature method based on the trapezoidal rule.

Furthermore, it has been shown that a particular attention has to be paid to the choice of the symplectic integrator. One has to bear in mind that both Hamiltonian systems associated to the equations of motion and the variational equations can present very different structures. For this reason, we argue for the use of Yoshida’s symplectic integrator.

Finally, our analysis shows that the GSI outperforms non-symplectic schemes. Indeed, large time steps are allowed, smaller computation times are needed and the energy loss is more limited. For all these considerations, we claim that the GSI method with the MEGNO indicator and Yoshida integrator turns out to be a reliable and time sparing method to correctly determine the behavior of orbits associated to Hamiltonian systems.

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