

# **Algorithms for the integration of variational equations of Hamiltonian systems**

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**Skokos Ch. and Gerlach E., 2010, PRE, 82, 036704**

**Gerlach E. and Skokos Ch., 2010, arXiv:nlin.CD/1008.1890**

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

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

$$\begin{aligned}\dot{\vec{q}} &= \vec{p} \\ \dot{\vec{p}} &= -\frac{\partial V}{\partial \vec{q}}\end{aligned}$$

# Variational Equations

The time evolution of a **deviation vector**

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

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

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

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

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

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

# 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**.

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

$\lambda_1 = 0 \rightarrow$  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  $k$  :

$$\text{GALI}_k(t) = \|\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \dots \wedge \hat{w}_k(t)\|$$

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

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

# Symplectic Integration schemes

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

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

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  $t+\tau$**  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  $\tau$  is described by a series of successive acts of Hamiltonians  $A$  and  $B$ .**

# Symplectic Integrator SBAB<sub>2</sub>C

We use a **symplectic integration scheme** developed for Hamiltonians of the form  $H=A+\varepsilon B$  where  $A, B$  are both integrable and  $\varepsilon$  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

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

**Hamilton equations of motion:**

$$\dot{x} = p_x$$

$$\dot{y} = p_y$$

$$\dot{p}_x = -x - 2xy$$

$$\dot{p}_y = y^2 - x^2 - y$$

**Variational equations:**

$$\dot{\delta x} = \delta p_x$$

$$\dot{\delta y} = \delta p_y$$

$$\dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y$$

$$\dot{\delta p}_y = -2x\delta x + (-1 + 2y)\delta y$$

**Tangent dynamics Hamiltonian (TDH) :**

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



# 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  $t_i = i\Delta t$ ,  $i=0,1,2,\dots$ , where  $\Delta t$  is the integration time step and **approximate the Tangent Dynamics Hamiltonian (TDH) with a quadratic form having constant coefficients for each time interval  $[t_i, t_i + \Delta t)$**

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

$H_{VH}$  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**.

$$\begin{aligned}\tilde{H}_{VH}(\delta x, \delta y, t, \delta p_x, \delta p_y, p_t) &= \frac{1}{2} (\delta p_x^2 + \delta p_y^2) + p_t \\ &+ \frac{1}{2} \{ [1 + 2y(t)] \delta x^2 + [1 - 2y(t)] \delta y^2 + 2 [2x(t)] \delta x \delta y \}\end{aligned}$$

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

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

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

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

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

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

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

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

# Tangent Map (TM) Method

Use symplectic integration schemes for the whole set of equations.

We apply the **SBABC<sub>2</sub>** integrator scheme to the Hénon-Heiles system (with  $\varepsilon=1$ ) by using **the splitting**:

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

with a **corrector term** which corresponds to the Hamiltonian function:

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

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

$$e^{\tau L_A} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ p'_x = p_x \\ p'_y = p_y \end{cases}, \quad e^{\tau L_C} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1 + 2x^2 + 6y + 2y^2)\tau \\ p'_y = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y)\tau \end{cases}.$$

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

# 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.**

$$\dot{x} = p_x$$

$$\dot{y} = p_y$$

$$\dot{p}_x = -x - 2xy$$

$$\dot{p}_y = y^2 - x^2 - y$$

$$\dot{\delta x} = \delta p_x$$

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$$\dot{\delta p}_x = -(1 + 2y)\delta x - 2x\delta y$$

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 \delta \dot{x} = \delta p_x \\
 \delta \dot{y} = \delta p_y \\
 \delta \dot{p}_x = -(1 + 2y)\delta x - 2x\delta y \\
 \delta \dot{p}_y = -2x\delta x + (-1 + 2y)\delta y
 \end{array}
 \xrightarrow{A(\vec{p})}
 \left. \begin{array}{l}
 \dot{x} = p_x \\
 \dot{y} = p_y \\
 \dot{p}_x = 0 \\
 \dot{p}_y = 0 \\
 \delta \dot{x} = \delta p_x \\
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 \delta \dot{p}_x = 0 \\
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 \end{array} \right\} \Rightarrow \frac{d\vec{u}}{dt} = L_{AV}\vec{u}$$

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

$$\left( \begin{array}{l}
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 \dot{p}_y = y^2 - x^2 - y \\
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 \end{array} \right) \xrightarrow{B(\vec{q})} \left\{ \begin{array}{l}
 x' = x \\
 y' = y \\
 p_x' = p_x - x(1 + 2y)\tau \\
 p_y' = p_y + (y^2 - x^2 - y)\tau \\
 \delta x' = \delta x \\
 \delta y' = \delta y \\
 \delta p_x' = \delta p_x - [(1 + 2y)\delta x + 2x\delta y]\tau \\
 \delta p_y' = \delta p_y + [-2x\delta x + (-1 + 2y)\delta y]\tau
 \end{array} \right.$$

# 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.**

$$e^{\tau L_A} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ p'_x = p_x \\ p'_y = p_y \end{cases}$$

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

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

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

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 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} \xrightarrow{\quad} 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 - [(1 + 2y)\delta x + 2x\delta y]\tau \\ \delta p'_y = \delta p_y + [-2x\delta x + (-1 + 2y)\delta 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^2y)\tau \end{cases}
 \end{array}$$

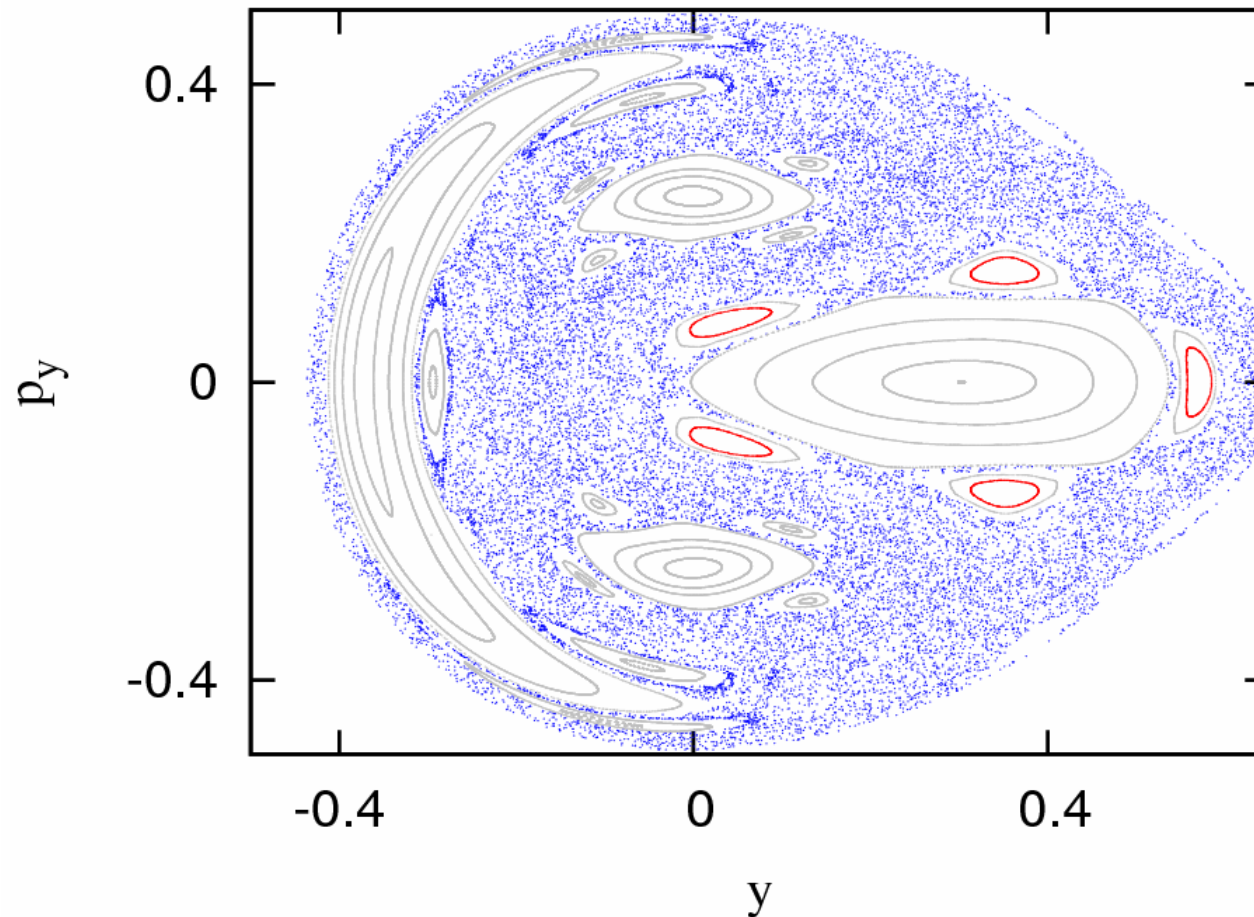
# Tangent Map (TM) Method

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.

$$\begin{array}{ccc}
 e^{\tau L_A} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ p'_x = p_x \\ p'_y = p_y \end{cases} & \xrightarrow{\quad} & e^{\tau L_{AV}} : \begin{cases} x' = x + p_x \tau \\ y' = y + p_y \tau \\ px' = p_x \\ py' = p_y \\ \delta x' = \delta x + \delta p_x \tau \\ \delta y' = \delta y + \delta p_y \tau \\ \delta p'_x = \delta p_x \\ \delta p'_y = \delta p_y \end{cases} \\
 e^{\tau L_B} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - x(1+2y)\tau \\ p'_y = p_y + (y^2 - x^2 - y)\tau \end{cases} & \xrightarrow{\quad} & e^{\tau L_{BV}} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - x(1+2y)\tau \\ p'_y = p_y + (y^2 - x^2 - y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_x = \delta p_x - [(1+2y)\delta x + 2x\delta y]\tau \\ \delta p'_y = \delta p_y + [-2x\delta x + (-1+2y)\delta y]\tau \end{cases} \\
 e^{\tau L_C} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1+2x^2+6y+2y^2)\tau \\ p'_y = p_y - 2(y-3y^2+2y^3+3x^2+2x^2y)\tau \end{cases} & \xrightarrow{\quad} & e^{\tau L_{CV}} : \begin{cases} x' = x \\ y' = y \\ p'_x = p_x - 2x(1+2x^2+6y+2y^2)\tau \\ p'_y = p_y - 2(y-3y^2+2y^3+3x^2+2x^2y)\tau \\ \delta x' = \delta x \\ \delta y' = \delta y \\ \delta p'_x = \delta p_x - 2[(1+6x^2+2y^2+6y)\delta x + 2x(3+2y)\delta y]\tau \\ \delta p'_y = \delta p_y - 2[2x(3+2y)\delta x + (1+2x^2+6y^2-6y)\delta y]\tau \end{cases}
 \end{array}$$

# 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  $\approx$

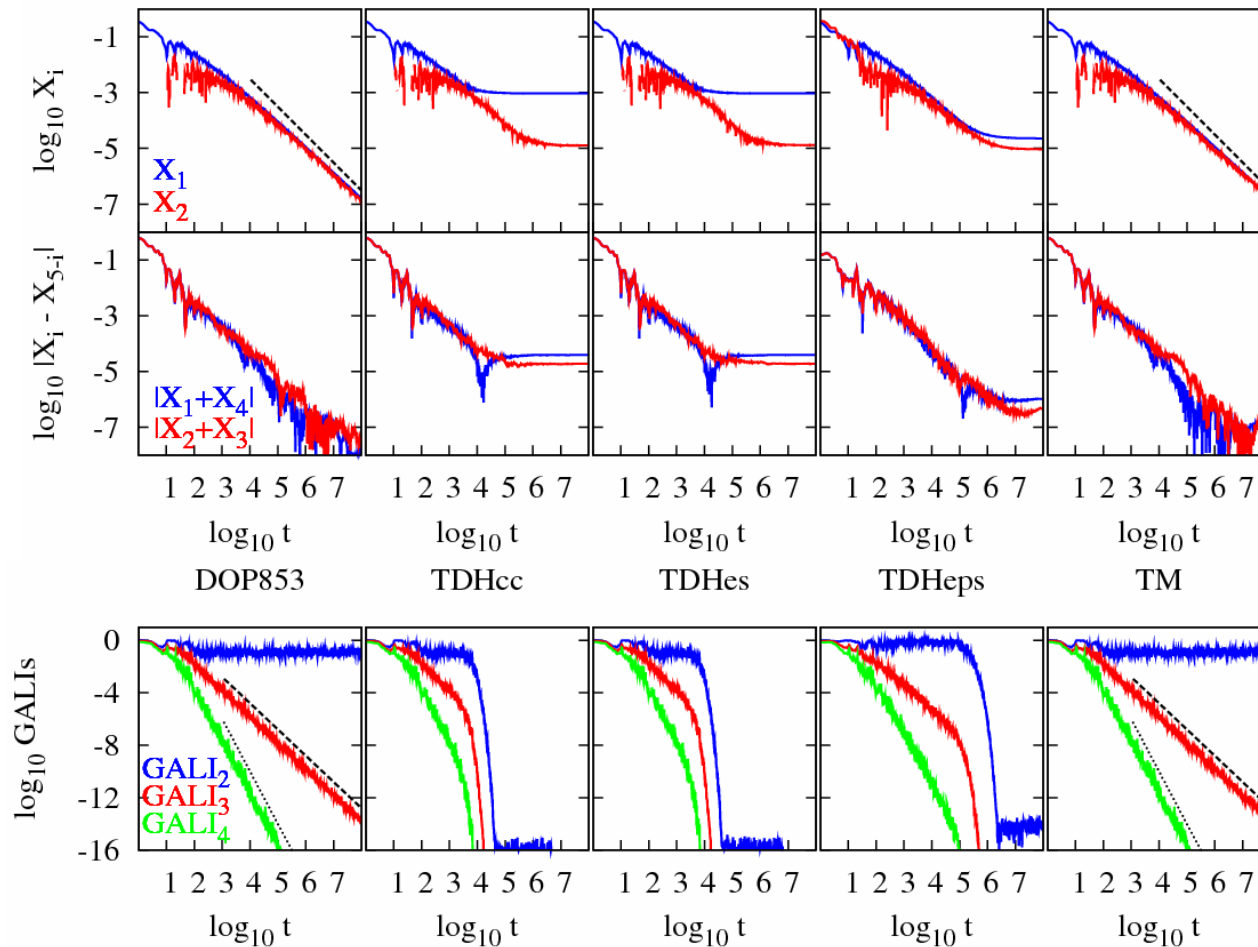
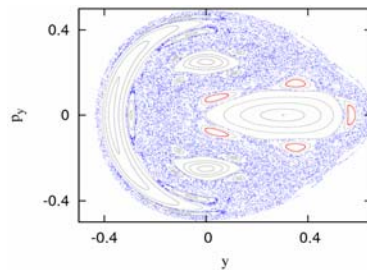
**15 h**  
DOP853

**6h**  
TDHcc

**6h**  
TDHes

**6h**  
TDHeps

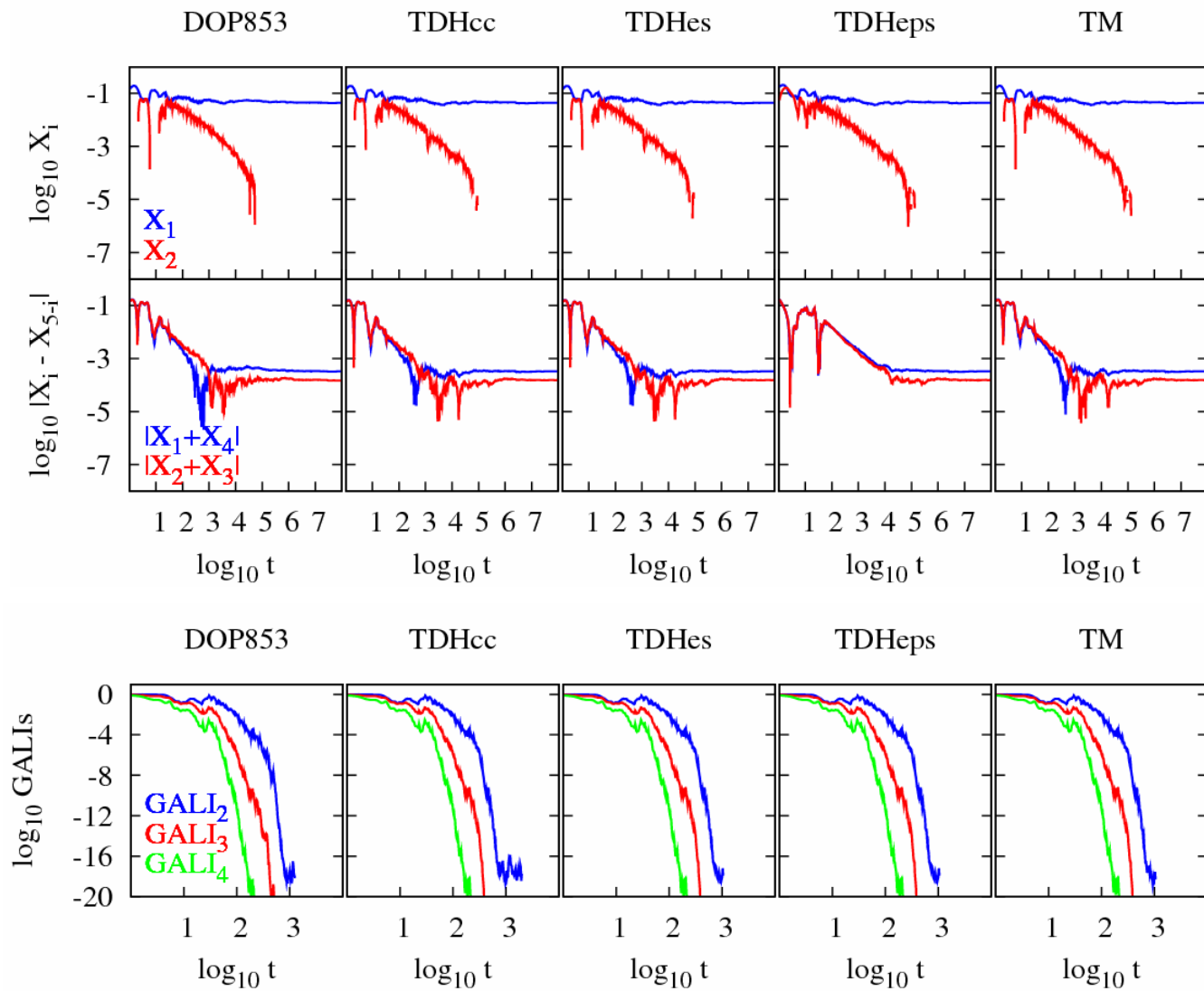
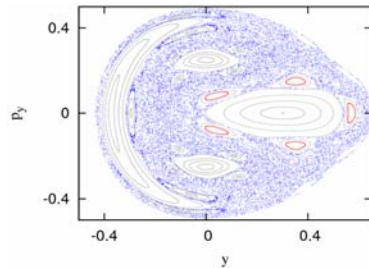
**5h**  
TM



H. Skokos

Seminar on Nonlinear Systems, University of Patras  
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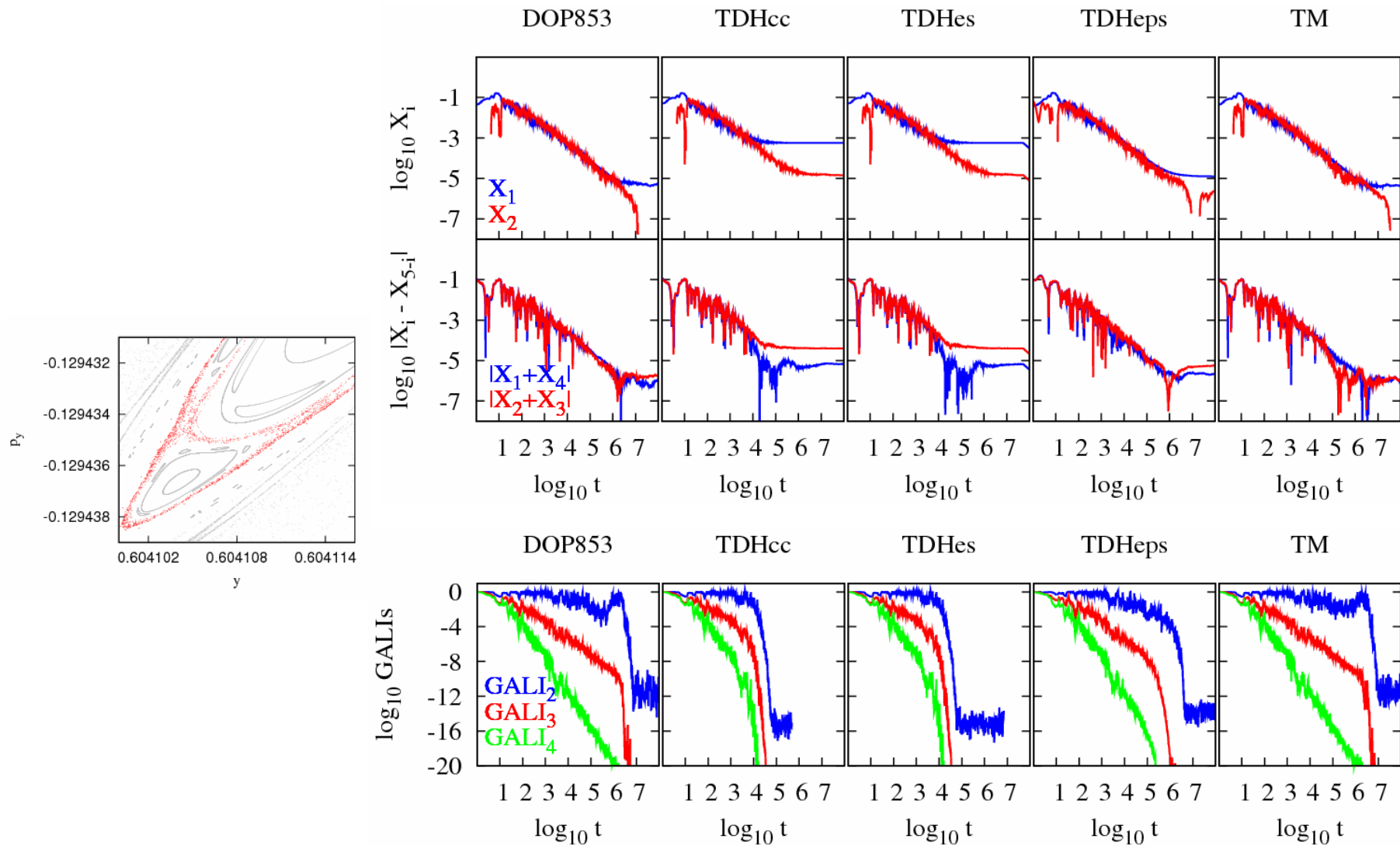
# Chaotic orbit



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# Slightly chaotic orbit



# Summary

- We presented and compared **different integration schemes** for the variational equations of autonomous Hamiltonian 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.**