Algorithms for the integration of variational equations of multidimensional Hamiltonian systems

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/

Work in collaboration with

Enrico Gerlach and Siegfried Eggl

Autonomous Hamiltonian systems

We study **N degree of freedom** autonomous Hamiltonian systems of the form:

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

As an example, we consider the 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:

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

Variational equations:

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

Integration of the variational equations

We use two general-purpose **numerical integration algorithms for the integration of the whole set of equations:**

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

a) the DOP853 integrator (Hairer et al. 1993, http://www.unige.ch/~hairer/software.html), which is an explicit non-symplectic Runge-Kutta integration scheme of order 8,

b) the TIDES integrator (Barrio 2005, http://gme.unizar.es/software/tides), which is based on a Taylor series approximation

$$\boldsymbol{y}(t_i+\tau) \simeq \boldsymbol{y}(t_i) + \tau \frac{\mathrm{d}\boldsymbol{y}(t_i)}{\mathrm{d}t} + \frac{\tau^2}{2!}\frac{\mathrm{d}^2\boldsymbol{y}(t_i)}{\mathrm{d}t^2} + \ldots + \frac{\tau^n}{n!}\frac{\mathrm{d}^n\boldsymbol{y}(t_i)}{\mathrm{d}t^n}$$

for the solution of system

$$\frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{y}(t))$$

Symplectic integration schemes

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 $e^{\tau L_H}$, i.e. the solution of Hamilton equations of motion, 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.

We consider a particular symplectic integrator (Laskar & Robutel, 2001)

$$\mathrm{SABA}_2 = e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A} \; e^{\frac{\tau}{2}L_B} \; e^{\frac{\sqrt{3}\tau}{3}L_A} \; e^{\frac{\tau}{2}L_B} \; e^{\left[\frac{(3-\sqrt{3})}{6}\tau\right]L_A}$$

Tangent Map (TM) Method

We use symplectic integration schemes for the integrating the equations of motion AND the variational equations.

The Hénon-Heiles system can be split as:

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

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

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

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.

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

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

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

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

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

Tangent Map (TM) Method

So any symplectic integration scheme used for solving the Hamilton equations of motion, which involves the act of Hamiltonians A and B, can be extended in order to integrate simultaneously the variational equations (Skokos & Gerlach 2010, Gerlach & Skokos 2011).

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

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

Chaos detection methods

The Lyapunov exponents of a given orbit characterize the mean exponential rate of divergence of trajectories surrounding it.

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

$\lambda_1=0 \rightarrow$ **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) the Generalized Alignment Index (GALI) of order k :

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

Chaotic motion:

$$GALI_k(t) \propto e^{-[(\lambda_1-\lambda_2)+(\lambda_1-\lambda_3)+...+(\lambda_1-\lambda_k)]t}$$

Regular motion on an s-dimensional torus with $s\leq N$:

$$GALI_k(t) \propto \begin{cases} \text{constant} & \text{if} \quad 2 \leq k \leq s \\ \frac{1}{t^{k-s}} & \text{if} \quad s < k \leq 2N-s \\ \frac{1}{t^{2(k-N)}} & \text{if} \quad 2N-s < k \leq 2N \end{cases}$$

Application: FPU system

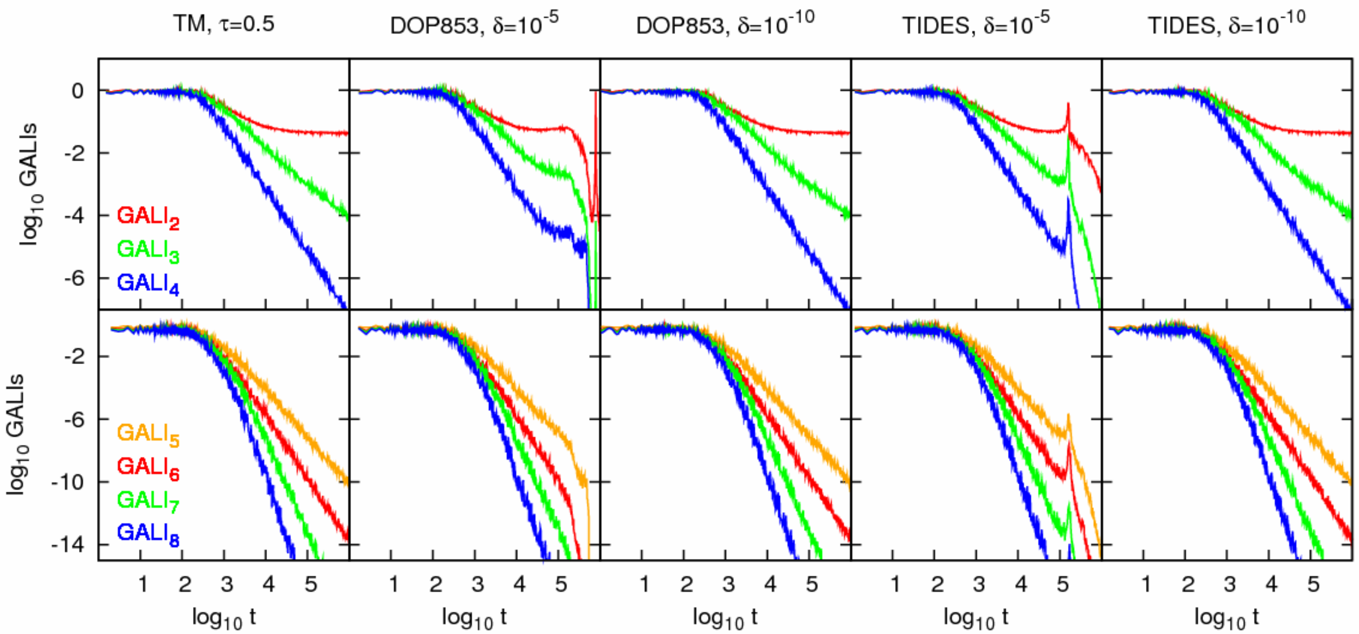
N particles Fermi-Pasta-Ulam (FPU) system:

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=0}^{N}\left[\frac{1}{2}(q_{i+1} - q_i)^2 + \frac{\beta}{4}(q_{i+1} - q_i)^4\right]$$

with fixed boundary conditions, β=1.5 and N=4 - 20.

N=4. Regular motion on 2d torus. Final time $t=10^6$.

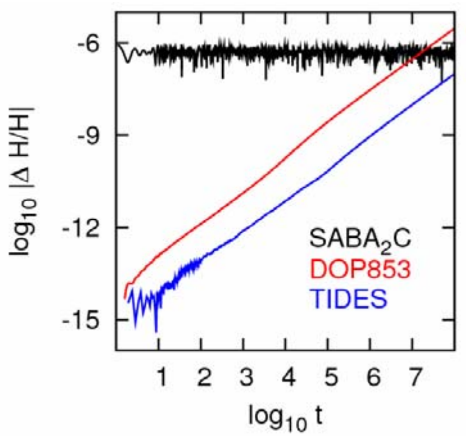
CPU times ≈ 9 s 54 s 1m 37s

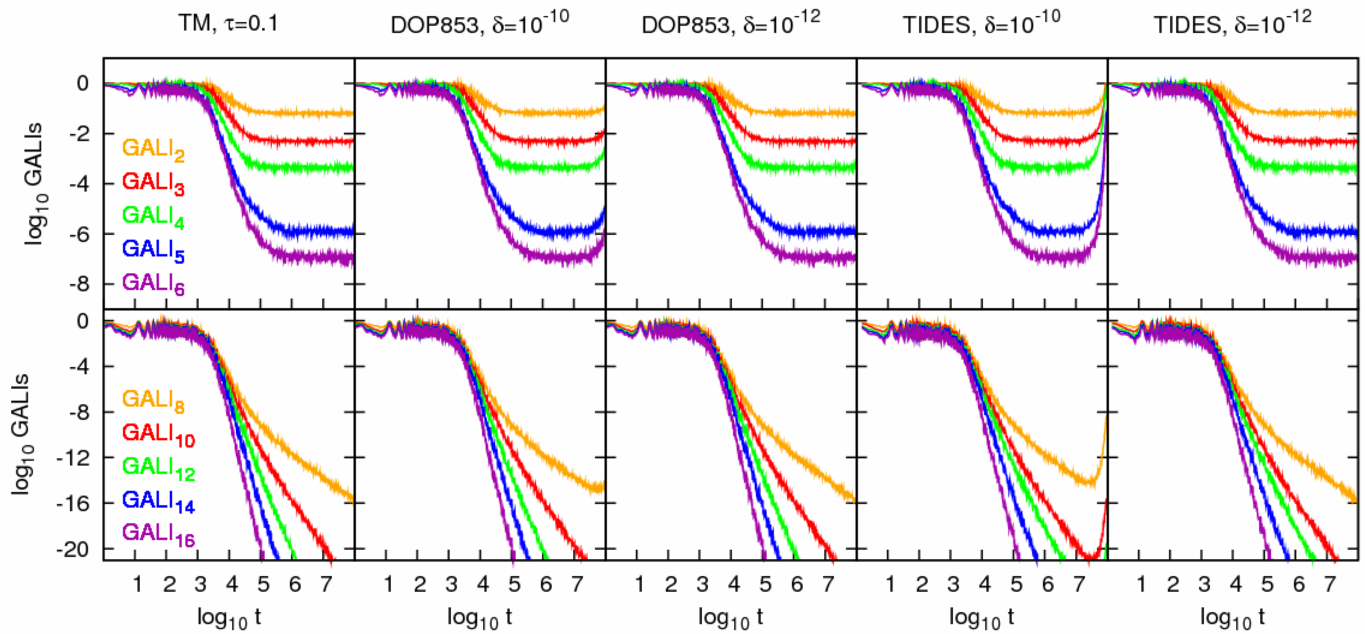


Application: FPU system

N=12. Regular motion on 6d torus. Final time t=10^8.

CPU times ≈ 8 h 22,5 h 38 h

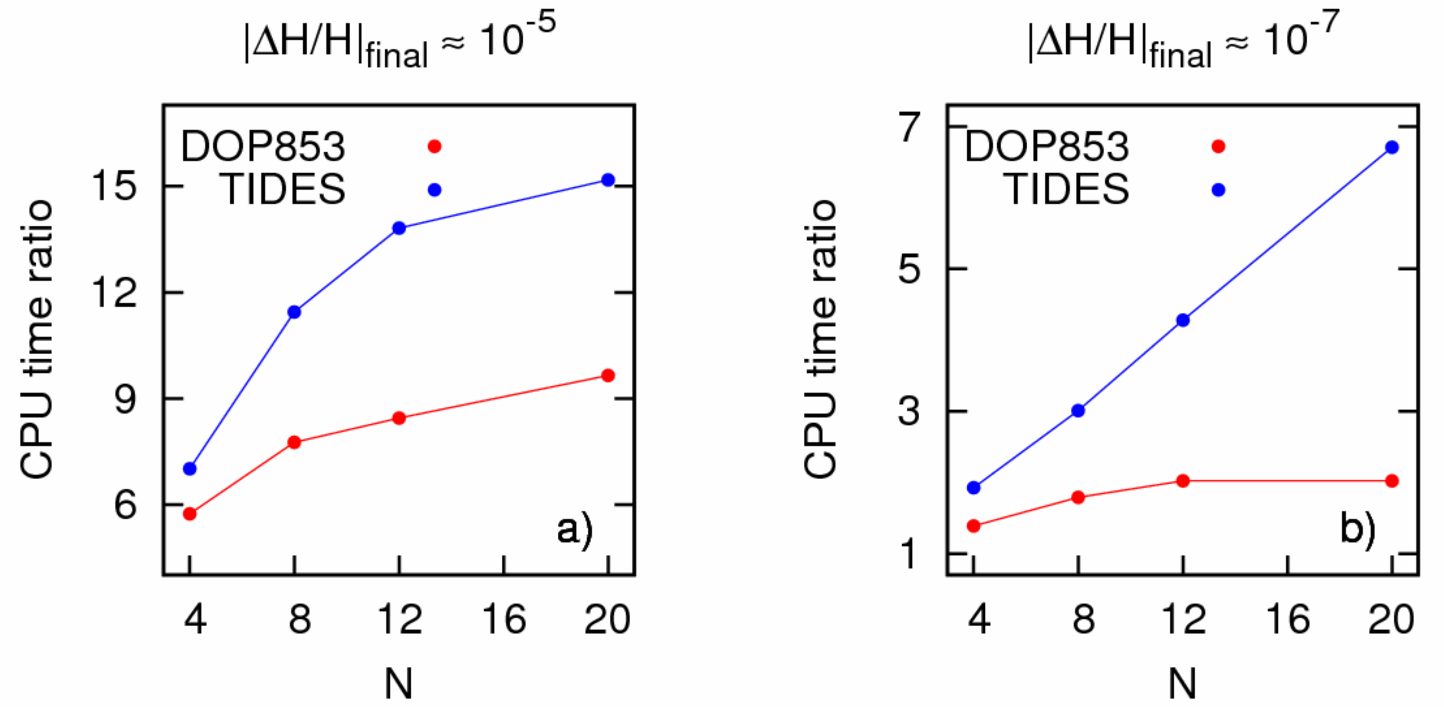




Application: FPU system

Efficiency of different algorithms

Final time $t=10^6$.



DOP853 $\delta=10^{-10}$ | **DOP853 $\delta=10^{-11}$**

TIDES $\delta=10^{-8}$ | **TIDES $\delta=10^{-10}$**

$SABA_2C$ $\tau=0.5$ | **$SABA_2C$ $\tau=0.1$**

Conclusions

Numerical schemes based on symplectic integrators can be used for the efficient integration of the variational equation of multidimensional Hamiltonian systems.

Papers:

- **Skokos Ch. and Gerlach E., 2010, PRE, 82, 036704**
- **Gerlach E. and Skokos Ch., 2011, arXiv:nlin.CD/1008.1890**
- **Gerlach E., Eggl S. and Skokos Ch., 2011, in preparation**