On the numerical integration of variational equations

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See also poster: Some aspects of the numerical integration of variational equations

Outline

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

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.

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

$\lambda_1 = 0 \rightarrow$ Regular motion
$\lambda_1 \neq 0 \rightarrow$ Chaotic motion

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

$$GALI_k(t) = \|\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \ldots \wedge \hat{w}_k(t)\|$$

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

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

Symplectic Integration schemes

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

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

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

$$L_H f = \sum_{j=1}^{3} \left\{ \frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right\}$$

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 appropratite values of constants c_i, d_i.

<u>So the dynamics over an integration time step τ is transformed into a series of successive acts of Hamiltonians A and B.</u>

Symplectic Integrator SABA$_2$C

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):

$$\mathrm{SABA}_2 = e^{c_1 \tau L_A}\, e^{d_1 \tau L_{\varepsilon B}}\, e^{c_2 \tau L_A}\, e^{d_1 \tau L_{\varepsilon B}}\, e^{c_1 \tau L_A}$$

with $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6},\ c_2 = \frac{\sqrt{3}}{3},\ d_1 = \frac{1}{2}.$

The integrator has only small 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 $c = \frac{2-\sqrt{3}}{24}.$

Thus the full integrator scheme becomes: $SABAC_2 = C\,(SABA_2)\,C$ 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) :

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

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

Integration of the variational equations

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

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

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

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 the integration time step and approximate the TDH with a quadratic form having constant coefficients for each time interval $[t_i, t_i+\Delta t)$

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

Tangent Map Method (TMM)

Use symplectic integration schemes for the whole set of equations.

We apply the SABAC$_2$ 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 Method (TMM)

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.

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

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

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

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

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

Tangent Map Method (TMM)

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.

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

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

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

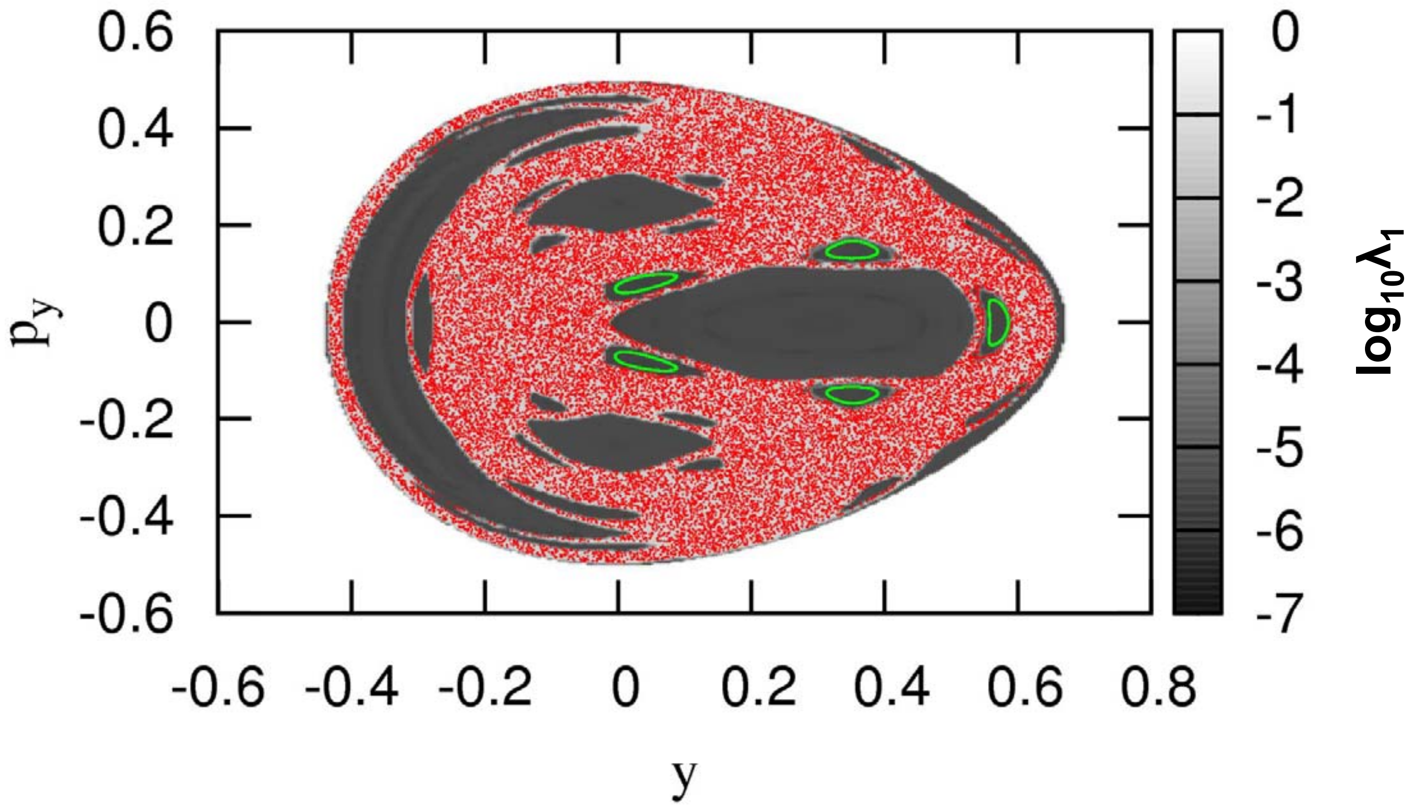
$$e^{\tau L_{BV}}: \begin{cases} x' &= x \\ y' &= y \\ p_x' &= p_x - x(1+2y)\tau \\ p_y' &= p_y + (y^2 - x^2 - y)\tau \\ \delta x' &= \delta x \\ \delta y' &= \delta y \\ \delta p_x' &= \delta p_x - \left[(1+2y)\delta x + 2x\delta y\right]\tau \\ \delta p_y' &= \delta p_y + \left[-2x\delta x + (-1+2y)\delta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

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

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

Application: Hénon-Heiles system

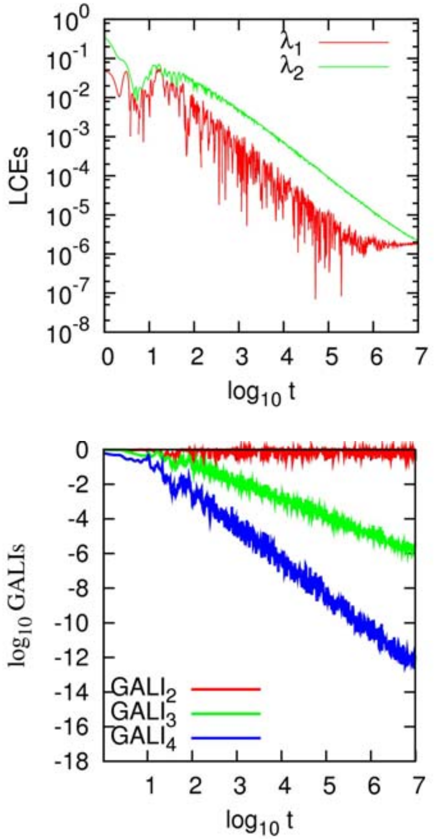
For H_2=0.125 we consider a regular and a chaotic orbit



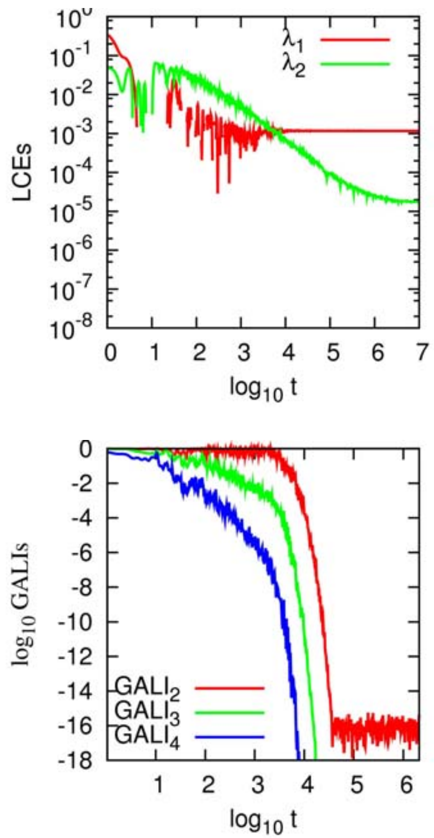
Hénon-Heiles system: Regular orbit

Integration step = 0.05

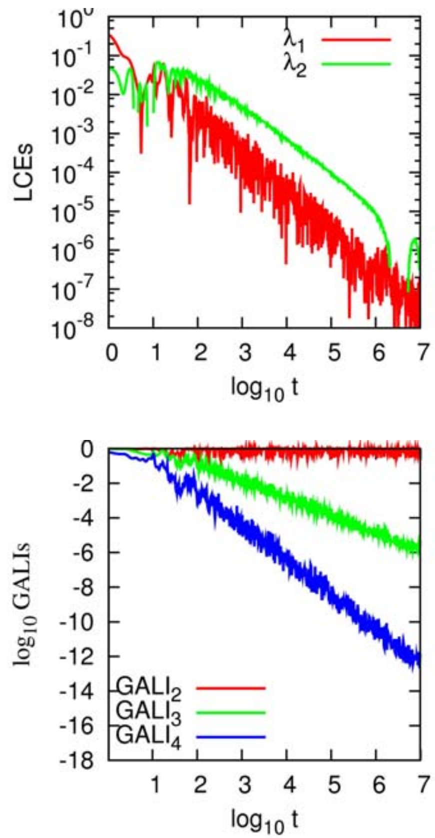
DOP



TDH



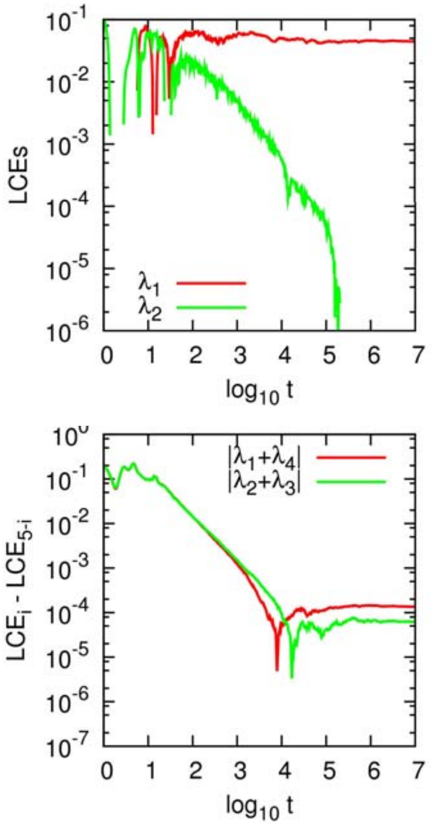
TMM – $SABA_2C$



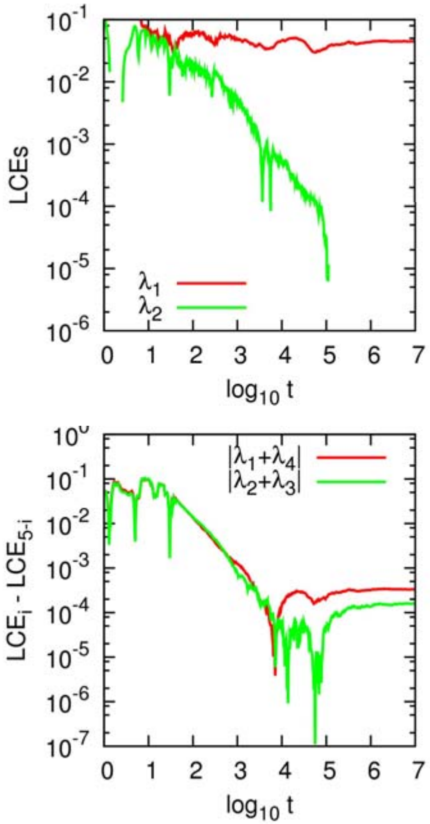
Hénon-Heiles system: Chaotic orbit

Integration step = 0.05

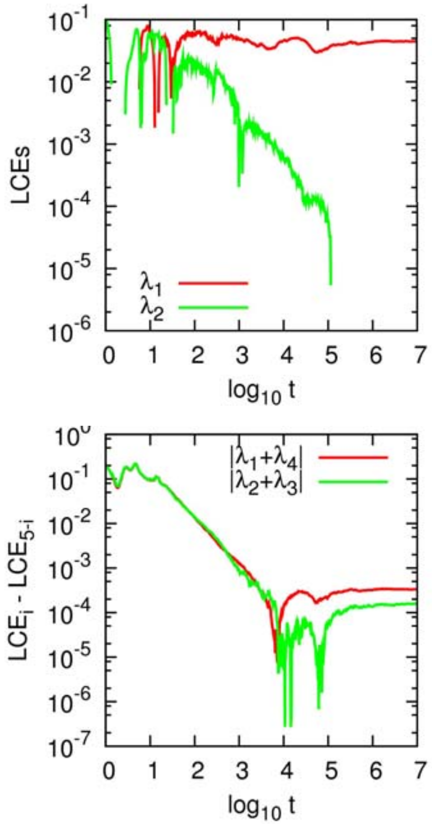
DOP (λ_1=0.042)



TDH (λ_1=0.045)



TMM – SABA$_2$C (λ_1=0.045)



Summary

- **We discussed different integration schemes for the variational equations of Hamilonian systems.**

- **Symplectic integration schemes can be used for the simultaneous integration of the Hamilton equations of motion and the veriational equations.**
  - ✓ **These algorithms have better performance than non-symplectic schemes in CPU time requirements. This characteristic is of great importance especially for high dimensional systems.**
  - ✓ **They reproduce the properties of the Lyapunov spectrum and of GALIs better than techniques based on the previous knowledge of the orbit's evolution.**