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

\[
\begin{align*}
\dot{\vec{q}} &= \vec{p} \\
\dot{\vec{p}} &= -\frac{\partial V}{\partial \vec{q}}
\end{align*}
\]
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:

\[ \begin{align*}
\dot{\delta q} &= \delta p \\
\dot{\delta p} &= -D^2V(\vec{q}(t))\delta q
\end{align*} \]

where

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

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

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

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

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

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

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

**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:

\[ \frac{d\tilde{X}}{dt} = \{H, \tilde{X}\} = L_H \tilde{X} \Rightarrow \tilde{X}(t) = \sum_{n \geq 0}^{t^n} L_H^n \tilde{X} = e^{tL_H} \tilde{X} \]

where \( \tilde{X} \) 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 \( B \).
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):

$$SBAB_2 = e^{d_1\tau L_B} e^{c_2\tau L_A} e^{d_2\tau L_B} e^{c_2\tau L_A} e^{d_1\tau L_B}$$

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 $O(\tau^4\varepsilon + \tau^4\varepsilon^2)$. 

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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:

\[ \delta \dot{x} = \delta p_x \]
\[ \delta \dot{y} = \delta p_y \]
\[ \delta \dot{p}_x = -(1 + 2y) \delta x - 2x \delta y \]
\[ \delta \dot{p}_y = -2x \delta x + (-1 + 2y) \delta y \]

Tangent dynamics Hamiltonian (TDH):

\[ H_{\text{VH}}(\delta x, \delta y, \delta p_x, \delta p_y; t) = \frac{1}{2} (\delta p_x^2 + \delta p_y^2) + \]
\[ + \frac{1}{2} \left\{ [1 + 2y(t)] \delta x^2 + [1 - 2y(t)] \delta y^2 + 2 [2x(t)] \delta x \delta y \right\} \]
Integration of the variational equations

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

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

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.

E.g. compute \(x(t_i), y(t_i)\) at \(t_i = i \Delta t, i=0,1,2,...\), 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 \([t_i, t_i+\Delta t)\)

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

\(H_{VH}\) 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.

\[
\tilde{H}_{VH}(\delta x, \delta y, t, \delta p_x, \delta p_y, p_t) = \frac{1}{2} (\delta p_x^2 + \delta p_y^2) + p_t \quad \tilde{A}
\]
\[
+ \frac{1}{2} \{ [1 + 2y(t)] \delta x^2 + [1 - 2y(t)] \delta y^2 + 2 [2x(t)] \delta x \delta y \} \quad \tilde{B}
\]

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

\[
e^{\tau L_A} : \quad \begin{cases} 
\delta x' = \delta x + \delta p_x \tau \\
\delta y' = \delta y + \delta p_y \tau \\
\delta p_x' = \delta p_x \\
\delta p_y' = \delta p_y \\
t' = t + \tau
\end{cases} \quad \tilde{C} = \{ \{ \tilde{A}, \tilde{B} \}, \tilde{B} \}
\]
\[
e^{\tau L_C} : \quad \begin{cases} 
\delta x' = \delta x \\
\delta y' = \delta y \\
t' = t \\
\delta p_x' = \delta p_x - 2 \{4x(t)\delta y + 4x^2(t) + (1 + 2y(t))^2 \} \delta x \\
\delta p_y' = \delta p_y - 2 \{4x(t)\delta x + 4x^2(t) + (1 - 2y(t))^2 \} \delta y \\
\end{cases}
\]

\[
e^{\tau L_B} : \quad \begin{cases} 
\delta x' = \delta x \\
\delta y' = \delta y \\
t' = t \\
\delta p_x' = \delta p_x - [1 + 2y(t)] \delta x + 2x(t) \delta y \tau \\
\delta p_y' = \delta p_y + [-2x(t)\delta x + [-1 + 2y(t)] \delta y] \tau
\end{cases}
\]
Tangent Map (TM) Method

Use symplectic integration schemes for the whole set of equations. We apply the \( \text{SBABC}_2 \) integrator scheme to the Hénon-Heiles system (with \( \varepsilon=1 \)) by using the splitting:

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

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:

\[
ed^{\tau L_A} : \begin{cases} 
    x' = x + p_x \tau \\
    y' = y + p_y \tau \\
    p'_x = p_x \\
    p'_y = p_y
\end{cases}, \quad 
\]

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

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

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

\[
\begin{aligned}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= 0 \\
\dot{p}_y &= 0 \\
\delta x &= \delta p_x \\
\delta y &= \delta p_y \\
\delta p_x &= 0 \\
\delta p_y &= 0
\end{aligned}
\] \Rightarrow \frac{d\vec{u}}{dt} = L_{AV} \vec{u} \Rightarrow e^{\tau L_{AV}}

\[
\begin{aligned}
\dot{x}' &= x + p_x\tau \\
\dot{y}' &= y + p_y\tau \\
\dot{p}_x' &= p_x \\
\dot{p}_y' &= p_y \\
\delta x' &= \delta x + \delta p_x\tau \\
\delta y' &= \delta y + \delta p_y\tau \\
\delta p_x' &= \delta p_x \\
\delta p_y' &= \delta p_y
\end{aligned}
\]
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.

\[
\begin{align*}
\left\{ \begin{array}{l}
x' = x + p_x \tau \\
y' = y + p_y \tau \\
p'_x = p_x \\
p'_y = p_y \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x + p_x \tau \\
y' = y + p_y \tau \\
p'_x = p_x \\
p'_y = p_y \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = p_x - x(1 + 2y) \tau \\
p'_y = p_y - \left( y^2 - x^2 - y \right) \tau \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = p_x - x(1 + 2y) \tau \\
p'_y = p_y - \left( y^2 - x^2 - y \right) \tau \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = p_x \left( 1 + 2x^2 + 6y + 2y^2 \right) \tau \\
p'_y = p_y \left( 2y^2 + 3x^2 + 2x^2 y \right) \tau \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = p_x \left( 1 + 2x^2 + 6y + 2y^2 \right) \tau \\
p'_y = p_y \left( 2y^2 + 3x^2 + 2x^2 y \right) \tau \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = 2 \left( 1 + 6x^2 + 2y^2 + 6y \right) \delta x + 2x \left( 3 + 2y \right) \delta y \tau \\
p'_y = -2 \left( 2x \left( 3 + 2y \right) \delta x + \left( 1 + 2x^2 + 6y^2 - 6y \right) \delta y \right) \tau \\
\end{array} \right. \\
\left\{ \begin{array}{l}
x' = x \\
y' = y \\
p'_x = 2 \left( 1 + 6x^2 + 2y^2 + 6y \right) \delta x + 2x \left( 3 + 2y \right) \delta y \tau \\
p'_y = -2 \left( 2x \left( 3 + 2y \right) \delta x + \left( 1 + 2x^2 + 6y^2 - 6y \right) \delta y \right) \tau \\
\end{array} \right. \\
\end{align*}
\]
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 \( \approx \)

<table>
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<tr>
<th>15 h</th>
<th>6h</th>
<th>6h</th>
<th>6h</th>
<th>5h</th>
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<tbody>
<tr>
<td>DOP853</td>
<td>TDHcc</td>
<td>TDHes</td>
<td>TDHeps</td>
<td>TM</td>
</tr>
</tbody>
</table>

![Graphs showing the integration results for different methods](image)
Chaotic orbit

DOP853  TDHcc  TDHcs  TDHeps  TM

\[ \log_{10} X_i \]

\[ \log_{10} |X_i - X_{i+1}| \]

\[ \log_{10} |X_i + X_{i+1}| \]

\[ \log_{10} G_{ALL} \]

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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.