THE LIE-INTEGRATOR AND THE HÉNON-HEILES SYSTEM

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Abstract. There are several integration schemes intended to solve the equations of motion in problems of celestial mechanics. The Lie-integration method is based on the idea to tackle systems of ODE via Lie series. It is applied to solve Hamiltonian systems by giving recurrence formulae for the calculation of the Lie-terms. Here we present these recurrence formulae, which considerably simplify the linearized equations of motion. To exemplify, we choose the famous chaotic Hénon-Heiles system. Then the Lie-integrator is compared with the well-known Runge-Kutta method and the symplectic integrator for the Hénon-Heiles system. The convergence of the Lie-integrator can be regarded as a kind of a symplectic integrator, which conserves the integrals of motion. The Lie-integrator method is found to be very well suited for a long-time integration of orbits in celestial mechanics.

Key words: celestial mechanics – numerical methods – Lie series – Hénon-Heiles' model.

1. INTRODUCTION

The Lie-integration method is a fast integration method for systems of ODE, especially for the motion equations of celestial bodies (Asghari et al. 2004). The basic ideas of solving differential equations with Lie-series can be found in Gröbner's (1967) book. Recurrent formulae for the solution of the *n*-body problem have been derived by means of Lie-series (Hanslmeier and Dvorak 1984; Pârv 1993; Pál and Süli 2007). Via these formulae we have a rapid numerical integration procedure, used in celestial mechanics to solve systems of ODE (Dvorak et al. 2005). In this paper we derive the corresponding recurrence relations and we construct the *n*th order Lie-integrator for the equations of the Hénon-Heiles system.

The famous Hénon-Heiles dynamical system is the simplest Hamiltonian system which exhibits chaotic behaviour. Since this two-degrees-of-freedom system of ODE admits only one first integral (the energy integral), hence only one constant of motion, it is nonintegrable, therefore chaotic. The level of chaoticity varies with the energy level (Hénon and Heiles 1964; see also Abraham and Marsden 1978; Arnold 1978; Zhong and Marsden 1988; Marsden and Rațiu 1994).

Lots of authors dealt with the Hénon-Heiles model and with the associated problems, from the most various standpoints. As a very short digression, here we limit ourselves to quoting arbitrarily some contributions of the Romanian authors: Anisiu and Pál (1999); Mioc and Bărbosu (2003a, b); Mioc (2004); Pricopi et al. (2006); Mioc and Pricopi (2007); Mioc et al. (2008, 2009).

Resuming, in this paper the Lie-integrator is compared with the Runge-Kutta method and a symplectic integrator (Dormand and Prince 1978; Sanz-Serna and Calvo 1984; Channel and Scovel 1990; Forest and Ruth 1990; Forest et al. 1990; Kinoshita et al. 1990; Yoshida 1990, 1993; Feng and Meng-Zhao 1991; Mei-Ging and Meng-Zhao 1991; Wisdom and Holman 1991; Cartwright and Piro 1992; McLachlan and Atela 1992; Sanz-Serna 1998; Guzzo 2001; Laskar and Robutel 2001; Stuchi 2002; Butcher 2003; Csillik 2003).

Section 2 presents the Lie-integrator and details the corresponding algorithm of fourth order (LIE4).

In Section 3 we deal briefly with the Runge-Kutta method, as well as with symplectic integrators. The Runge-Kutta scheme of fourth order (RK4) is presented, followed by the symplectic integration scheme for the Lie-integrator (SI4).

In Section 4, the central section of the paper, we present the Hénon-Heiles system, then we derive the corresponding Lie operator. We write the approximate solution of the system in both terms of the Lie operator and in explicit form. To compare the effectiveness of the methods considered, we resort to numerical approaches.

Section 5 surveys the main results of our analysis. The advantages and shortcomings of the Lie-integrator are pointed out.

2. THE LIE-INTEGRATOR

Gröbner (1967) defined the Lie-operator D as follows:

$$D = \theta_1(z)\frac{\partial}{\partial z_1} + \theta_2(z)\frac{\partial}{\partial z_2} + \ldots + \theta_n(z)\frac{\partial}{\partial z_n}, \tag{1}$$

D being a linear differential operator. The point $z = (z_1, z_2, \ldots, z_n)$ lies in the n-dimensional z-space, the functions $\theta_i(z)$, $i = \overline{1,n}$ are holomorphic within a certain domain G (they can be expanded in a convergent power series).

Let the function $f(z)$ be holomorphic in the same region as $\theta_i(z)$, $i=\overline{1,n}$. Then D can be applied to $f(z)$, and if we proceed applying D to f we get

$$\begin{aligned}
&D^0 f = f\,,\\
&D^1 f = \theta_1(z)\frac{\partial f}{\partial z_1} + \theta_2(z)\frac{\partial f}{\partial z_2} + \ldots + \theta_n(z)\frac{\partial f}{\partial z_n}\,,\\
&D^2 f = D(Df)\,,\\
&\vdots\\
&D^n f = D(D^{n-1} f)\,.
\end{aligned} \tag{2}$$

The *Lie series* will be defined in the following way:

$$L(z,t) = \sum_{\upsilon=0}^{\infty}\frac{t^\upsilon}{\upsilon!}D^\upsilon f(z) = D^0 f(z) + tD^1 f(z) + \frac{t^2}{2!}D^2 f(z) + \ldots \tag{3}$$

Because we can write the Taylor-expansion of the exponential function as

$$\mathrm{e}^{tD} f = (D^0 + tD^1 + \frac{t^2}{2!}D^2 + \ldots) f\,, \tag{4}$$

$L(z,t)$ can be written in the symbolic form

$$L(z,t) = \mathrm{e}^{tD} f(z)\,. \tag{5}$$

One of the most useful properties of Lie-series is

THEOREM 1 (Exchange Theorem). *Let $F(z)$ be a holomorphic function in the neighborhood of $z=(z_1,z_2,\ldots,z_n)$, where the corresponding power series expansion converges at the point $Z=(Z_1,Z_2,\ldots,Z_n)$. Then we have:*

$$F(Z) = \sum_{\upsilon=0}^{\infty}\frac{t^\upsilon}{\upsilon!}D^\upsilon F(Z)\,, \tag{6}$$

or

$$F(\mathrm{e}^{tD})z = \mathrm{e}^{tD} F(z)\,. \tag{7}$$

Making use of it we can demonstrate how Lie-series solve differential equations. Let us consider the system of differential equations:

$$\frac{dz_i}{dt} = \theta_i(z), \quad i = \overline{1,n}, \tag{8}$$

with $z = (z_1, z_2, \ldots, z_n)$. The solution of (8) can be written as

$$z_i = e^{tD}\xi_i, \tag{9}$$

where the ξ_i are the initial conditions $z_i(t=0)$ and D is the Lie-operator as defined in formula (1). In order to prove (9), we differentiate it with respect to the time t:

$$\frac{dz_i}{dt} = De^{tD}\xi_i = e^{tD}D\xi_i. \tag{10}$$

Because of the fact that

$$D\xi_i = \theta_i(\xi_i), \tag{11}$$

we obtain the following result, which turns out to be the original ODE (8):

$$\frac{dz_i}{dt} = e^{tD}\theta_i(\xi_i) = \theta_i(e^{tD}\xi_i) = \theta_i(z_i). \tag{12}$$

Now we present the fourth order Lie-integrator (LIE4) for a $H(x, y, \dot{x}, \dot{y})$ Hamiltonian.

The system of differential equations is written as:

$$\begin{cases} \dot{x} = \dfrac{dx}{dt} = \theta_1(x, y, u, v), \\ \dot{y} = \dfrac{dy}{dt} = \theta_2(x, y, u, v), \\ \dot{u} = \dfrac{d\dot{x}}{dt} = \theta_3(x, y, u, v), \\ \dot{v} = \dfrac{d\dot{y}}{dt} = \theta_4(x, y, u, v), \end{cases} \tag{13}$$

(where $u = \dot{x}$, $v = \dot{y}$) with the initial conditions at time $t = 0$:

$$\begin{aligned} x(0) = \xi,\ \ y(0) = \eta, \\ u(0) = \varphi,\ \ v(0) = \psi. \end{aligned} \tag{14}$$

The corresponding Lie-operator is

$$D = \theta_1 \frac{\partial}{\partial \xi} + \theta_2 \frac{\partial}{\partial \eta} + \theta_3 \frac{\partial}{\partial \varphi} + \theta_4 \frac{\partial}{\partial \psi}. \tag{15}$$

For a time $(t + \Delta t)$, we obtain the solution under the following form (up to the fourth order):

$$x(t+\Delta t) = D^0(\xi) + \Delta\tau D^1(\xi) + \frac{\Delta\tau^2}{2!} D^2(\xi) + \frac{\Delta\tau^3}{3!} D^3(\xi) + \frac{\Delta\tau^4}{4!} D^4(\xi), \tag{16}$$

$$y(t+\Delta t) = D^0(\eta) + \Delta\tau D^1(\eta) + \frac{\Delta\tau^2}{2!} D^2(\eta) + \frac{\Delta\tau^3}{3!} D^3(\eta) + \frac{\Delta\tau^4}{4!} D^4(\eta), \tag{17}$$

$$u(t+\Delta t) = D^0(\varphi) + \Delta\tau D^1(\varphi) + \frac{\Delta\tau^2}{2!} D^2(\varphi) + \frac{\Delta\tau^3}{3!} D^3(\varphi) + \frac{\Delta\tau^4}{4!} D^4(\varphi), \tag{18}$$

$$v(t+\Delta t) = D^0(\psi) + \Delta\tau D^1(\psi) + \frac{\Delta\tau^2}{2!} D^2(\psi) + \frac{\Delta\tau^3}{3!} D^3(\psi) + \frac{\Delta\tau^4}{4!} D^4(\psi), \tag{19}$$

where

$$\begin{aligned} &D^0(\xi) = \xi, \quad D^1(\xi) = \theta_1, \\ &D^2(\xi) = D^1(D^1(\xi)) = D^1(\theta_1) \\ &D^3(\xi) = D^1(D^2(\xi)), \\ &D^4(\xi) = D^1(D^3(\xi)); \end{aligned} \tag{20}$$

$$\begin{aligned} &D^0(\eta) = \eta, \quad D^1(\eta) = \theta_2, \\ &D^2(\eta) = D^1(D^1(\eta)) = D^1(\theta_2), \\ &D^3(\eta) = D^1(D^2(\eta)), \\ &D^4(\eta) = D^1(D^3(\eta)); \end{aligned} \tag{21}$$

$$\begin{aligned} &D^0(\varphi) = \varphi, \quad D^1(\varphi) = \theta_3, \\ &D^2(\varphi) = D^1(D^1(\varphi)) = D^1(\theta_3) = D^3(\xi), \\ &D^3(\varphi) = D^1(D^2(\varphi)) = D^4(\xi), \\ &D^4(\varphi) = D^1(D^3(\varphi)) = D^5(\xi); \end{aligned} \tag{22}$$

$$
\begin{aligned}
&D^0(\psi)=\psi\,, \quad D^1(\psi)=\theta_4\,,\\
&D^2(\psi)=D^1(D^1(\psi))=D^1(\theta_4)=D^3(\eta)\,,\\
&D^3(\psi)=D^1(D^2(\psi))=D^4(\eta)\,,\\
&D^4(\psi)=D^1(D^3(\psi))=D^5(\eta)\,.
\end{aligned} \tag{23}
$$

3. RUNGE-KUTTA AND SYMPLECTIC INTEGRATORS

In numerical analysis, the Runge-Kutta methods constitute an important family of implicit and explicit iterative methods for the approximation of solutions of ordinary differential equations (Butcher 2003). One member of the family of Runge-Kutta methods is so commonly used that it is often referred to as RK4.

The family of explicit Runge-Kutta methods is given by

$$y_{i+1}=y_i+h(b_1k_1+\ldots+b_sk_s)\,, \tag{24}$$

where

$$k_1=f(t_i,y_i)\,, \tag{25}$$

$$k_2=f(t_i+c_2h,y_i+ha_{21}k_1)\,, \tag{26}$$

$$k_3=f(t_i+c_3h,y_i+h(a_{31}k_1+a_{32}k_2))\,, \tag{27}$$

$$\ldots$$

$$k_s=f(t_i+c_sh,y_i+h(a_{s1}k_1+\ldots+a_{s,s-1}k_s)) \tag{28}$$

and s is an integer number (stage number); $a_{21},a_{31},\ldots,a_{s1},\ldots,a_{s,s-1}$, $b_1,\ldots,b_s$, $c_1,\ldots,c_s$ are coefficients. In general, the coefficients $c_1,\ldots,c_s$, which characterize the partition of the step *h*, satisfy the following condition:

$$
\begin{aligned}
&c_2=a_{21}\,,\\
&c_3=a_{31}+a_{32}\,,\\
&\quad\ldots\\
&c_s=a_{s1}+\ldots+a_{s,s-1}\,.
\end{aligned} \tag{29}
$$

They are determined by the condition that the approximate solution x_{i+1} is equal to the exact solution corresponding to the first s terms of the Taylor series. The Runge-Kutta method is *consistent* if the following relations are satisfied:

$$\sum_{j=1}^{i-1} a_{ij} = c_i, \quad i = \overline{2,s}; \qquad (30)$$
$$\sum_{j=1}^{s} b_j = 1$$

The Runge-Kutta method of fourth order (RK4) is a numerical technique used to solve ordinary differential equation of the form

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y), \qquad (31)$$
$$y(0) = y_0 .$$

The RK4 method is based on the following algorithm:

$$y_{i+1} = y_i + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4), \qquad (32)$$
$$t_{i+1} = t_i + h, \qquad i = \overline{0,n},$$

where y_{i+1} is the RK4 approximation of $y(t_{i+1})$, and

$$k_1 = f(t_i, y_i), \qquad (33)$$

$$k_2 = f\left(t_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right), \qquad (34)$$

$$k_3 = f\left(t_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right), \qquad (35)$$

$$k_4 = f(t_i + h, y_i + k_3 h). \qquad (36)$$

The *fourth order* of the RK4 method means that the error per step is of order h^5, while the total accumulated error is of order h^4.

As regards the *symplectic integrators*, it is very well known that they have the following properties (e.g., Yoshida 1990): area preserving, time reversibility, and constant step-size (this guarantees that there is no secular change in the error of the total energy).

It is known that for Hamiltonian systems of the form

$$H = T(\mathbf{p}) + V(\mathbf{q}) \qquad (37)$$

explicit symplectic schemes exist. In this formula the $\mathbf{q}$ variables are generalized coordinates, the $\mathbf{p}$ variables are conjugate generalized momenta, whereas the Hamiltonian H corresponds to the total mechanical energy (T and V stand for the kinetic energy and potential energy of the system, respectively).

Here we dwell on Neri's (1987) explicit symplectic integrator in terms of Lie algebraic language. To do this, we begin by writing the Hamiltonian equations in the following form (using Poisson bracket):

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \{\mathbf{z}, H(\mathbf{z})\} = \frac{\partial \mathbf{z}}{\partial \mathbf{q}}\frac{\partial H}{\partial \mathbf{p}} - \frac{\partial \mathbf{z}}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{q}} . \tag{38}$$

Introducing the differential operator $D_H(\mathbf{z}) = \{\mathbf{z}, H\}$, (38) can be written as

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = D_H(\mathbf{z}) . \tag{39}$$

Therefore, the exact time-evolution of the solution of equation (39), $\mathbf{z}(t)$, from $t = 0$ to $t = \tau$, is given by

$$\mathbf{z}(\tau) = \exp[\tau D_H]\,\mathbf{z}(0) . \tag{40}$$

For the Hamiltonian of the form (37), where $D_H = D_T + D_V$, we have the formal solution

$$\mathbf{z}(\tau) = \exp[\tau(A + B)]\mathbf{z}(0) , \tag{41}$$

where $A := D_T$ and $B := D_V$ are two operators which do not commute. Further, we suppose that the set of the real numbers (c_i, d_i), $i = \overline{1,n}$, satisfies the equality

$$\exp[\tau(A + B)] = \prod_{i=1}^{n} \exp(c_i \tau A)\exp(d_i \tau B) + O(\tau^{n+1}) , \tag{42}$$

where n is the integrator's order. Let a mapping from $\mathbf{z} = \mathbf{z}(0)$ to $\mathbf{z}' = \mathbf{z}(\tau)$ be given by

$$\mathbf{z}' = \left[\prod_{i=1}^{n} \exp(c_i \tau A)\exp(d_i \tau B)\right]\mathbf{z} . \tag{43}$$

The above application is symplectic because it is a product of elementary symplectic mappings. We can write the explicit equation (43) in the following form:

$$\begin{cases} q_i = q_{i-1} + \tau c_i \left(\dfrac{\partial T}{\partial \mathbf{p}} \right)_{\mathbf{p}=p_{i-1}} \\ p_i = p_{i-1} + \tau d_i \left(\dfrac{\partial V}{\partial \mathbf{q}} \right)_{\mathbf{q}=q_i} \end{cases}, \quad i = \overline{1,n}, \tag{44}$$

where $\mathbf{z} = (q_0, p_0)$ and $\mathbf{z}' = (q_n, p_n)$. This system of equations is an nth order symplectic integration scheme. The numerical coefficients (c_i, d_i), $i = \overline{1,n}$, are not uniquely determined from the requirement that the local truncation error is of order τ^n. If one requires the time reversibility of the numerical solution, one can determine it uniquely.

In this context, the fourth order Lie-integrator schema is given by the system of equations (44) for $i = \overline{1,4}$, where the values of the coefficients (c_i, d_i), $i = \overline{1,4}$, are:

$$\begin{aligned} c_1 &= c_4 = \frac{1}{2(2-\sqrt[3]{2})}, \\ c_2 &= c_3 = \frac{1-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}, \\ d_1 &= d_3 = \frac{1}{2-\sqrt[3]{2}}, \\ d_2 &= -\frac{\sqrt[3]{2}}{2-\sqrt[3]{2}}, \qquad d_4 = 0. \end{aligned} \tag{45}$$

4. HÉNON-HEILES SYSTEM AND APPLICATION

In 1964, Michel Hénon and Carl Heiles modelled the motion of a star within a galaxy, representing the gravitational attraction of the galaxy by a potential having cylindrical symmetry (Hénon and Heiles 1964). The chosen potential energy is given by that of a planar oscillator to which two cubic terms were added:

$$V(x,y) = \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3} y^3. \tag{46}$$

Those terms made the problem nonlinear and nonintegrable. This two-dimensional system has only one constant of motion, hence nonintegrable, in fact chaotic. Hénon and Heiles found that, for very low values of the total energy

($E=1/12$), the system is very close to being integrable, since the majority of intersection points are placed along the curves corresponding to the intersections with the tori. By increasing the energy, the regular curves progressively disappear, through a phase where they are reduced to tiny isolated zones persists. For $E=1/6$ the whole area is filled by points generated by a single trajectory. So, at low energies, the system is practically integrable. Numerical methods could then provide much help in guessing if a system is very close to the condition of integrability or not. In the Hénon-Heiles problem, the system, as the energy grows, becomes a chaotic system, the intersections of the trajectories with the surface of section thickly fill the area determined by energy conservation. The exponential divergence of the trajectories is determined by the initial conditions according to the equations of the system. This fact does not help in predicting the system's behaviour, because in practical cases one has to deal with experimental errors.

We introduce the Hénon-Heiles Hamiltonian in the most general form:

$$H=\frac{1}{2}(u^2+v^2+Ax^2+By^2)+Dx^2y-\frac{1}{3}Cy^3. \tag{47}$$

The corresponding equations of motion are

$$\begin{cases} \dot{x}=u, \\ \dot{y}=v, \\ \dot{u}=-Ax-2Dxy, \\ \dot{v}=-By-Dx^2+Cy^2. \end{cases} \tag{48}$$

For the values $A=B=C=D=1$ of the coefficients, we obtain the nonintegrable Hénon-Heiles Hamiltonian:

$$H(x,y,u,v)=\frac{1}{2}(u^2+v^2+x^2+y^2)+x^2y-\frac{1}{3}y^3. \tag{49}$$

The equations of motion for the coordinates and momenta of the Hénon-Heiles system are given by:

$$\begin{cases} \dot{x}=\dfrac{\mathrm{d}x}{\mathrm{d}t}=\dfrac{\partial H}{\partial u}=u, \\ \dot{y}=\dfrac{\mathrm{d}y}{\mathrm{d}t}=\dfrac{\partial H}{\partial v}=v, \\ \dot{u}=\dfrac{\mathrm{d}u}{\mathrm{d}t}=-\dfrac{\partial H}{\partial x}=-x-2xy, \\ \dot{v}=\dfrac{\mathrm{d}v}{\mathrm{d}t}=-\dfrac{\partial H}{\partial y}=-y-x^2+y^2. \end{cases} \tag{50}$$

The initial conditions for a time τ are denoted as follows:

$$x(\tau)=\xi,\ y(\tau)=\eta,\ u(\tau)=\varphi,\ v(\tau)=\psi. \tag{51}$$

To derive the corresponding Lie operator, we use the following system of equations:

$$\dot{\xi}=\varphi=\theta_1\,,\quad \dot{\eta}=\psi=\theta_2\,,\quad \dot{\varphi}=-\xi-2\xi\eta=\theta_3\,,\quad \dot{\psi}=\eta-\xi^2+\eta^2=\theta_4\,, \tag{52}$$

and the Lie operator is:

$$D=\theta_1\frac{\partial}{\partial\xi}+\theta_2\frac{\partial}{\partial\eta}+\theta_3\frac{\partial}{\partial\varphi}+\theta_4\frac{\partial}{\partial\psi}\,, \tag{53}$$

which, substituting (52), can be written as:

$$D=\varphi\frac{\partial}{\partial\xi}+\psi\frac{\partial}{\partial\eta}+(-\xi-2\xi\eta)\frac{\partial}{\partial\varphi}+(\eta-\xi^2+\eta^2)\frac{\partial}{\partial\psi}\,. \tag{54}$$

So, for a time $(\tau+\Delta\tau)$ the solution is:

$$\begin{aligned} &x(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\xi}\ ,\ y(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\eta}\ ,\\ &u(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\varphi}\ ,\ v(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\psi}\ . \end{aligned} \tag{55}$$

We can write the solution in the following form:

$$x(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\xi}=\xi+\Delta\tau D^1(\xi)+\frac{\Delta\tau^2}{2!}D^2(\xi)+\ldots+\frac{\Delta\tau^{n-1}}{(n-1)!}D^{n-1}(\xi)+O(n)\ , \tag{56}$$

$$y(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\eta}=\eta+\Delta\tau D^1(\eta)+\frac{\Delta\tau^2}{2!}D^2(\eta)+\ldots+\frac{\Delta\tau^{n-1}}{(n-1)!}D^{n-1}(\eta)+O(n)\ , \tag{57}$$

$$u(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\varphi}=\varphi+\Delta\tau D^1(\varphi)+\frac{\Delta\tau^2}{2!}D^2(\varphi)+\ldots+\frac{\Delta\tau^{n-1}}{(n-1)!}D^{n-1}(\varphi)+O(n)\ , \tag{58}$$

$$v(\tau+\Delta\tau)=\mathrm{e}^{\Delta\tau D_\psi}=\psi+\Delta\tau D^1(\psi)+\frac{\Delta\tau^2}{2!}D^2(\psi)+\ldots+\frac{\Delta\tau^{n-1}}{(n-1)!}D^{n-1}(\psi)+O(n)\ , \tag{59}$$

where the expressions of $D^i(\xi)$, $i=\overline{1,n}$, are:

$$\begin{aligned} &D^1(\xi)=\varphi,\quad D^2(\xi)=D^1(\varphi),\\ &D^3(\xi)=-D^1(\xi)-2D^1(\xi\eta),\\ &\ldots \end{aligned} \tag{60}$$

whereas the expressions of $D^i(\eta)$, $i=\overline{1,n}$, are:

$$D^1(\eta)=\psi,\quad D^2(\eta)=D^1(\psi),$$
$$D^3(\eta)=-D^1(\eta)-D^1(\xi^2)+D^1(\eta^2), \tag{61}$$
$$\ldots$$

We explicitly write for $i=\overline{0,n}$:

$$\begin{aligned}
&D^0(\xi)=\xi,\quad D^1(\xi)=\varphi,\quad D^2(\xi)=-\xi-2\xi\eta,\\
&D^3(\xi)=-\varphi-2(\xi\psi+\eta\varphi),\quad D^4(\xi)=\xi+6\xi\eta-4\varphi\psi+2\xi(\xi^2+\eta^2),\\
&D^5(\xi)=\varphi+10(\xi\psi+\eta\varphi)+2\varphi(5\xi^2-\eta^2)+12\xi\eta\psi,\\
&D^6(\xi)=-\xi-22\xi\eta+20\varphi\psi-20\xi(\xi^2+\eta^2)-\\
&\qquad -16\xi\eta(2\xi^2-\eta^2)+4\xi(5\varphi^2+3\psi^2)+8\eta\varphi\psi,\\
&D^7(\xi)=-\varphi-42(\xi\psi+\eta\varphi)-8\varphi(15\xi^2+\eta^2)-56\xi\psi(\xi^2-\eta^2)-\\
&\qquad -8\eta\varphi(23\xi^2-3\eta^2)+20\varphi(\varphi^2+\psi^2)-114\xi\eta\psi,\\
&\ldots\\
&D^n(\xi)=-D^{n-2}(\xi)-2\sum_{k=0}^{n-2}C_{n-2}^k D^k(\xi)D^{n-2-k}(\eta),
\end{aligned} \tag{62}$$

and

$$\begin{aligned}
&D^0(\eta)=\eta,\quad D^1(\eta)=\psi,\quad D^2(\eta)=-\eta-\xi^2+\eta^2,\\
&D^3(\eta)=-\psi-2(\xi\varphi-\eta\psi),\\
&D^4(\eta)=\eta+3(\xi^2-\eta^2)+2\eta(\xi^2+\eta^2)-2(\varphi^2-\psi^2),\\
&D^5(\eta)=\psi+10(\xi\varphi-\eta\psi)-2\psi(\xi^2-5\eta^2)+12\xi\eta\varphi,\\
&D^6(\eta)=-\eta-11(\xi^2-\eta^2)-20\eta(\xi^2+\eta^2)+10(\varphi^2-\psi^2)+\\
&\qquad +4\eta(3\varphi^2+5\psi^2)+2\xi^4+10\eta^4-36\xi^2\eta^2+8\xi\varphi\psi,\\
&D^7(\eta)=-\psi-42(\xi\varphi-\eta\psi)-8\eta(\xi^2+15\eta^2)+20\psi(\varphi^2+\psi^2)-\\
&\qquad -16\eta\psi(8\xi^2-5\eta^2)-112\xi\eta\varphi-122\xi\eta^2\varphi,\\
&\ldots\\
&D^n(\eta)=-D^{n-2}(\eta)-\sum_{k=0}^{n-2}C_{n-2}^k\left(D^k(\xi)D^{n-2-k}(\xi)-D^k(\eta)D^{n-2-k}(\eta)\right),
\end{aligned} \tag{63}$$

The expressions for $D^i(\varphi)$ and $D^i(\psi)$, where $i=\overline{1,n}$, can be obtained easily:

$$D^i(\varphi)=D^{i+1}(\xi),$$
$$D^i(\psi)=D^{i+1}(\eta). \tag{64}$$

Now the equations of motion of the Hénon-Heiles system can be integrated numerically with the Lie-integrator method (up to order *n*; see Pál and Süli 2007).

LIE4: Using (62)–(64), the numerical solutions (56)–(59) of the Hénon-Heiles system (50) with the initial conditions (51) are:

$$x(\tau+\Delta\tau)=\xi+\varphi\Delta\tau-(\xi+2\xi\eta)\frac{\Delta\tau^2}{2}-(\varphi+2(\xi\psi+\eta\varphi))\frac{\Delta\tau^3}{6}+$$
$$+(\xi+6\xi\eta-4\varphi\psi+2\xi(\xi^2+\eta^2))\frac{\Delta\tau^4}{24},$$

$$y(\tau+\Delta\tau)=\eta+\psi\Delta\tau+(-\eta-\xi^2+\eta^2)\frac{\Delta\tau^2}{2}-(\psi+2(\xi\varphi-\eta\psi))\frac{\Delta\tau^3}{6}+$$
$$+(\eta+3(\xi^2-\eta^2)+2\eta(\xi^2+\eta^2)-2(\varphi^2-\psi^2))\frac{\Delta\tau^4}{24},$$

$$u(\tau+\Delta\tau)=\varphi-(\xi+2\xi\eta)\Delta\tau-(\varphi+2(\xi\psi+\eta\varphi))\frac{\Delta\tau^2}{2}+(\xi+6\xi\eta-4\varphi\psi+$$
$$+2\xi(\xi^2+\eta^2))\frac{\Delta\tau^3}{6}+(\varphi+10(\xi\psi+\eta\varphi)+2\varphi(5\xi^2-\eta^2)+12\xi\eta\psi)\frac{\Delta\tau^4}{24},$$

$$v(\tau+\Delta\tau)=\psi+(-\eta-\xi^2+\eta^2)\Delta\tau-(\psi+2(\xi\varphi-\eta\psi))\frac{\Delta\tau^2}{2}+(\eta+3(\xi^2-\eta^2)+$$
$$+2\eta(\xi^2+\eta^2)-2(\varphi^2-\psi^2))\frac{\Delta\tau^3}{6}+(\psi+10(\xi\varphi-\eta\psi)-2\psi(\xi^2-5\eta^2)+12\xi\eta\varphi)\frac{\Delta\tau^4}{24}. \tag{65}$$

RK4: The numerical solutions of the Hénon-Heiles system (50), with the notation $x=y^{(1)}$, $y=y^{(2)}$, $\dot{x}=y^{(3)}$, $\dot{y}=y^{(4)}$ and initial conditions $y_0^{(j)}$, $j=\overline{1,4}$, are:

$$y_{i+1}^{(j)} = y_i^{(j)} + \frac{1}{6}h(k_1^{(j)} + 2k_2^{(j)} + 2k_3^{(j)} + k_4^{(j)}), \quad j = \overline{1,4}, \; i = \overline{0,n},$$
$$t_{i+1} = t_i + h, \tag{66}$$

where

$$k_1^{(j)} = f(t_i, y_i^{(j)}), \tag{67}$$

$$k_2^{(j)} = f\left(t_i + \frac{1}{2}h, y_i^{(j)} + \frac{1}{2}k_1^{(j)}h \right), \tag{68}$$

$$k_3^{(j)} = f\left(t_i + \frac{1}{2}h, y_i^{(j)} + \frac{1}{2}k_2^{(j)}h \right), \tag{69}$$

$$k_4^{(j)} = f(t_i + h, y_i^{(j)} + k_3^{(j)}h). \tag{70}$$

SI4 (Csillik 2004): Using the system of equations (50)–(51) (notation: $x = q_1$, $y = q_2$, $\dot{x} = p_1$, $\dot{y} = p_2$), equations (44) for the Hénon-Heiles system are:

$$\begin{aligned}
q_1^j &= q_1^{j-1} + \tau c_j p_1^{j-1}, \\
q_2^j &= q_2^{j-1} + \tau c_j p_2^{j-1}, \\
p_1^j &= q_1^{j-1} - \tau d_j (q_1^j + 2q_1^j q_2^j), \\
p_2^j &= q_2^{j-1} - \tau d_j (q_2^j + (q_1^j)^2 - (q_2^j)^2),
\end{aligned} \qquad j = \overline{1,4}, \tag{71}$$

where the values of the coefficients (c_j, d_j) are given by (45).

A surface of section (SOS), also called a Poincaré section (see, e.g., Rasband 1990), is a way of presenting a trajectory in an n-dimensional phase space in an (n–1)-dimensional space. By picking one phase element constant (in our Hénon-Heiles system case: $x = 0$) and plotting the values of the other elements, each time the chosen element has the desired value, an intersection surface is obtained. The surfaces of section for the Hénon-Heiles equation (49) with energy $E = 1/8$, plotting $y(t)$ versus $\dot{y}(t)$ at values where $x(t) = 0$, are presented in Fig. 1 (using RK4 integrator), in Fig. 2 (using SI4 integrator), and in Fig. 3 (using LIE4 integrator). All three integrators are made with MATLAB and MAPLE (Baker 1981; Lynch 2000; Moler 2004).

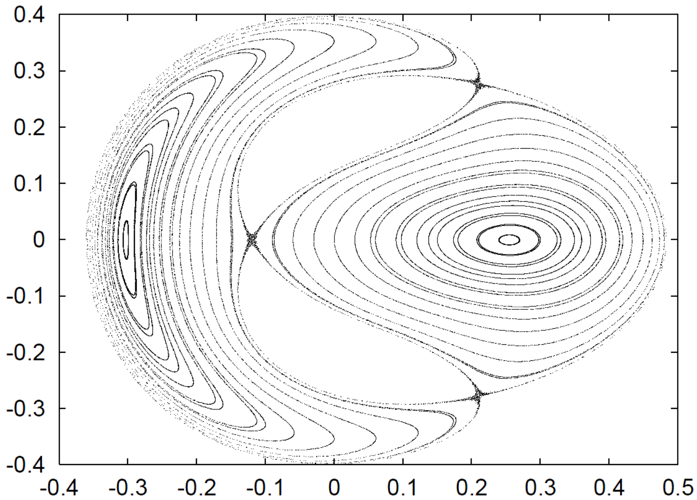

Fig. 1 – Poincaré section of the Hénon-Heiles equation (49) using RK4 integrator.

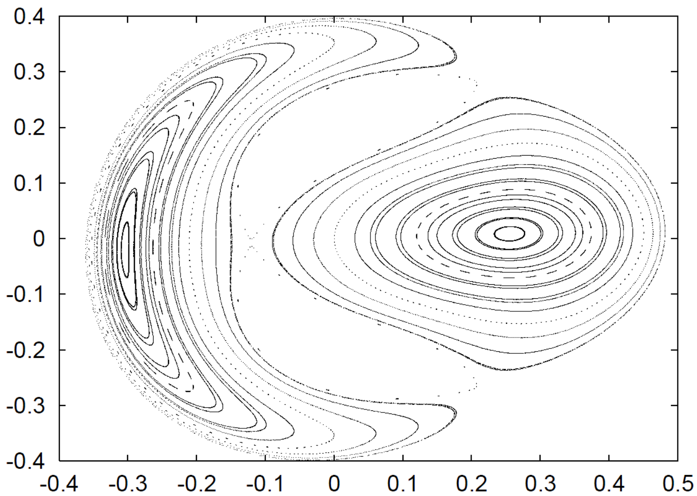

Fig. 2 – Poincaré section of the Hénon-Heiles equation (49) using SI4 integrator.

A Poincaré map can be interpreted as a discrete dynamical system with a state space of codimension 1 with respect to the original continuous dynamical system. Because it preserves many properties of periodic and quasiperiodic orbits of the original system and has a lower dimensional state space it is often used for analyzing the original system. In practice this is not always possible as there is no general method to construct a Poincaré map. The Hénon-Heiles system was used to study the motion of stars in a galaxy, because the path of a star projected onto a plane looks like a tangled mess and the Poincaré map shows the structure more clearly. Comparing Figs. 1, 2 and 3, one can see that Fig. 3 with LIE4 integrator has more details.

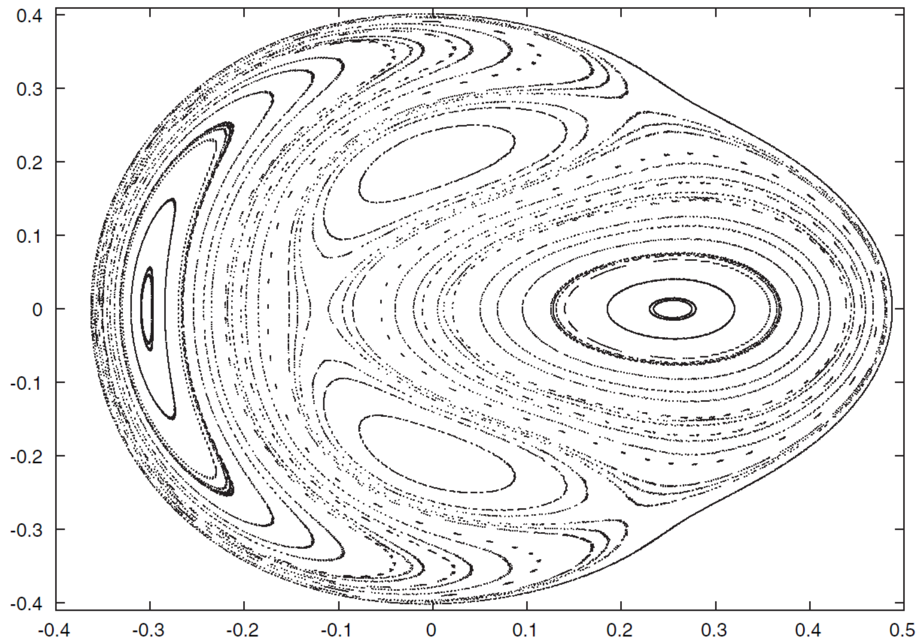

Fig. 3 – Poincaré section of the Hénon-Heiles equation (49) using LIE4 integrator.

5. CONCLUSIONS

The Lie-integrator method appears to be very effective as compared with other numerical integrators of differential equations. The solution written in the power series expansions of the independent variable τ can be slightly different for every step. The Lie-integrator method (LIE4) is quite precise and fast, as has been shown in our comparative test computations with the Runge-Kutta (RK4) and symplectic integrators (SI4). Symplectic integrators are very effective when eccentricities are small; the Lie-integrator is a better choice in studies such as this one, where very large eccentricity orbits are explored (Pál and Süli 2007). The convergence of the Lie-integrator can be regarded as a kind of a symplectic integrator, which conserves the integrals of motion. The desired accuracy can be fixed and controlled by two different parameters: the time step and the number of Lie-terms. The only disadvantage is that the derivation of recurrence in the Lie-terms may nevertheless lead to very lengthy expressions when the right-hand sides are complicated and lengthy themselves (Dvorak et al. 2005). The Lie integrator is straightforward and comprehensible in its construction; it allows an easy handling. So, the method is very well suited for the calculation of orbits in celestial mechanics. Many practical differential equations evolve on a Lie group; it preserves the geometry of the configuration space.

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