On the numerical integration of variational equations

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Outline

- **Definitions: Variational equations, Lyapunov exponents, the Generalized Alignment Index – GALI, Symplectic Integrators**
- **Different integration schemes: Application to the Hénon-Heiles system**
- **Numerical results**
- **Conclusions**

Autonomous Hamiltonian systems

Consider an N degree of freedom autonomous Hamiltonian system having a Hamiltonian function of the form:

$$H(\vec{q},\vec{p}) = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + V(\vec{q})$$

with $\vec{q} = (q_1(t), q_2(t), \ldots, q_N(t))$ $\vec{p} = (p_1(t), p_2(t), \ldots, p_N(t))$ being respectively the coordinates and momenta.

The time evolution of an orbit is governed by the Hamilton equations of motion

$$\dot{\vec{q}} = \vec{p}$$
$$\dot{\vec{p}} = -\frac{\partial V}{\partial \vec{q}}$$

Variational Equations

The time evolution of a deviation vector

$$\vec{w}(t) = (\delta q_1(t), \delta q_2(t), \ldots, \delta q_N(t), \delta p_1(t), \delta p_2(t), \ldots, \delta p_N(t))$$

from a given orbit is governed by the so-called variational equations:

$$\dot{\vec{\delta q}} = \vec{\delta p}$$
$$\dot{\vec{\delta p}} = -\mathbf{D}^2\mathbf{V}(\vec{q}(t))\vec{\delta q}$$

where $$\mathbf{D}^2\mathbf{V}(\vec{q}(t))_{jk} = \left.\frac{\partial^2 V(\vec{q})}{\partial q_j \partial q_k}\right|_{\vec{q}(t)}, \quad j,k = 1,2,\ldots,N.$$

The variational equations are the equations of motion of the time dependent tangent dynamics Hamiltonian (TDH) function

$$H_V(\vec{\delta q}, \vec{\delta p}; t) = \frac{1}{2}\sum_{j=1}^{N} \delta p_i^2 + \frac{1}{2}\sum_{j,k}^{N} \mathbf{D}^2\mathbf{V}(\vec{q}(t))_{jk}\delta q_j \delta q_k$$

Chaos detection methods

The Lyapunov exponents of a given orbit characterize the **mean exponential rate of divergence** of trajectories surrounding it. The 2N exponents are ordered in **pairs of opposite sign numbers and two of them are 0.**

$$\mathrm{mLCE} = \lambda_1 = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\|\vec{w}(t)\|}{\|\vec{w}(0)\|}$$

$\lambda_1 = 0 \rightarrow$ Regular motion

$\lambda_1 \neq 0 \rightarrow$ Chaotic motion

Following the evolution of **k deviation vectors with $2 \leq k \leq 2N$**, we define **(Skokos et al., 2007, Physica D, 231, 30)** the **Generalized Alignment Index (GALI) of order k :**

$$\mathrm{GALI}_k(t) = \left\| \hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \ldots \wedge \hat{w}_k(t) \right\|$$

Chaotic motion: $\mathrm{GALI}_k(t) \propto e^{-[(\lambda_1-\lambda_2)+(\lambda_1-\lambda_3)+\ldots+(\lambda_1-\lambda_k)]t}$

Regular motion: $\mathrm{GALI}_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq N \\ \dfrac{1}{t^{2(k-N)}} & \text{if} \quad N < k \leq 2N \end{cases}$

Symplectic Integration schemes

Formally the solution of the Hamilton equations of motion can be written as:

$$\frac{d\vec{X}}{dt} = \left\{H, \vec{X}\right\} = L_H \vec{X} \Rightarrow \vec{X}(t) = \sum_{n\geq 0} \frac{t^n}{n!} L_H^n \vec{X} = e^{tL_H} \vec{X}$$

where $\vec{X}$ is the full coordinate vector and L_H the Poisson operator:

$$L_H f = \sum_{j=1}^{N} \left\{ \frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right\}$$

If the Hamiltonian H can be split into two integrable parts as H=A+B, a symplectic scheme for integrating the equations of motion from time t to time t+τ consists of approximating the operator $e^{\tau L_H}$ by

$$e^{\tau L_H} = e^{\tau(L_A + L_B)} \approx \prod_{i=1}^{j} e^{c_i \tau L_A} e^{d_i \tau L_B}$$

for appropriate values of constants c_i, d_i.

So the dynamics over an integration time step τ is described by a series of successive acts of Hamiltonians A and B.

Symplectic Integrator $SBAB_2C$

We use a symplectic integration scheme developed for Hamiltonians of the form $H=A+\varepsilon B$ where A, B are both integrable and ε a parameter. The operator $e^{\tau L_H}$ can be approximated by the symplectic integrator (Laskar & Robutel, Cel. Mech. Dyn. Astr., 2001, 80, 39):

$$SBAB_2 = e^{d_1 \tau L_{\varepsilon B}}\ e^{c_2 \tau L_A}\ e^{d_2 \tau L_{\varepsilon B}}\ e^{c_2 \tau L_A}\ e^{d_1 \tau L_{\varepsilon B}}$$

with $c_2 = \frac{1}{2},\ d_1 = \frac{1}{6},\ d_2 = \frac{2}{3}.$

The integrator has only positive steps and its error is of order $O(\tau^4\varepsilon+\tau^2\varepsilon^2)$.

In the case where *A* is quadratic in the momenta and *B* depends only on the positions the method can be improved by introducing a corrector $C=\{\{A,B\},B\}$, having a small negative step: $e^{-\tau^3\varepsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}}$

with $c = \frac{1}{72}.$

Thus the full integrator scheme becomes: $SBABC_2 = C\ (SBAB_2)\ C$ and its error is of order $O(\tau^4\varepsilon+\tau^4\varepsilon^2)$.

Example: Hénon-Heiles system

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3$$

Hamilton equations of motion:

$$\begin{aligned} \dot{x} &= p_x \\ \dot{y} &= p_y \\ \dot{p}_x &= -x - 2xy \\ \dot{p}_y &= y^2 - x^2 - y \end{aligned}$$

Variational equations:

$$\begin{aligned} \dot{\delta x} &= \delta p_x \\ \dot{\delta y} &= \delta p_y \\ \dot{\delta p}_x &= -(1 + 2y)\delta x - 2x\delta y \\ \dot{\delta p}_y &= -2x\delta x + (-1 + 2y)\delta y \end{aligned}$$

Tangent dynamics Hamiltonian (TDH) :

$$H_{VH}(\delta x, \delta y, \delta p_x, \delta p_y; t) = \frac{1}{2}\left(\delta p_x^2 + \delta p_y^2\right) +$$

$$+\frac{1}{2}\left\{\left[1 + 2y(t)\right]\delta x^2 + \left[1 - 2y(t)\right]\delta y^2 + 2\left[2x(t)\right]\delta x \delta y\right\}$$

Integration of the variational equations

Use any non-symplectic numerical integration algorithm for the integration of the whole set of equations.

$$
\begin{aligned}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y \\
\dot{\delta x} &= \delta p_x \\
\dot{\delta y} &= \delta p_y \\
\dot{\delta p_x} &= -(1 + 2y)\delta x - 2x\delta y \\
\dot{\delta p_y} &= -2x\delta x + (-1 + 2y)\delta y
\end{aligned}
$$

In our study we use the DOP853 integrator, which is an explicit non-symplectic Runge-Kutta integration scheme of order 8.

Integration of the TDH

Solve numerically the Hamilton equations of motion by any, symplectic or non-symplectic, integration scheme and obtain the time evolution of the reference orbit. Then, use this numerically known solution for solving the equations of motion of the TDH.

$$\begin{aligned}\dot{x} &= p_x\\ \dot{y} &= p_y\\ \dot{p}_x &= -x-2xy\\ \dot{p}_y &= y^2-x^2-y\end{aligned}$$

E.g. compute $x(t_i)$, $y(t_i)$ at $t_i=i\Delta t$, $i=0,1,2,\ldots$, where Δt is the integration time step and approximate the Tangent Dynamics Hamiltonian (TDH) with a quadratic form having constant coefficients for each time interval $[t_i, t_i+\Delta t)$

$$H_{VH} = \frac{1}{2}\left(\delta p_x^2 + \delta p_y^2\right) + \frac{1}{2}\left\{\left[1+2y(t_i)\right]\delta x^2 + \left[1-2y(t_i)\right]\delta y^2 + 2\left[2x(t_i)\right]\delta x \delta y\right\}$$

H_{VH} can be

- **integrated by any symplectic integrator (TDHcc method), or**
- **it can be explicitly solved by performing a canonical transformation to new variables, so that the transformed Hamiltonian becomes a sum of uncoupled 1D Hamiltonians, whose equations of motion can be integrated immediately (TDHes method).**

Integration of the TDH

Considering the TDH as a time dependent Hamiltonian we can transform it to a time independent one having time t as an additional generalized position.

$$\widetilde{H}_{VH}(\delta x, \delta y, t, \delta p_x, \delta p_y, p_t) = \underbrace{\boxed{\frac{1}{2}\left(\delta p_x^2 + \delta p_y^2\right) + p_t}}_{\tilde{A}}$$

$$\underbrace{\boxed{+\frac{1}{2}\left\{\left[1 + 2y(t)\right]\delta x^2 + \left[1 - 2y(t)\right]\delta y^2 + 2\left[2x(t)\right]\delta x \delta y\right\}}}_{\tilde{B}}$$

This new Hamiltonian has one more degree of freedom (extended phase space) and can be integrated by a symplectic integrator (TDHeps method).

$$e^{\tau L_{\tilde{A}}}: \begin{cases} \delta x' &= \delta x + \delta p_x \tau \\ \delta y' &= \delta y + \delta p_y \tau \\ t' &= t + \tau \\ \delta p_x' &= \delta p_x \\ \delta p_y' &= \delta p_y \end{cases}$$

$$\tilde{C} = \left\{\left\{\tilde{A}, \tilde{B}\right\}, \tilde{B}\right\}$$

$$e^{\tau L_{\tilde{C}}}: \begin{cases} \delta x' &= \delta x \\ \delta y' &= \delta y \\ t' &= t \\ \delta p_x' &= \delta p_x - 2\left\{4x(t)\delta y + \right. \\ & \quad \left. + \left[4x^2(t) + \left(1 + 2y(t)\right)^2\right]\delta x\right\}\tau \\ \delta p_y' &= \delta p_y - 2\left\{4x(t)\delta x + \right. \\ & \quad \left. + \left[4x^2(t) + \left(1 - 2y(t)\right)^2\right]\delta y\right\}\tau \end{cases}$$

$$e^{\tau L_{\tilde{B}}}: \begin{cases} \delta x' &= \delta x \\ \delta y' &= \delta y \\ t' &= t \\ \delta p_x' &= \delta p_x - \left\{\left[1 + 2y(t)\right]\delta x + 2x(t)\delta y\right\}\tau \\ \delta p_y' &= \delta p_y + \left\{-2x(t)\delta x + \left[-1 + 2y(t)\right]\delta y\right]\tau \end{cases}$$

Tangent Map (TM) Method

Use symplectic integration schemes for the whole set of equations.

We apply the SBABC$_2$ integrator scheme to the Hénon-Heiles system (with ε=1) by using the splitting:

$$A = \frac{1}{2}(p_x^2 + p_y^2), \qquad B = \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3,$$

with a corrector term which corresponds to the Hamiltonian function:

$$C = \{\{A, B\}, B\} = (x + 2xy)^2 + \left(x^2 - y^2 + y\right)^2$$

We approximate the dynamics by the act of Hamiltonians A, B and C, which correspond to the symplectic maps:

$$e^{\tau L_A} : \begin{cases} x' &= x + p_x \tau \\ y' &= y + p_y \tau \\ p_x' &= p_x \\ p_y' &= p_y \end{cases},$$

$$e^{\tau L_B} : \begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - x(1+2y)\tau \\ p_y' &= p_y + (y^2 - x^2 - y)\tau \end{cases},$$

$$e^{\tau L_C} : \begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p_y' &= p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2 y)\tau \end{cases}.$$

Tangent Map (TM) Method

Let $\vec{u} = (x, y, p_x, p_y, \delta x, \delta y, \delta p_x, \delta p_y)$

The system of the Hamilton equations of motion and the variational equations is split into two integrable systems which correspond to Hamiltonians A and B.

$$
\begin{aligned}
\dot{x} &= p_x\\
\dot{y} &= p_y\\
\dot{p}_x &= -x - 2xy\\
\dot{p}_y &= y^2 - x^2 - y
\end{aligned}
$$

$$
\begin{aligned}
\dot{\delta x} &= \delta p_x\\
\dot{\delta y} &= \delta p_y\\
\dot{\delta p}_x &= -(1+2y)\delta x - 2x\delta y\\
\dot{\delta p}_y &= -2x\delta x + (-1+2y)\delta y
\end{aligned}
$$

$$\xrightarrow{A(\vec{p})}$$

$$
\left.
\begin{aligned}
\dot{x} &= p_x\\
\dot{y} &= p_y\\
\dot{p}_x &= 0\\
\dot{p}_y &= 0\\
\dot{\delta x} &= \delta p_x\\
\dot{\delta y} &= \delta p_y\\
\dot{\delta p}_x &= 0\\
\dot{\delta p}_y &= 0
\end{aligned}
\right\}
\Rightarrow \frac{d\vec{u}}{dt} = L_{AV}\vec{u} \quad \Rightarrow \quad e^{\tau L_{AV}}:
\left\{
\begin{aligned}
x' &= x + p_x\tau\\
y' &= y + p_y\tau\\
px' &= p_x\\
py' &= p_y\\
\delta x' &= \delta x + \delta p_x\tau\\
\delta y' &= \delta y + \delta p_y\tau\\
\delta p_x' &= \delta p_x\\
\delta p_y' &= \delta p_y
\end{aligned}
\right.
$$

$$\xrightarrow{B(\vec{q})}$$

$$
\left.
\begin{aligned}
\dot{x} &= 0\\
\dot{y} &= 0\\
\dot{p}_x &= -x - 2xy\\
\dot{p}_y &= y^2 - x^2 - y\\
\dot{\delta x} &= 0\\
\dot{\delta y} &= 0\\
\dot{\delta p}_x &= -(1+2y)\delta x - 2x\delta y\\
\dot{\delta p}_y &= -2x\delta x + (-1+2y)\delta y
\end{aligned}
\right\}
\Rightarrow \frac{d\vec{u}}{dt} = L_{BV}\vec{u} \quad \Rightarrow \quad e^{\tau L_{BV}}:
\left\{
\begin{aligned}
x' &= x\\
y' &= y\\
p_x' &= p_x - x(1+2y)\tau\\
p_y' &= p_y + (y^2 - x^2 - y)\tau\\
\delta x' &= \delta x\\
\delta y' &= \delta y\\
\delta p_x' &= \delta p_x - [(1+2y)\delta x + 2x\delta y]\,\tau\\
\delta p_y' &= \delta p_y + [-2x\delta x + (-1+2y)\delta y]\,\tau
\end{aligned}
\right.
$$

Tangent Map (TM) Method

So any symplectic integration scheme used for solving the Hamilton equations of motion, which involves the act of Hamiltonians A, B and C, can be extended in order to integrate simultaneously the variational equations.

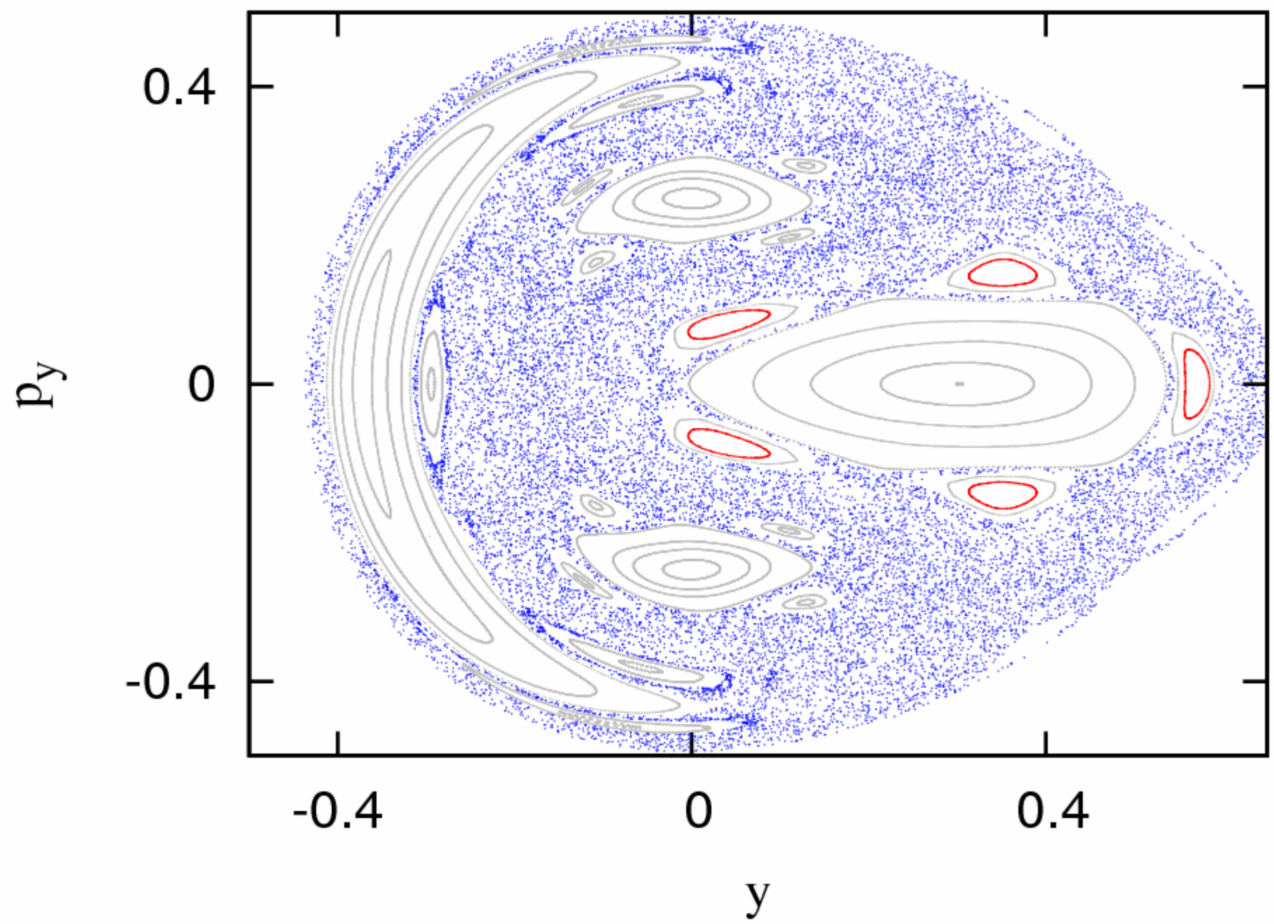
$$e^{\tau L_A}:\begin{cases} x' &= x + p_x\tau \\ y' &= y + p_y\tau \\ p_x' &= p_x \\ p_y' &= p_y \end{cases} \longrightarrow e^{\tau L_{AV}}:\begin{cases} x' &= x + p_x\tau \\ y' &= y + p_y\tau \\ px' &= p_x \\ py' &= p_y \\ \delta x' &= \delta x + \delta p_x\tau \\ \delta y' &= \delta y + \delta p_y\tau \\ \delta p_x' &= \delta p_x \\ \delta p_y' &= \delta p_y \end{cases}$$

$$e^{\tau L_B}:\begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - x(1+2y)\tau \\ p_y' &= p_y + (y^2 - x^2 - y)\tau \end{cases} \longrightarrow e^{\tau L_{BV}}:\begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - x(1+2y)\tau \\ p_y' &= p_y + (y^2 - x^2 - y)\tau \\ \delta x' &= \delta x \\ \delta y' &= \delta y \\ \delta p_x' &= \delta p_x - \left[(1+2y)\delta x + 2x\delta y\right]\tau \\ \delta p_y' &= \delta p_y + \left[-2x\delta x + (-1+2y)\delta y\right]\tau \end{cases}$$

$$e^{\tau L_C}:\begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - 2x(1+2x^2+6y+2y^2)\tau \\ p_y' &= p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \end{cases} \longrightarrow e^{\tau L_{CV}}:\begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - 2x(1+2x^2+6y+2y^2)\tau \\ p_y' &= p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \\ \delta x' &= \delta x \\ \delta y' &= \delta y \\ \delta p_x' &= \delta p_x - 2\left[(1+6x^2+2y^2+6y)\delta x + \right. \\ & \quad \left. +2x(3+2y)\delta y\right]\tau \\ \delta p_y' &= \delta p_y - 2\left[2x(3+2y)\delta x + \right. \\ & \quad \left. +(1+2x^2+6y^2-6y)\delta y\right]\tau \end{cases}$$

Application: Hénon-Heiles system

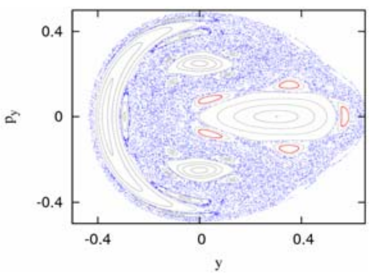
For H_2=0.125 we consider a regular and a chaotic orbit

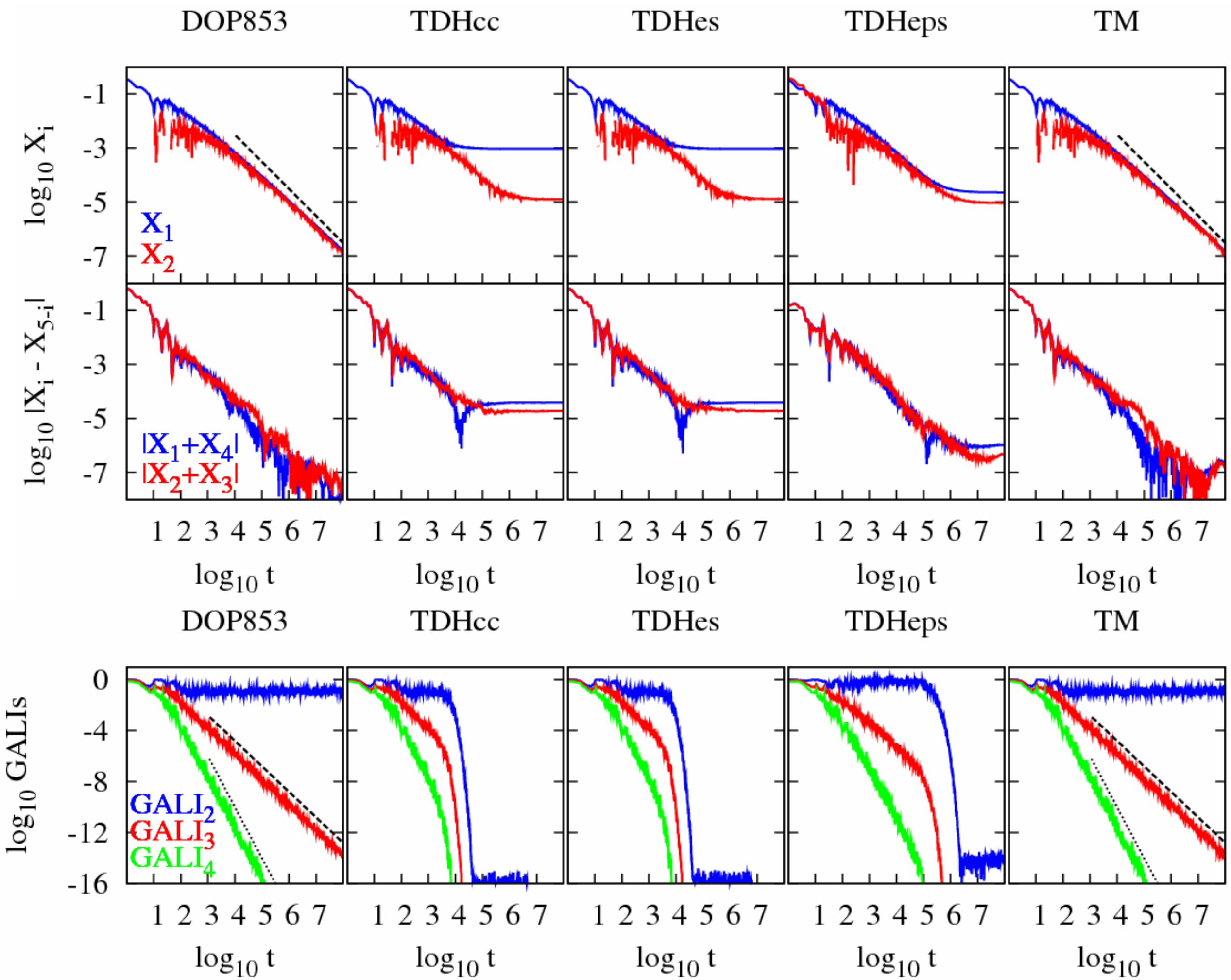


Regular orbit

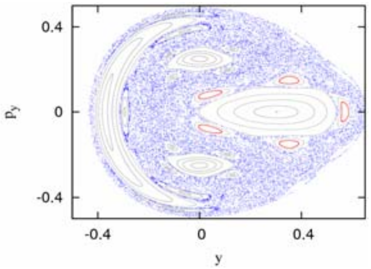
Integration step, $\tau = 0.05$. Relative energy error $\approx 10^{-10} - 10^{-8}$

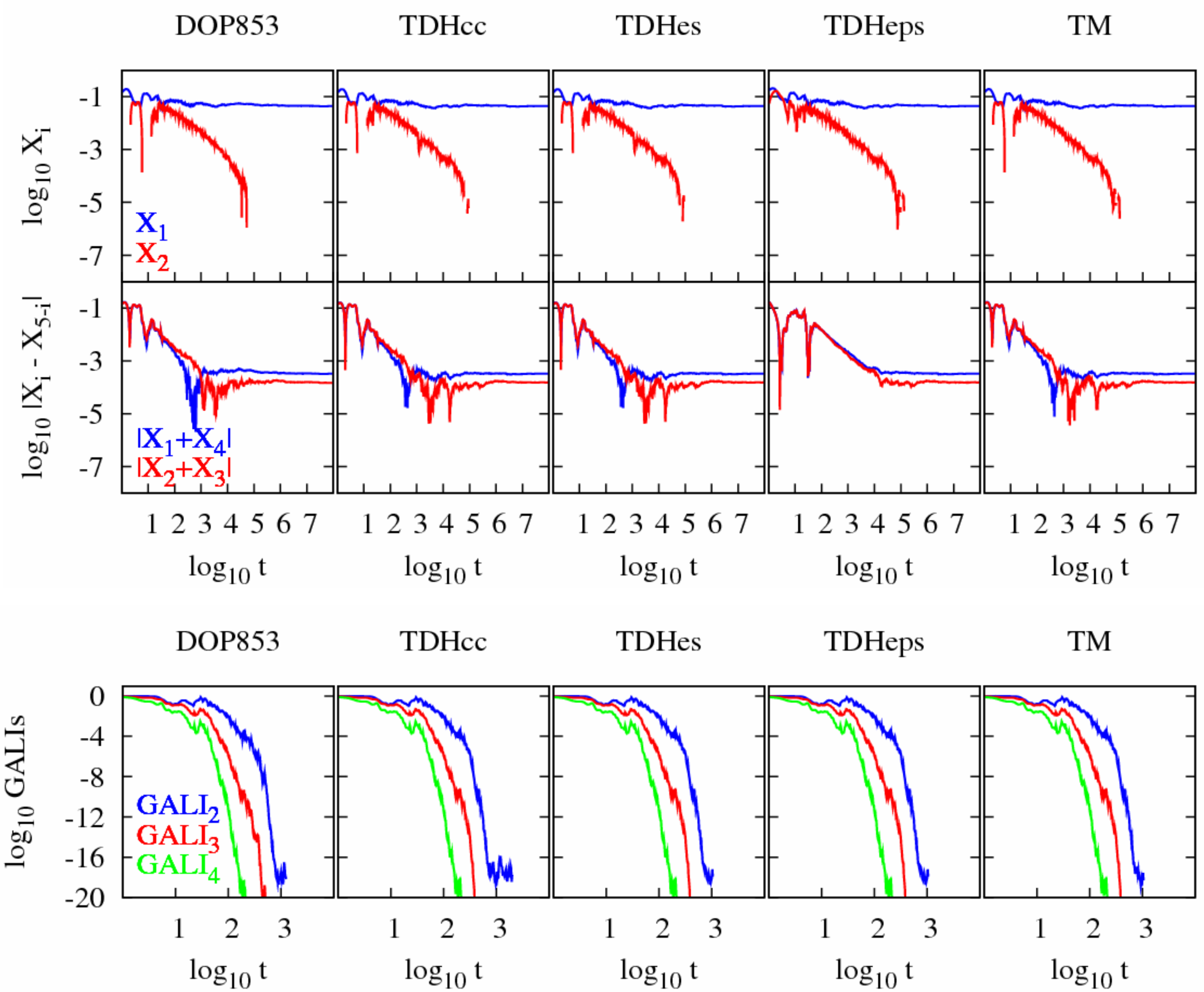
CPU times ≈ 15 h, 6h, 6h, 6h, 5h



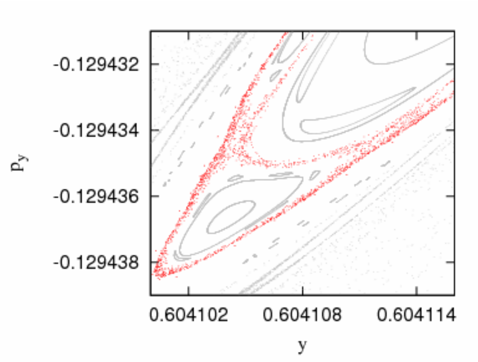


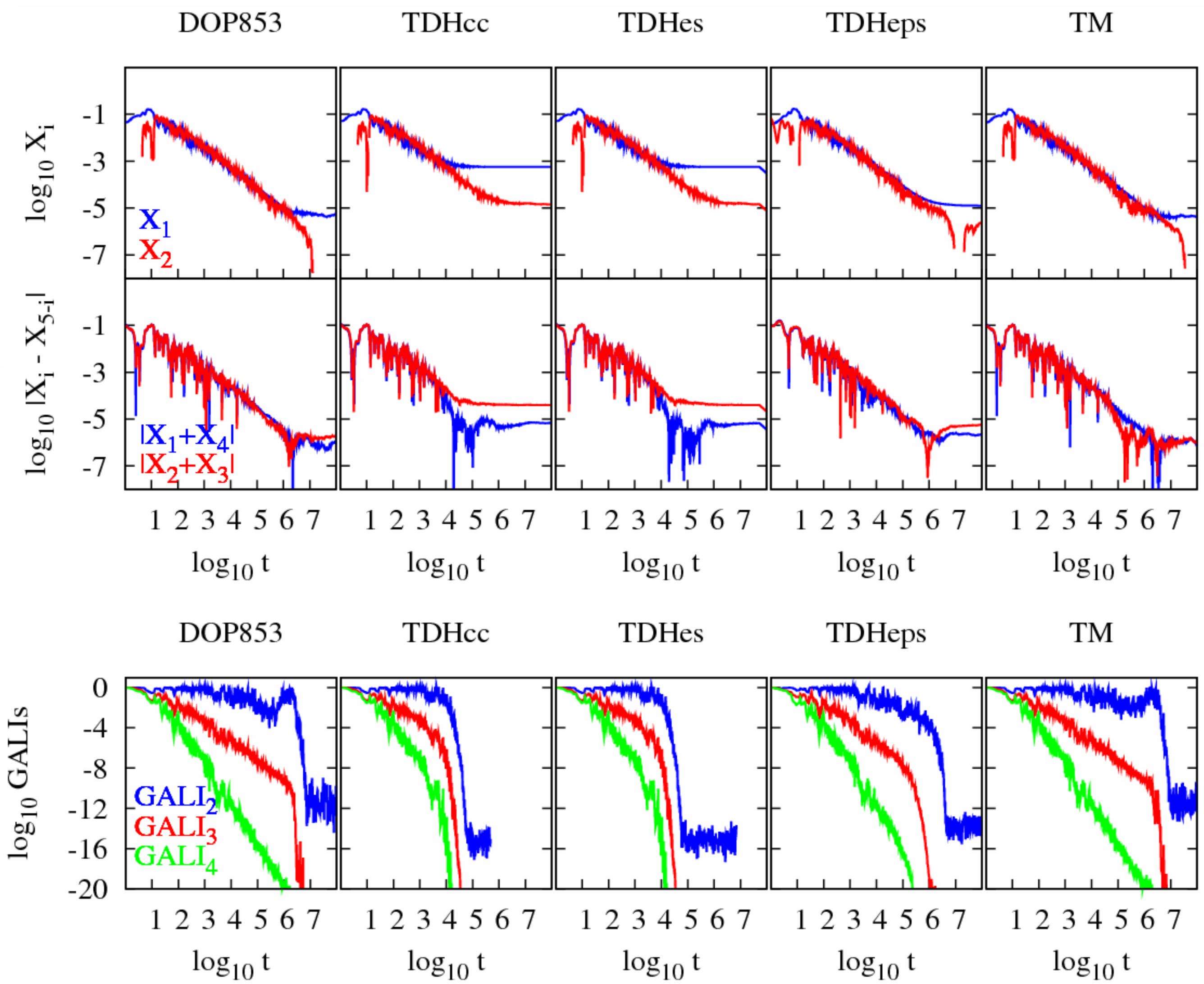
Chaotic orbit





Slightly chaotic orbit





Summary

- We presented and compared different integration schemes for the variational equations of autonomous Hamilonian systems.
- Non-symplectic schemes, like the DOP853 integrator, are very reliable and reproduce correctly the behavior of the LCEs and GALIs, although they require relative large CPU times.
- Techniques based on the previous knowledge of the orbit's evolution (TDHcc, TDHes, TDHeps) have a rather poor numerical performance: they can overestimate the mLCE of chaotic orbits, while regular orbits could be characterized as slightly chaotic.
- Tangent map (TM) method: Symplectic integrators can be used for the simultaneous integration of the Hamilton equations of motion and the variational equations.
  - ✓ They reproduce accurately the properties of the LCEs and GALIs.
  - ✓ These algorithms have better performance than non-symplectic schemes in CPU time requirements. This characteristic is of great importance especially for high dimensional systems.