Numerical integration of variational equations

Haris Skokos
Max Planck Institute for the Physics of Complex Systems
Dresden, Germany
E-mail: hskokos@pks.mpg.de,
URL: http://www.pks.mpg.de/~hskokos/

Enrico Gerlach
Lohrmann Observatory, Technical University
Dresden, Germany
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 $\vec{q} = (q_1(t), q_2(t), \ldots, q_N(t))$ and $\vec{p} = (p_1(t), p_2(t), \ldots, p_N(t))$ 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

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

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

\[ \ddot{\delta q} = \dot{\delta p} \]
\[ \dot{\delta p} = -D^2V(\mathbf{\overline{q}}(t))\delta q \]

where

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

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

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

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

\[\lambda_1 = 0 \rightarrow \text{Regular motion}\]
\[\lambda_1 \neq 0 \rightarrow \text{Chaotic motion}\]

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:
\[
\frac{d\vec{X}}{dt} = \{H, \vec{X}\} = L_H \vec{X} \Rightarrow \vec{X}(t) = \sum_{n\geq0} t^n L^n_H \vec{X} = e^{tL_H} \vec{X}
\]

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 \(e^{tL_H}\) by
\[
e^{tL_H} = e^{(L_A+L_B)} \approx \prod_{i=1}^{j} e^{c_i \tau L_A} e^{d_i \tau L_B}
\]

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 \( SBAB_2C \)

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

\[
SBAB_2 = e^{d_1\tau L_{\epsilon B}} e^{c_2\tau L_A} e^{d_2\tau L_{\epsilon B}} e^{c_2\tau L_A} e^{d_1\tau L_{\epsilon B}}
\]

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 \( O(\tau^4\epsilon+\tau^2\epsilon^2) \).

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:

\[
\exp\left(-\tau^3\epsilon^2\frac{c}{2}L_{\{\{A,B\},B\}}\right)
\]

with \( c = \frac{1}{72} \).

Thus the full integrator scheme becomes: \( SBABC_2 = C (SBAB_2) C \) and its error is of order \( O(\tau^4\epsilon+\tau^4\epsilon^2) \).
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:
\[
\begin{align*}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y
\end{align*}
\]

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

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

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

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

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 \( t_i = i\Delta t \), \( i=0,1,2,\ldots \), 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 \([t_i, t_i+\Delta t)\)

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

\( H_{VH} \) 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.

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

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

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

\[
e^{\tau \tilde{A}} : \begin{cases} 
\delta x' = \delta x + \delta p_x \tau \\
\delta y' = \delta y + \delta p_y \tau \\
\delta p_x' = \delta p_x \\
\delta p_y' = \delta p_y 
\end{cases}
\]

\[
e^{\tau \tilde{C}} = \left\{ \{ \tilde{A}, \tilde{B} \}, \tilde{B} \right\}
\]

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

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

H. Skokos  
NDC2010, Thessaloniki, Greece - 13 July 2010
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.

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

\[
\Rightarrow \frac{d\vec{u}}{dt} = L_{AV} \vec{u} \Rightarrow e^{\tau L_{AV}}:
\]

\[
\begin{align*}
x' &= x + p_x \tau \\
y' &= y + p_y \tau \\
p_x' &= p_x \\
p_y' &= p_y \\
\delta x' &= \delta x + \delta p_x \tau \\
\delta y' &= \delta y + \delta p_y \tau \\
\delta p_x' &= \delta p_x \\
\delta p_y' &= \delta p_y
\end{align*}
\]

\[
\begin{align*}
\dot{x} &= p_x \\
\dot{y} &= p_y \\
\dot{p}_x &= -x - 2xy \\
\dot{p}_y &= y^2 - x^2 - y \\
\delta x &= 0 \\
\delta y &= 0 \\
\delta p_x &= -(1 + 2y)\delta x - 2x\delta y \\
\delta p_y &= -2x\delta x + (-1 + 2y)\delta y
\end{align*}
\]

\[
\Rightarrow \frac{d\vec{u}}{dt} = L_{BV} \vec{u} \Rightarrow e^{\tau L_{BV}}:
\]

\[
\begin{align*}
x' &= x \\
y' &= y \\
p_x' &= p_x - x(1 + 2y) \tau \\
p_y' &= p_y + (y^2 - x^2 - y) \tau \\
\delta x' &= \delta x \\
\delta y' &= \delta y \\
\delta p_x' &= \delta p_x - [(1 + 2y)\delta x + 2x\delta y] \tau \\
\delta p_y' &= \delta p_y + [-2x\delta x + (-1 + 2y)\delta y] \tau
\end{align*}
\]
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.

\[
\begin{align*}
\mathcal{L}_A: & \quad \begin{cases} 
    x' = x + p_x \tau \\
    y' = y + p_y \tau \\
    p_x' = p_x \\
    p_y' = p_y
\end{cases} \\
\mathcal{L}_{AV}: & \quad \begin{cases} 
    x' = x + p_x \tau \\
    y' = y + p_y \tau \\
    p_x' = p_x + \delta p_x \tau \\
    p_y' = p_y + \delta p_y \tau
\end{cases} \\
\mathcal{L}_{B}: & \quad \begin{cases} 
    x' = x \\
    y' = y \\
    p_x' = p_x - x(1 + 2y) \tau \\
    p_y' = p_y + (y^2 - x^2 - y) \tau
\end{cases} \\
\mathcal{L}_{BV}: & \quad \begin{cases} 
    x' = x \\
    y' = y \\
    p_x' = p_x - [(1 + 2y) \delta x + 2x \delta y] \tau \\
    p_y' = p_y + [-2x \delta x + (-1 + 2y) \delta y] \tau
\end{cases} \\
\mathcal{L}_{C}: & \quad \begin{cases} 
    x' = x \\
    y' = y \\
    p_x' = p_x - 2x(1 + 2x^2 + 6y + 2y^2) \tau \\
    p_y' = p_y - 2(y - 3y^2 + 2y^3 + 3x^2 + 2x^2y) \tau
\end{cases} \\
\mathcal{L}_{CV}: & \quad \begin{cases} 
    x' = x \\
    y' = y \\
    p_x' = p_x - 2[(1 + 6x^2 + 2y^2 + 6y) \delta x + +2x(3 + 2y) \delta y] \tau \\
    p_y' = p_y - 2[2x(3 + 2y) \delta x + +(1 + 2x^2 + 6y^2 - 6y) \delta y] \tau
\end{cases}
\]
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 $\approx$

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

![Graph showing log10 of various variables over time](image.png)
Chaotic orbit
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 relatively 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.