Solving linearized equations of the $N$-body problem using the Lie-integration method

András Pál* and Áron Süli*

Department of Astronomy, Loránd Eötvös University, Pázmány Péter sétány 1/A, Budapest H-1117, Hungary

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ABSTRACT

Several integration schemes exist to solve the equations of motion of the $N$-body problem. The Lie-integration method is based on the idea to solve ordinary differential equations with Lie-series. In the 1980s, this method was applied to solve the equations of motion of the $N$-body problem by giving the recurrence formulae for the calculation of the Lie-terms. The aim of this work is to present the recurrence formulae for the linearized equations of motion of $N$-body systems. We prove a lemma which greatly simplifies the derivation of the recurrence formulae for the linearized equations if the recurrence formulae for the equations of motions are known. The Lie-integrator is compared with other well-known methods. The optimal step-size and order of the Lie-integrator are calculated. It is shown that a fine-tuned Lie-integrator can be 30–40 per cent faster than other integration methods.

Key words: methods: $N$-body simulations – methods: numerical – celestial mechanics.

1 INTRODUCTION

The classical problems of celestial mechanics are described by a system of ordinary differential equations (ODEs). The investigation of the motions in the Solar system, exoplanetary systems, satellites around the Earth or other celestial objects is based on the solutions of such ODEs. However, several modern analyses, including many chaos-detection methods, require to solve the linearized equations of the problem.

The integration method based on the Lie-series (Gröbner & Knapp 1967) is widely used in celestial mechanics to solve ODEs (see Hanslmeier & Dvorak 1984, hereafter H&D and papers referring to it). The basis of this method is to generate the coefficients of the Taylor expansion of the solution by using recurrence relations. The principal application, that is, the integration of the $N$-body problem is described in details in H&D.

1.1 Lie-integration

Here, we summarize the key points of this method of numerical integration, using almost identical notations to those used by H&D.

Let us write the differential equation to be solved as

$$\dot{x} = f(x),$$

where $x \equiv (x_1, \ldots, x_N)$ is an $\mathbb{R} \rightarrow \mathbb{R}^N$ and $f \equiv (f_1, \ldots, f_N)$ is an $\mathbb{R}^N \rightarrow \mathbb{R}^N$ continuous function and $N$ is the dimension of the vector $x$ and the vector space where $f$ maps from and maps to. Let us introduce the differential operator

$$D_i := \frac{\partial}{\partial x_i},$$

(2)

and the derivation

$$L_0 := \sum_{i=1}^{N} f_i \frac{\partial}{\partial x_i},$$

(3)

which is known as the Lie-derivation or Lie-operator. $L_0$ is a linear differential operator and one can apply Leibniz’s rule,

$$L_0(ab) = aL_0(b) + bL_0(a),$$

(4)

where $a$ and $b$ are $\mathbb{R}^N \rightarrow \mathbb{R}^N$ differentiable functions. It can easily be proven that the solution of equation (1) at a given instance $t + \Delta t$ is formally

$$x(t + \Delta t) = \exp(\Delta t L_0) x(t),$$

(5)

where

$$\exp(\Delta t L_0) = \sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} L_0^k = \sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} \left( \sum_{i=1}^{N} f_i D_i \right)^k.$$  

(6)

The method of Lie-integration is finite approximation of the sum in the right-hand side of equation (6), up to the order of $M$, namely

$$x(t + \Delta t) \approx \left( \sum_{k=0}^{M} \frac{\Delta t^k}{k!} L_0^k \right) x(t) = \sum_{k=0}^{M} \frac{\Delta t^k}{k!} (L_0^k x(t)).$$

(7)

The proof of equation (5) and other related properties of the Lie-derivation can be found in Gröbner & Knapp (1967) or H&D.
In spite of the fact that the Lie-derivatives can be analytically calculated up to an arbitrary order, the formulae yielded by these expansions are highly complicated even if all kinds of new variables are introduced (see e.g. equations 19d and 19e in H&D at page 204). A definitely more efficient way to evaluate the Lie-derivatives is to find a set of recurrence relations. These relations allow us to express the \((n+1)\)th Lie-derivative, for example, \(L^{n+1}x\) as the function of the derivatives with a lower order, namely \(L^jx\) where \(0 \leq j \leq n\). The initialization of such a recurrence relation is evident, because \(L^0x \equiv x\). We note that in several applications, well-chosen auxiliary variables have to be introduced to gain a compact set of recurrence relations which can efficiently be evaluated.

1.2 The importance of linearized equations

A wide range of problems related to celestial mechanics require to solve simultaneously the linearized form of the original equations too. The numerous experiments conducted in the last decades show that chaotic behaviour is typical and already occurs in simple but non-linear systems. This finding throws completely new light on these systems and the study of the chaotic behaviour becomes of high concern. A major part of the frontline research focuses on the structure of the phase space; therefore, the problem to separate ordered and chaotic motion in systems, which possess only a few degrees of freedom and are described by ODEs, has become a fundamental task in a wide area of modern research. The phase space of these non-linear systems cannot be described by the known mathematical tools. To map the phase space and study the chaotic behaviour of a given system, fast and reliable numerical tools are needed. These tools are extremely useful in those cases when the inspected dynamical system has more than two degrees of freedom and accordingly its phase space cannot be explored in a direct way or the classical method of surface of section (SoS) cannot be applied which is widely used in the case of conservative systems with two degrees of freedom. The basic idea of the method of SoS was invented by Poincaré (1899) and its application was renewed by Hénon & Heiles (1964).

The mathematical foundation of the theory of Lyapunov characteristic exponents (LCEs) is approximately of the same age as the SoS and arose progressively in the literature. The use of such exponents dates back to Lyapunov (1907), but was first applied by Oseledec (1968) to characterize trajectories. Hénon & Heiles (1964) found that in an integrable region of the phase space of a dynamical system nearby orbits diverge linearly whereas in a chaotic region they diverge exponentially. The LCEs express these facts in a precise form and many papers were devoted to the application of LCEs in several non-linear problems.

Unfortunately, both methods have a serious drawback. To compute the LCEs, the equations have to be integrated for infinity, which is numerically impossible. The method of SoS becomes hard to handle and greatly deceiving for systems with more than two degrees of freedom. To overcome these problems was the main motivation in the 1980s that initiated the research to develop new numerical methods to characterize the stochasticity of the trajectories in the phase space in short time-span and in an arbitrary dimension. The developed methods can be classified into two groups: one group consists of the methods which are based on the analysis of the orbits, (e.g. SoS or frequency analysis, see Laskar 1990), while the other one is based on the time-evolution of the tangent vector, that is, the solution of the linearized equations of motion (e.g. LCE). There are complete software packages designed to analyse systems of celestial mechanics, both for general integration of motion (e.g. MERCURY6, see Chambers 1999) and for solving linearized equations and calculating LCEs (ORBIT9, see Milani & Nobili 1988). We also have to mention that there are several improved chaos-detection methods which are based on the solution of the linearized equations. Instead of a complete review, we only mention two of them: the method of fast Lyapunov indicators (FLIs, see Froeschlé, Lega & Gončzi 1997) and the method of mean exponential growth of nearby orbits (MEGNO, see Cincotta & Simó 2000; Godziewski et al. 2001). The aim of this paper is to present a lemma which advances the derivation of the same kind of recurrence relations for the linearized equations. We present these relations for certain classical dynamic systems: for the general N-body problem and for the N-body problem in the reference frame of one of the bodies. In the last section, we compare the efficiency of this method with well-known other ones.

2 LINEARIZED EQUATIONS

The chaos indicators mentioned in the previous section can be obtained if the linearized form of the equations of motion is solved. The solution of the linearized equations is a \(\xi \equiv (\xi_1, \ldots , \xi_N) : \mathbb{R} \rightarrow \mathbb{R}^N\) function having the same dimension as the equations of motion have. In practice, any ODE can be written in the form of equation (1), and the linearized form of this equation is

\[ \dot{\xi}_i = \sum_{m=1}^{N} \xi_m \frac{\partial f_i(x)}{\partial x_m}. \]

where the variables \(\xi_i \equiv \xi_i(t) : \mathbb{R} \rightarrow \mathbb{R}\) are the so-called linearized variables and \(x \equiv x(t)\) is the solution of equation (1). Equation (8) is linear in \(\xi\); therefore, if \(\xi^{(1)}_i(t)\) and \(\xi^{(2)}_i(t)\) are two independent solutions, then \(a\xi^{(1)}_i(t) + b\xi^{(2)}_i(t)\) is also a solution. Using the Einstein summation convention, equation (8) can be written in a more compact form:

\[ \dot{\xi}_i = \xi_m D_m f_i. \]

2.1 Lie-derivatives of the linearized equations

Introducing the differential operator

\[ \partial_i := \frac{\partial}{\partial \xi_i}, \]

the coupled system of equations (both the original and the linearized) is

\[ \dot{x}_i = f_i, \]

\[ \dot{\xi}_i = \xi_m D_m f_i, \]

and the Lie-operator of equations (11) and (12) is

\[ L = L_0 + L_c = f_i D_i + \xi_m D_m f_i \partial_i. \]

Lemma Using the same notations as above, the Lie-deriva-tives of \(\dot{x}_i\) can be written as

\[ L^n \xi_k = \xi_m D_m L^n x_k = \xi_m D_m L^n x_k. \]

Proof Obviously, equation (14) is true for \(n = 0\):

\[ D_m L^0 x_k = D_m x_k = \delta_{mk}, \]

hence

\[ \xi_m D_m L^0 x_k = \xi_m \delta_{mk} = \xi_k. \]
Let us suppose that it is true for all $0 \leq j \leq n$ and calculate the $(n+1)$th Lie-derivative of $\xi_k$:

$$L^{n+1}\xi_k = L\left(\xi_m D_m L^n x_k\right)$$

$$= \left(f_j D_j + \xi_j D_j f_j \partial_0\right) \left(\xi_m D_m L^n x_k\right)$$

$$= f_j D_j \xi_m D_m L^n x_k + \xi_j D_j f_j \left(\xi_m D_m L^n x_k\right) + \xi_m D_m \partial_0 L^n x_k.$$  \hfill (17)

Here, the term $\xi_m D_m \partial_0 L^n x_k$ equals to zero, because $x_k$ and $L^n x_k$ for all $n \geq 2$ do not depend on $\xi_k$.

$$L^{n+1}\xi_k = f_j D_j \xi_m D_m L^n x_k + \xi_j D_j f_j \left(\xi_m D_m L^n x_k\right)$$

$$= \xi_m f_j D_m D_l L^n x_k + \xi_m \xi_m f_j (D_l L^n x_k)$$

$$= \xi_m (f_m D_m + D_m f_j) (D_l L^n x_k)$$

$$= \xi_m D_m (f_j D_l) (L^n x_k)$$

$$= \xi_m D_m L(L^n x_k) = \xi_m D_m L^{n+1} x_k = L\xi_m D_m L^n x k.$$  \hfill (18)

We have applied Young’s theorem, namely

$$D_m D_l X = D_m f_j (D_l X)$$

and Leibniz rule,

$$D_m (f_j D_l X) = D_m f_j (D_l X) + (D_m f_j) (D_l X),$$  \hfill (20)

where $X$ can be an arbitrary function of $x$; in equation (18) $X \equiv L^n x_k$. Therefore, equation (18) is the same relation for $n+1$ as equation (14) for $n$. Continuing the scheme described above, equation (14) can be proven for all positive integer values of $n$. \hfill \blacksquare

### 2.2 An example: applying to the Hénon–Heiles system

Demonstrating the power of the lemma proven in the previous section, we derive the recurrence relations for the equation of the Hénon–Heiles dynamical system and its linearized form. The Hénon–Heiles system is one of the simplest Hamiltonian systems which shows chaotic behaviour under certain initial conditions (see Hénon & Heiles 1964).

The equations of motion are derived from the Hamiltonian function

$$H(x, y; v, w) = \frac{1}{2} \left( x^2 + y^2 + 2x^2 y - \frac{2}{3} y^3 \right) + \frac{1}{2} (v^2 + w^2),$$  \hfill (21)

where $\dot{x} = v$ and $\dot{y} = w$. The equations of motion are

$$\dot{x} = v,$$  \hfill (22)

$$\dot{y} = w,$$  \hfill (23)

$$\dot{v} = -x - 2xy,$$  \hfill (24)

$$\dot{w} = -y - x^2 + y^2,$$  \hfill (25)

and the Lie-operator of this system of equations is

$$L_0 = v \partial_x + w \partial_y + (-x - 2xy) \partial_v + (-y - x^2 + y^2) \partial_w.$$  \hfill (26)

According to equation (3), it can easily be shown that the recurrence relations of the equations (22)–(25) are the following:

$$L_0^{n+1} x = L_0^n v,$$  \hfill (27)

$$L_0^{n+1} y = L_0^n w,$$  \hfill (28)

$$L_0^{n+1} v = -L_0^n x - 2 \sum_{k=0}^{n} \binom{n}{k} L_0^k x L_0^{n-k} y,$$  \hfill (29)

$$L_0^{n+1} w = -L_0^n y - 2 \sum_{k=0}^{n} \binom{n}{k} \left( L_0^k x L_0^{n-k} x - L_0^k y L_0^{n-k} y \right).$$  \hfill (30)

Let us denote the linearized variables related to $x, y, v$ and $w$ by $\xi, \eta, \phi$ and $\rho$, respectively. According to equation (14), the Lie-derivatives of these variables are

$$L^n \xi = \xi_m D_m L^n x,$$  \hfill (31)

$$L^n \eta = \xi_m D_m L^n y,$$  \hfill (32)

$$L^n \phi = \xi_m D_m L^n v,$$  \hfill (33)

$$L^n \rho = \xi_m D_m L^n w,$$  \hfill (34)

where $\xi_1 \equiv \xi, \xi_2 \equiv \eta, \xi_3 \equiv \phi$ and $\xi_4 \equiv \rho$. The pure recurrence relations can be almost automatically derived. For the first two variables, it is evidently

$$L^{n+1} \xi = \xi_m D_m L^{n+1} x = \xi_m D_m L^n v = L^n \phi.$$  \hfill (35)

$$L^{n+1} \eta = \xi_m D_m L^{n+1} y = \xi_m D_m L^n w = L^n \rho.$$  \hfill (36)

For the third variable, one gets

$$L^{n+1} \phi = \xi_m D_m L^{n+1} v$$

$$= \xi_m D_m \left( -L^n x - 2 \sum_{k=0}^{n} \binom{n}{k} L^k x L^{n-k} y \right)$$

$$= -\xi_m D_m L^n x$$

$$- 2 \sum_{k=0}^{n} \binom{n}{k} D_m \left[ L^k x L^{n-k} y \right]$$

$$= -L^n \xi - 2 \sum_{k=0}^{n} \binom{n}{k} \xi_m \left[ (D_m L^k x)(L^{n-k} y) \right] + (L^k x)(\xi_m D_m L^{n-k} y)$$

$$= -L^n \xi - 2 \sum_{k=0}^{n} \binom{n}{k} \left[ L^k \xi L^{n-k} y + L^k x L^{n-k} y \right].$$  \hfill (37)

The same procedure can be performed for $\rho$ and the result is

$$L^{n+1} \rho = -L^n \eta - 2 \sum_{k=0}^{n} \binom{n}{k} \left[ L^k \xi L^{n-k} x + L^k x L^{n-k} \xi \right]$$

$$- L^k \eta L^{n-k} y - L^k y L^{n-k} \eta.$$  \hfill (38)

### 3 THE LIE-DERIVATIVES FOR THE N-BODY PROBLEM AND ITS LINEARIZED FORM

Let us have $K$ point masses $m_i (i = 1, \ldots, K)$ moving under the mutual gravitational attraction described by Newton’s universal law.
3.1 Equations of motion

Using the above notations, the equations of motion of the N-body problem are the following:

\[ x_{im} = v_{im}, \quad (39) \]

\[ \dot{v}_{im} = -G \sum_{j=1, j \neq i}^{K} \frac{m_j (x_{jm} - x_{im})}{\rho_{ij}^3}, \quad (40) \]

where \( G \) is the Newtonian gravitational constant and \( \rho_{ij} \) is the distance between the \( i \)th and \( j \)th body, that is,

\[ \rho_{ij}^2 = \sum_{m} (x_{im} - x_{jm})^2 = A_{ijm} A_{ijm}. \quad (41) \]

We also introduce the following new variables and differential operators:

\[ A_{ijm} := x_{im} - x_{jm}, \quad (42) \]

\[ B_{ijm} := v_{im} - v_{jm}, \quad (43) \]

\[ \Lambda_{ij} := A_{ijm} B_{ijm}, \quad (44) \]

\[ \phi_{ij} := \rho_{ij}^{-3}, \quad (45) \]

\[ D_{im} := \frac{\partial}{\partial x_{im}}, \quad (46) \]

\[ \Delta_{im} := \frac{\partial}{\partial v_{im}}. \quad (47) \]

With these notations, the Lie-operator of the equations of motion can be written as

\[ L_0 = v_{im} D_{im} - G \sum_{i} \left[ \left( \sum_{j=1, j \neq i}^{K} m_j \phi_{ij} A_{ijm} \right) \Delta_{im} \right]. \quad (48) \]

In Appendix A, we prove that the recurrence relations for the variables \( x_{im}, A_{ijm}, B_{ijm}, \Lambda_{ij}, v_{im} \) and \( \phi_{ij} \) is the following system of equations:

\[ L_0^{n+1} x_{im} = L_0^n v_{im}, \quad (49) \]

\[ L_0^n A_{ijm} = L_0^n x_{im} - L_0^n x_{jm}, \quad (50) \]

\[ L_0^n B_{ijm} = L_0^n v_{im} - L_0^n v_{jm}, \quad (51) \]

\[ L_0^{n+1} v_{im} = -G \sum_{j=1, j \neq i}^{K} m_j \left( \sum_{k=0}^{n} \binom{n}{k} L_0^k \phi_{ij} L_0^{n-k} A_{ijm} \right), \quad (52) \]

\[ L_0^n \Lambda_{ij} = \sum_{k=0}^{n} \binom{n}{k} L_0^k A_{ijm} L_0^{n-k} B_{ijm}, \quad (53) \]

\[ L_0^n \phi_{ij} = \rho_{ij}^{-2} \sum_{k=0}^{n} F_{nk} L_0^{n-k} \phi_{ij} L_0^k \Lambda_{ij}, \quad (54) \]

where \( F_{nk} = (-3)^k \binom{n}{k} + (-2)^k \binom{n}{k} \). We note that \( F_{nk} \) is equivalent to the matrix \( A_{nk} \) introduced in H&D.

3.2 Linearized equations

For the linearized coordinates and velocities, we introduce the variables \( \xi_{im} \) and \( \eta_{im} \), respectively. Therefore, using the Lemma, we get the Lie-derivatives of the linearized variables, namely,

\[ L^n \xi_{im} = (\xi_{kp} D_{kp} + \eta_{kp} \Delta_{kp}) L^n x_{im}, \quad (55) \]

\[ L^n \eta_{im} = (\xi_{kp} D_{kp} + \eta_{kp} \Delta_{kp}) L^n v_{im}. \quad (56) \]

To obtain recurrence relations, we have to introduce other auxiliary quantities. First, we form two vectors which contain all the linearized variables and the differential operators:

\[ \Xi_{kp} := (\xi_{kp}, \eta_{kp}), \quad (57) \]

\[ D_{kp} := (D_{kp}, \Delta_{kp}). \quad (58) \]

Therefore, one can write \( \Xi D = \Xi_{kp} D_{kp} = \xi_{kp} D_{kp} + \eta_{kp} \Delta_{kp} \) which simplifies the notation of the scalar products appearing in equations (55) and (56):

\[ L^n \xi_{im} = \Xi D L^n x_{im}, \quad (59) \]

\[ L^n \eta_{im} = \Xi D L^n v_{im}. \quad (60) \]

Secondly, let us introduce \( \alpha_{ijm} := \xi_{im} - \xi_{jm} \) and \( \beta_{ijm} := \eta_{im} - \eta_{jm} \). With these newly introduced variables and expressions, we can derive the recurrence formulae for the linearized variables. The calculations are presented in Appendix B in more details, and the result is

\[ L^{n+1} \xi_{im} = L^n \eta_{im}, \quad (61) \]

\[ L^n \alpha_{ijm} = L^n \xi_{im} - L^n \xi_{jm}, \quad (62) \]

\[ L^n \beta_{ijm} = L^n \eta_{im} - L^n \eta_{jm}, \quad (63) \]

\[ \Xi D L^n \Lambda_{ij} = \sum_{k=0}^{n} \binom{n}{k} \left[ L^k \alpha_{ijm} L^{n-k} B_{ijm} + L^k \Lambda_{ijm} L^{n-k} \beta_{ijm} \right], \quad (64) \]

\[ L^{n+1} \eta_{im} = -G \sum_{j=1, j \neq i}^{K} m_j \left( \sum_{k=0}^{n} \binom{n}{k} [ \text{per cent}_1 ] \right), \quad (65) \]

per cent$_1 = (\Xi D L^n \phi_{ij}) L^{n-k} A_{ijm} + L^n \phi_{ij} L^{n-k} \alpha_{ijm}$

\[ \Xi D L^{n+1} \phi_{ij} = -2 \rho_{ij}^{-2} \alpha_{ijm} L^{n+1} \phi_{ij} + \rho_{ij}^{-2} \sum_{k=0}^{n} F_{nk} [ \text{per cent}_2 ], \quad (66) \]

per cent$_2 = (\Xi D L^{n-k} \phi_{ij}) L^k \Lambda_{ij} + L^{n-k} \phi_{ij} (\Xi D L^n \Lambda_{ij})$. 

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For the initialization of the recursion, we have to calculate \( \Xi \mathcal{D}L^0\phi_{ij} \equiv \Xi \mathcal{D}\phi_{ij} \). It is easy to show that \( \Xi \mathcal{D}\phi_{ij} = \Xi \mathcal{D}\rho_{ij} = -3\rho_{ij}^2\alpha_{ijim}A_{ijm} \).

(67)

We have some remarks concerning the derivation and evaluation of the above formulae. First, we did not need the linearized equations explicitly to derive the recurrence relations for the linearized variables. Secondly, because of the symmetry properties of the variables, we do not have to calculate all the matrix elements: we know that the tensors \( A_{ijm}, \beta_{ijm}, \alpha_{ijm} \) and \( \beta_{ijm} \) are antisymmetric for swapping the indices \( i \) and \( j \) and the matrices \( \Lambda_{ij}, \phi_{ij}, \Xi \mathcal{D}\Lambda_{ij} \) and \( \Xi \mathcal{D}\phi_{ij} \) are symmetric. Because distances are defined only between different bodies, the diagonal matrix elements of \( \rho_{ij} \) and their derivatives (\( \phi_{ij}, L^p\rho_{ij}, L^p\phi_{ij}, \Xi \mathcal{D}L^p\rho_{ij}, \ldots \)) are not defined.

3.3 Motion in the reference frame of one of the bodies

In the description of the Solar system or in perturbation theory, the equations of motion are transformed into a reference frame whose origin coincides with one of the bodies. Practically, it is the body with the largest mass; in the Solar system, it is the Sun (where all orbital elements are defined relative to the Sun). Therefore, it could prove useful to have the recurrence relations both for the equations of motion and for the linearized part of the equations in this reference frame.

Let us define the central body as the body with the index of \( i = 0 \). Altogether we have \( 1 + K \) bodies, whereas the other ones are indexed by \( i = 1, \ldots, K \). For simplicity, we denote its mass by \( M = m_0 \). In an inertial frame, the equations of motion can be split into two parts, namely

\[
\dot{x}_{in} = v_{in},
\]

(68)

\[
v_{in} = -G \sum_{j=0,j\neq i}^{K} m_j \rho_{ij}^{-3} (x_{in} - x_{jm}),
\]

(69)

and

\[
\dot{v}_{in} = v_{in},
\]

(70)

\[
v_{0m} = -G \sum_{j=1}^{K} m_j \rho_{ij}^{-3} (x_{0m} - x_{jm}).
\]

(71)

Following the usual steps, the equations of motion in the fixed frame can easily be derived by subtracting equation (70) from equation (68) and equation (71) from equation (69) for all \( i \) indices. Let us define new variables

\[
r_{in} := x_{in} - x_{0m},
\]

(72)

\[
u_{in} := v_{in} - v_{0m},
\]

(73)

\[
\rho_i := \rho_{ii},
\]

(74)

\[
\phi_i := \phi_{ii}.
\]

(75)

Note that the quantities \( \rho_i, \rho_{ij}, \phi_i, \phi_{ij} \) are distinguished only by the number of their indices. Obviously, \( A_{ijm} = x_{in} - x_{jm} = r_{in} - r_{jm} \) and \( B_{ijm} = v_{in} - v_{jm} = w_{in} - w_{jm} \). Thus, using the relative (non-inertial) coordinates and velocities, the equations of motion in more compact form are

\[
r_{in} = w_{in},
\]

(74)

\[
\dot{w}_{in} = -G (M + m_i) \phi_i r_{in}
\]

(75)

Without going into details, we preset the recurrence relations of the Lie-derivatives, including the linearized variables in Appendix C. Some speed-up considerations with which the required number of operations can definitely be decreased are presented in Appendix D.

4 PERFORMANCE AND COMPARISONS

We have implemented the method of Lie-integration as a stand-alone program, written in ANSI C with the following capabilities. The program is able to integrate the equations of motion of the \( N \)-body problem in the reference frame of one of the bodies (see equations 74 and 75) and, parallelly, the program approximates the LCE by the Lyapunov characteristic indicator (LCI) of the system using the solution of the linearized equations. For the method of integration, one could use the classical fourth-order Runge–Kutta (see Press et al. 1992) and Runge–Kutta–Nystrom integrators (namely, RKN5/6/ and RKN7/8/, see Fehlberg 1972; Dormand & Prince 1978), the Bulirsch–Stoer integrator (BS, see also Press et al. 1992) as well as the Lie-integration method (see equations C1–C8 and equations C9–C16 in Appendix C), up to an arbitrary order \( M \). The program is also able to figure out the optimal step-sizes to satisfy a pre-defined accuracy. The accuracy is derived using the differences in the mean longitude which is the fastest-changing orbital element. This type of accuracy control can be found in many integrators (e.g. ORBIT9) where the dimensionless accuracy is defined as the difference in the mean longitudes between the exact and approximated solution (in radians) divided by the square of the number of revolutions, namely

\[
\varepsilon = \frac{|\Delta \lambda| \text{(radians)}}{N^2 \text{revolution}}.
\]

(76)

(see Milani & Nobili 1988, for a more detailed explanation).

As an initial test, we have compared the LCIs computed by two different integration methods, namely RKN7/8/ and the Lie-integration of the order of \( M = 8 \). The dynamical system is the spatial Sun–Jupiter–Saturn–test particle spatially restricted four-body system where the latter has the same orbit as the Jupiter has. The LCIs are calculated as the function of the difference in the mean longitudes of Jupiter (\( \lambda_i \)) and the test particle (\( \lambda_{0m} \)), while all other five initial orbital elements are equal to those of Jupiter. The results are plotted in Fig. 1. In the left-hand panel of Fig. 1, one can see the derived indicators by the method of RKN7/8/, LCI RKN7/8/, and using Lie-integration, LCI Lie, as the function of \( \Delta \lambda = \lambda_{0m} - \lambda_{jm} \). In the right-hand panel, the absolute value of the base-10 logarithm of the ratio of the indicators, namely

\[
\chi = \frac{\log_{10} |\text{LCI RKN7/8/}}{\text{LCI Lie}} |,
\]

(77)

is plotted, resulted by these two integration methods. Note that the integration length is \( 10^8 \) yr; therefore, the LCIs concerning to regular solutions are saturated around \( 10^{-5} - 10^{-4} \) yr\(^{-1}\). It can easily be seen that in the stable regions (around the two Lagrangian points at \( \Delta \lambda = -60^\circ \) and \( +60^\circ \)) the results of the two methods are very similar, and the magnitude of the differences between them is \( \approx 10^{-5} \). In the chaotic regions, the two methods yielded different LCIs but their magnitudes were always the same.

4.1 Performance analysis

We have compared the efficiency of the Lie-integrator and the other implemented integrators. Here, we give how much CPU time is required to integrate the equations of motion with RK4, RKN5/6/, RKN7/8/, BS and with the Lie-integration and parallelly the linearized equations to get the result with a previously given accuracy.
Figure 1. The LCIs for a fictitious asteroid having the same orbit as that of Jupiter. In the left-hand panel, one can see the derived indicators by the method of RKN7/8/ (crosses) and using Lie-integration (empty squares) as the function of $\Delta \lambda$. In the right-hand panel, the ratios $\chi(\Delta \lambda)$ defined by equation (77) are plotted.

The ratio of the net CPU times is the relative cost:

$$\text{cost}^{[\text{other}]} := \frac{\tau_{[\text{method}]}^{[\text{other}]}}{\tau_{[\text{method}]}^{[\text{method}]}},$$

As one can see, the smaller the cost is, the more efficient the Lie-integration is. It should be kept in mind that this relative cost does not only depend on the other method but also depend on the order of the Lie-integration and the desired accuracy. Going into the details, the cost has been measured indirectly in the following way. It can be said that any of the integration algorithms, the RK-based ones, the BS and the Lie-integration, uses the same CPU time per step independent of the step-size.¹ Let us denote this atomic CPU time by $t_{(0)}^{[\text{method}]}$. Therefore, if the optimal step-size $\Delta t_{(i)}^{[\text{method}]}$ is known for a given method and accuracy, the total CPU time can easily be calculated:

$$\tau_{[\text{method}]}^{[\text{method}]} = \frac{\tau_{(0)}^{[\text{method}]} T}{\Delta t_{(i)}^{[\text{method}]}},$$

where $T$ is the total length of the integration. Because the relative cost is the ratio of two such values of $\tau_{CPU}$ for two methods, the total length of the integration cancels. The atomic CPU time can easily be measured; the only unknown is the $\Delta t$ optimal step-size for the different methods. The latter is determined in the following way.

The exact mean longitude for the fastest-rotating planet is derived in the above sections of the appropriate values taken from this table, namely

$$\text{cost}^{[\text{m1}]\text{against}[\text{m2}]} = \frac{\tau_{(0)}^{[\text{m1}]} \Delta t_{(i)}^{[\text{m1}]} \chi_{[\text{m1}]}(\Delta \lambda)}{\tau_{(0)}^{[\text{m2}]} \Delta t_{(i)}^{[\text{m2}]} \chi_{[\text{m2}]}(\Delta \lambda)},$$

where [m1] and [m2] index the two methods to be compared. We should note that timing values were not only derived for these values of accuracy as it can be read from Table 1 and we have made timing measurements when the linearized equations are omitted. See the next sections for more details and for other plots.

4.2 Efficiency as the function of the accuracy

In Fig. 2, the relative cost of the Lie-integration against the RKN7/8/ and the Bulirsch–Stoer integration methods is plotted for the three-body problem of Sun–Jupiter–Saturn as the function of the accuracy. Different curves show the cost for different orders of the Lie-integration between 6 and 16. It can easily be seen that for higher orders and below a critical accuracy the Lie-integration is more efficient than RKN7/8/ and for higher orders, the Lie-integration is more efficient than the Bulirsch–Stoer method almost independent of the accuracy. Note that in this plot the linearized equations are omitted from the calculations.

In Fig. 3, we have plotted the cost of the Lie-integration against the methods as above but the dynamical system is extended with a particle extended with the linearized equations of the latter. The second column contains the atomic CPU time,² while the other three columns show the optimal step-size $\Delta t_{(i)}^{[\text{method}]}$, derived in the above manner for the accuracies of $\epsilon = 2.4 \times 10^{-11}, 2.4 \times 10^{-12}$ and $2.4 \times 10^{-13}$, respectively. Thus, the cost can be derived by the fraction of the atomic CPU time $\tau_{CPU}$ by the optimal step-size $\Delta t_{(i)}^{[\text{method}]}$.

Table 1. Timing data for the Runge–Kutta integrators, the Bulirsch–Stoer integrator and for the Lie-integrator for different orders. See the text for further details.

| Integrator (method) | CPU time $T$ | Stepsize, $\Delta t^{[\text{method}]}$ for $\epsilon =$ |
|---------------------|-------------|-----------------------------------------------|
| RK4                | 0.302       | $2.4 \times 10^{-11}$                           |
| RKN5/6/            | 0.460       | $2.4 \times 10^{-12}$                           |
| RKN7/8/            | 0.941       | $2.4 \times 10^{-12}$                           |
| BS                 | 8.578       | $2.4 \times 10^{-13}$                           |
| $M = 6$            | 0.916       | $2.4 \times 10^{-13}$                           |
| $M = 7$            | 1.109       | $2.4 \times 10^{-13}$                           |
| $M = 8$            | 1.271       | $2.4 \times 10^{-13}$                           |
| $M = 9$            | 1.706       | $2.4 \times 10^{-13}$                           |
| $M = 10$           | 2.004       | $2.4 \times 10^{-13}$                           |
| $M = 11$           | 2.336       | $2.4 \times 10^{-13}$                           |
| $M = 12$           | 2.689       | $2.4 \times 10^{-13}$                           |
| $M = 13$           | 3.048       | $2.4 \times 10^{-13}$                           |
| $M = 14$           | 3.411       | $2.4 \times 10^{-13}$                           |
| $M = 15$           | 3.810       | $2.4 \times 10^{-13}$                           |
| $M = 16$           | 4.223       | $2.4 \times 10^{-13}$                           |

¹ In our tests, in the BS method, the adaptive variation in the number of MMID substeps has been disabled, that is, the extrapolation is performed after the same sequence of a number of substeps: it yields an evaluation time which is independent of the step-size.

² Measured on an Athlon XP 1800+ processor with gcc v4.1.2 compiler, in units of $10^{-6}$ s.
massless test particle and for the latter the linearized equations are also solved. The qualitative behaviour of the cost as the function of the accuracy and the orders of the Lie-series are almost the same as in Fig. 2. We note that the different methods used in the RKN, BS and Lie-integration methods to evaluate the linearized equations result in different number of operations; therefore, the costs will not be exactly the same. Namely, the relative CPU time cost of the Lie-integration against the other methods is slightly larger when the linearized equations are solved parallel.

As a conclusion, we can say that omitting the linearized part order below $M \approx 10$ the Lie-integration method is inferior than the RKN7/8/ method, while the equations are extended with the linearized equations for the massless particle; the Lie-integration method is more effective than RKN7/8 for orders larger than $M \approx 12$ below a certain accuracy of about $\varepsilon \approx 10^{-11}$. Comparing with the BS method, the Lie-integration method is more effective for orders larger than $M \approx 8$ and $M \approx 10$ when the linearized equations are omitted or not, almost independent of the accuracy. We note that the Lie-integration is effective with more than a magnitude (or more) than the lower-order Runge–Kutta methods, as it can easily be derived from Table 1 and equation (80).

### 4.3 Efficiency as the function of the order

As it was written in the Introduction section, the method of Lie-integration approximates the Taylor-expansion of the solution up to a finite order. One can easily prove that the appropriate order, $n$, of a Taylor-series to obtain a certain accuracy of a periodic function defined on an interval is proportional to the length, $L$, of this interval. The concept of the proof is as follows. An adequately smooth periodic function can be approximated as a sum of sine (and cosine) functions, the so-called Fourier terms. The sine function, sin ($x$) can be expanded as

$$\sin(x) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!}.$$  

(81)

To obtain an accuracy of unity, the last ($n = 2k + 1$) term of the series should be the solution of $x^n \equiv L^n \approx n!$. Therefore, using Stirling's approximation, one gets

$$n \log L = \log(n!) \approx n \log n - n,$$  

(82)

so $n \approx e L$, which means $n \sim L$. This is true for all Fourier terms of the expansion of a periodic function.

Thus, one can assume that to obtain a certain accuracy, the $M$ number of the terms in the Lie-series is proportional to the length of the integration step-size, namely $\Delta t \approx k M$. The total number of arithmetical operations, therefore the required CPU time, is a quadratic function of the order of $M$: $\tau_{CPU} = \text{Ordo } (M^2)$. To be more precise, the required CPU time is $\tau_{CPU} = \alpha + \beta M + \gamma M^2$, for smaller values of $M$; the first two terms, $\alpha$ and $\beta M$, are not negligible. Therefore, to integrate the equations over an interval $T$
Figure 4. The relative cost in the CPU time as the function of the order of the Lie-integration against the RKN7/8 method for the model system of Sun–Jupiter–Saturn–fictitious asteroid. In these runs, the linearized equations are also evaluated for the massless test particle. The thin solid line, the long-dashed line and the dashed line show the cost for the accuracy of $2.4 \times 10^{-11}$, $2.4 \times 10^{-12}$ and $2.4 \times 10^{-13}$, respectively. The thick line marks the unity cost, below which the Lie-integration is more efficient.

requires

$$\frac{\text{CPU time}}{\alpha + \beta M + \gamma M^2} \frac{T}{\Delta t} = \frac{\alpha + \beta M + \gamma M^2}{\gamma M}$$

The relative cost in the CPU time as the function of the order of the Lie-integration against the RKN7/8 and RKN5/6 methods is shown in Figure 4. The results are plotted for three values of accuracy, while the dynamical system is the restricted four-body problem of Sun–Jupiter–Saturn–test particle extended with the linearized equations with respect to the latter. As it was assumed above, the relative cost has a minimum corresponding to the optimal order of the Lie-integration method.

We have tested this type of dependency of the CPU time on the order of the Lie-integration. The results are plotted in Figure 4, for three values of accuracy, while the dynamical system is the restricted four-body problem of Sun–Jupiter–Saturn–test particle extended with the linearized equations with respect to the latter. As it was assumed above, the relative cost has a minimum corresponding to the optimal order of the Lie-integration method.

4.4 Implementation of the method

We have implemented the method of Lie-integration of the N-body problem as a stand-alone ANSI C program, extended with the linearized equations and the capability to calculate the LCIs. The version of the program which can integrate the motion of 1+3 bodies and was used in our benchmarks can be downloaded from the address http://cm.elte.hu/lie as a single .tar.gz archive. The full version which is capable of integrating the motion of arbitrary number of bodies can be requested from the first author via e-mail. All versions of this code are designed to work on UNIX-like environments.

5 DISCUSSION AND SUMMARY

In this paper, we have presented a lemma with which recurrence relations can be derived for the Lie-integration of linearized equations. We have demonstrated the usage of this lemma on the Hénon–Heiles system, and thereafter applied it to the equations of the N-body problem, including the non-inertial equations where the origin of the reference frame is fixed to one of the bodies. Our performance comparisons have shown that although these recurrence formulae are rather complicated, they can efficiently be used for integrations where high accuracy is required. We have investigated realistic dynamical systems for these comparisons: using the lemma, the recurrence relations were determined and using the Lie-integration technique, the LCIs for a fictitious asteroid were computed. The method of LCIs is the basis for many modern chaos-detection methods; therefore, our lemma and the derived Lie-integration method can widely be used in various kinds of dynamical investigations, providing a faster alternative to the currently used techniques. We have checked the efficiency as the function of the order and accuracy. These tests have shown that the Lie-integration is definitely more effective than the classical RK4 and RKN5/6 integration methods and above a certain accuracy of about $\varepsilon \approx 10^{-11}$; the Lie-integration is more effective than the method of RKN7/8 for orders larger than $M = 10$ or 8, whether the linearized equations are evaluated parallelly or not. We found that the Lie-integration is more effective than the BS integrator for orders larger than $M = 10$, almost independent of the accuracy.

Further studies are already ongoing concerning this problem. First, there could be several possibilities for optimization in the actual implementation of the Lie-integration: we expect that the reordering of the highly nested loops and/or the introduction of new auxiliary variables yield better performance. Secondly, some aspects of the Lie-integration should better be analysed and understood, including the long-term error propagation in higher orders which is the basis of the adaptive extensions of this integration method, and finally, we are going to develop a more general code which is not only capable of the calculation of LCIs but also can be extended with other chaos indicators.

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APPENDIX A: RECURRENT RELATIONS FOR THE N-BODY PROBLEM

Using the notations defined in Section 3.1, we derive the recurrence relations for the equations of motion for the N-body problem.

As we have shown in Section 3.1, the Lie-operator of the equations of motion is

\[ L_0 = v_{im} D_{im} - G \sum_i \left( \sum_{j=1,j \neq i}^K m_j \phi_{ij} A_{ijm} \right) \Delta_{im} . \]  

(A1)

This implies that the first Lie-derivatives of the coordinates and velocities are the right-hand side of the equations of motion, namely

\[ L_0 x_{jm} = v_{im} , \]

\[ L_0 v_{jm} = -G \sum_{j=1,j \neq i}^K m_j \rho_{ij}^{-2} (x_{jm} - x_{im}) = -G \sum_{j=1,j \neq i}^K m_j \phi_{ij} A_{ijm} . \]  

(A2)

The distance \( \rho_{ij} \) does not depend on the velocities, like so \( \phi_{ij} \), therefore their Lie-derivatives can easily be calculated:

\[ L_0 \rho_{ij} = \sum_k v_{km} D_{kim} \rho_{ij} . \]  

(A3)

Therefore,

\[ L_0 \rho_{ij} = \sum_k v_{km} \frac{\partial}{\partial x_{im}} \left( \sum_m (x_{jm} - x_{im})(x_{jm} - x_{im}) \right) = \sum_k v_{km} \frac{\partial}{\partial x_{im}} \left( \sum_m (x_{jm} - x_{im})(x_{jm} - x_{im}) \right) \]

\[ = \sum_k v_{km} \left( \frac{1}{2} \rho_{ij}^{-2} (2(x_{jm} - x_{im})(\delta_{kj} - \delta_{ki})) \right) = \sum_k v_{km} \rho_{ij}^{-1} \left( (x_{jm} - x_{im})(\delta_{kj} - \delta_{ki}) \right) \]

\[ = \rho_{ij}^{-1} [(x_{jm} - v_{im})(x_{jm} - x_{im})] = \rho_{ij}^{-1} B_{jm} A_{jim} = \rho_{ij}^{-1} A_{ij} = \rho_{ij}^{-1} L_{0j} . \]  

(A4)

Now one can calculate the Lie-derivative of \( \phi_{ij} = \rho_{ij}^{-1} \):

\[ L_0 \phi_{ij} = L_0 (\rho_{ij}^{-1}) = -3 \rho_{ij}^{-3} L_0 \rho_{ij} = -3 \rho_{ij}^{-3} B_{jm} A_{jim} . \]  

(A5)

With mathematical induction, one can prove that

\[ L_0^{n+1} \phi_{ij} = \rho_{ij}^{-2} \sum_{k=0}^n \left[ -3 \left( \frac{n}{k} \right) - 2 \left( \frac{n}{k} \right) \right] L_0^{n-k} \phi_{ij} L_0^k A_{ij} . \]  

(A6)

For \( n = 0 \) this equation is equivalent to equation (A5). Let us assume that this is true for all \( m \leq n \), and calculate \( L_0^{n+1} \phi_{ij} \):

\[ L_0^{n+1} \phi_{ij} = L_0 \left( \rho_{ij}^{-2} \sum_{k=0}^n \left[ -3 \left( \frac{n}{k} \right) - 2 \left( \frac{n}{k} \right) \right] L_0^{n-k} \phi_{ij} L_0^k A_{ij} \right) \]

\[ = L_0 \left( \rho_{ij}^{-2} \right) \left( \rho_{ij}^2 L_0^{n+1} \phi_{ij} \right) + \rho_{ij}^{-2} \sum_{k=0}^n \left[ -3 \left( \frac{n}{k} \right) - 2 \left( \frac{n}{k} \right) \right] L_0^{n-k} \phi_{ij} L_0^k A_{ij} \]

\[ + \rho_{ij}^{-2} \sum_{k=0}^n \left[ -3 \left( \frac{n}{k} \right) - 2 \left( \frac{n}{k} \right) \right] L_0^{n-k} \phi_{ij} L_0^k A_{ij} = \text{per cent.} \]  

(A7)

The first term is

\[ L_0 \left( \rho_{ij}^{-2} \right) \left( \rho_{ij}^2 L_0^{n+1} \phi_{ij} \right) = -2 \rho_{ij}^{-1} A_{ij} \phi_{ij} \rho_{ij}^2 L_0^{n+1} \phi_{ij} = -2 \rho_{ij}^{-1} L_0^{n+1} \phi_{ij} A_{ij} . \]  

(A8)

We can increase the upper limit of the first summation of term 2 in equation (A7) from \( n \) to \( n + 1 \), since in the appearing new terms, the factors \( \left( \frac{n}{k+1} \right) \) and \( \left( \frac{n}{k+2} \right) \) are zero by definition. To unify term 1 and term 3, we introduce a new index, \( k' = k + 1 \) in term 3 of equation (A7):

\[ \rho_{ij}^{-2} \sum_{k=0}^n \left[ -3 \left( \frac{n}{k} \right) - 2 \left( \frac{n}{k} \right) \right] L_0^{n-k} \phi_{ij} L_0^k A_{ij} = \rho_{ij}^{-2} \sum_{k'=1}^{n+1} \left[ -3 \left( \frac{n}{k'-1} \right) - 2 \left( \frac{n}{k'} \right) \right] L_0^{n+1-k'} \phi_{ij} L_0^{k'} A_{ij} . \]  

(A9)

Note that if we substitute \( k' = 0 \) into the expression after the summation, we get the same what equation (A8) is; therefore, the latter can be inserted into the summation of equation (A9) while the lower limit of \( k' = 1 \) is replaced by \( k' = 0 \). Therefore,

\[ \text{per cent} = \rho_{ij}^{-2} \sum_{k'=0}^{n+1} \left[ -3 \left( \frac{n}{k'} \right) - 2 \left( \frac{n}{k'+1} \right) - 3 \left( \frac{n}{k'-1} \right) - 2 \left( \frac{n}{k'} \right) \right] L_0^{n+1-k'} \phi_{ij} L_0^{k'} A_{ij} = \text{per cent.} \]  

(A10)
The only unknown factor in equation (B7) is the quantity \( \Lambda_{ij} \) coordinates:

\[
-3 \binom{n}{k} - 2 \binom{n}{k+1} - 3 \binom{n}{k-1} - 2 \binom{n}{k} = -3 \binom{n+1}{k} - 2 \binom{n+1}{k+1},
\]

therefore we could simplify equation (A10):

\[
\text{per cent} = \rho_{ij}^{-2} \sum_{k=0}^{n+1} \left[ -3 \binom{n+1}{k} - 2 \binom{n+1}{k+1} \right] L_{0}^{n+1-k} \phi_{ij} L_{0}^{k} \Lambda_{ij}.
\]

Comparing equation (A12) with equation (A6), we conclude that the relation is proven. For simplicity, we define

\[
F_{nk} := -3 \binom{n}{k} - 2 \binom{n}{k+1}.
\]

Continuing the derivation of the recurrence formulae, we calculate the higher order Lie-derivatives of \( \Lambda_{ij} \) using the binomial theorem:

\[
L_{n}^{0} \Lambda_{ij} = \sum_{k=0}^{n} \binom{n}{k} L_{0}^{k} A_{ijm} L_{n-k}^{0} B_{ijm} = \sum_{k=0}^{n} \binom{n}{k} \left( L_{0}^{k} x_{jm} - L_{0}^{k} x_{jm} \right) \left( L_{0}^{n-k} v_{jm} - L_{0}^{n-k} v_{jm} \right).
\]

In the equations of motion, the term \( \phi_{ij} A_{ijm} \) appears; its higher order Lie-derivatives can also be calculated like the last relation for \( L_{n}^{0} \Lambda_{ij} \):

\[
L_{0}^{n} (\phi_{ij} A_{ijm}) = \sum_{k=0}^{n} \binom{n}{k} L_{0}^{k} \phi_{ij} \left( L_{0}^{n-k} x_{jm} - L_{0}^{n-k} x_{jm} \right).
\]

To summarize our results, the complete set of the recurrence relations for the equations of motion can be found in equations (49)–(54).

**APPENDIX B: DERIVATION OF THE LINEARIZED EQUATIONS**

To obtain the recurrence relations for the linearized equations, we apply the operator \( \Sigma D \) to equations (49)–(54). We note that the operator \( \Sigma D \) is linear,

\[
\Sigma D(pa + qb) = p(\Sigma D a) + q(\Sigma D b),
\]

where \( a \) and \( b \) are continuous functions while \( p \) and \( q \) are constants, and one can use Leibniz’s rule:

\[
\Sigma D(ab) = (\Sigma D a)b + a(\Sigma D b).
\]

Moreover, we should note that the operators \( \Sigma D \) and \( L \) cannot be commuted, \( \Sigma D L \neq L \Sigma D \).

For the first three equations, we get

\[
L_{n+1}^{0} \xi_{jm} = \Sigma D L_{n+1}^{0} x_{jm} = \Sigma D L_{n}^{0} v_{jm} = L_{n}^{0} \eta_{jm},
\]

\[
L_{n}^{0} \alpha_{ijm} = L_{n}^{0} \xi_{jm} = L_{n}^{0} \xi_{jm},
\]

\[
L_{n}^{0} \beta_{ijm} = L_{n}^{0} \eta_{jm} = L_{n}^{0} \eta_{jm}.
\]

For \( \Sigma D \Lambda_{ij} \) we can use the linear property and apply Leibniz’s rule:

\[
\Sigma D L_{n}^{0} \Lambda_{ij} = \sum_{k=0}^{n} \binom{n}{k} \left[ \left( \Sigma D L_{k}^{0} A_{ijm} \right) L_{n-k}^{0} B_{ijm} + L_{k}^{0} A_{ijm} \left( \Sigma D L_{n-k}^{0} B_{ijm} \right) \right]
\]

\[
= \sum_{k=0}^{n} \binom{n}{k} \left[ L_{k}^{0} \alpha_{ijm} L_{n-k}^{0} B_{ijm} + L_{k}^{0} A_{ijm} L_{n-k}^{0} \beta_{ijm} \right].
\]

Here, we applied the identities \( \Sigma D L_{n}^{0} A_{ijm} = L_{n}^{0} \alpha_{ijm} \) and \( \Sigma D L_{n}^{0} B_{ijm} = L_{n}^{0} \beta_{ijm} \). For the calculation of \( \Sigma D L_{n+1}^{0} \phi_{ij} \), we follow the same procedure:

\[
\Sigma D L_{n+1}^{0} \phi_{ij} = \left( \Sigma D \right) \left[ \rho_{ij}^{-2} \sum_{k=0}^{n} F_{nk} L_{n-k}^{0} \phi_{ij} L_{k}^{0} \Lambda_{ij} \right]
\]

\[
= \left( \Sigma D \rho_{ij}^{-2} \right) \left( \rho_{ij}^{n+1} \phi_{ij} \right) + \rho_{ij}^{-2} \sum_{k=0}^{n} F_{nk} \left[ \left( \Sigma D L_{n-k}^{0} \phi_{ij} \right) L_{k}^{0} \Lambda_{ij} + L_{n-k}^{0} \phi_{ij} \left( \Sigma D L_{k}^{0} \Lambda_{ij} \right) \right].
\]

The only unknown factor in equation (B7) is the quantity \( \Sigma D \rho_{ij}^{-2} \). We can calculate it easily, because \( \rho_{ij}^{-2} \) only depends by definition on the coordinates:

\[
\Sigma D \rho_{ij}^{-2} = \xi_{km} D_{km} (\rho_{ij}^{-2}) = \xi_{km} (-2 \rho_{ij}^{-3} D_{km} \rho_{ij} = (-2 \rho_{ij}^{-3}) \xi_{km} D_{km} \rho_{ij} = \text{per cent}.
\]
Throughout the derivation of the recurrence relations, we can use the fact that the partial differential operators $\partial_1/\Lambda_1$ and $\partial/\Lambda$ are equivalent to $D_\nu = \partial/\partial V_\nu$ and $\Delta_\nu = \partial^2/\partial V_\nu^2$, because the variables differ only in a constant ($\xi_\nu$ and $\nu_\nu$, respectively). We have to define the new variable $\Lambda_1 = r_{\nu\nu}/w_{\nu\nu}$. The derivation of the recurrence relations can be done following the steps of Appendix A and Appendix B: the quantities $\rho_i$, $\phi_i$ and $\Lambda_i$ have the same properties for the Lie-derivation as $\partial/\partial x_i$, $\partial/\partial \phi_i$ and $\Lambda_i$, respectively; therefore, all the induction steps can be done in the appropriate way.

Thus, the recurrence relations for the N-body problem around a fixed centre can be written as

\[ L^n r_{\nu\nu} = L^n w_{\nu\nu}, \]
\[ L^n A_{\nu\nu} = L^n r_{\nu\nu} - L^n r_{\nu\nu}, \]
\[ L^n B_{\nu\nu} = L^n w_{\nu\nu} - L^n w_{\nu\nu}, \]
\[ L^n \Lambda_1 = \sum_{k=0}^n \binom{n}{k} L^k r_{\nu\nu} L^{n-k} w_{\nu\nu}, \]
\[ L^n \Lambda_{ij} = \sum_{k=0}^n \binom{n}{k} L^k A_{\nu\nu} L^{n-k} B_{\nu\nu}, \]
\[ L^n w_{\nu\nu} = -G(M + m) \sum_{k=0}^n \binom{n}{k} L^k \phi_i L^{n-k} r_{\nu\nu} - G \sum_{j=1,j\neq i}^K m_j \sum_{k=0}^n \binom{n}{k} \left[ L^k \phi_j L^{n-k} A_{\nu\nu} + L^k \phi_j L^{n-k} r_{\nu\nu} \right], \]
\[ L^n \phi_i = \rho_i^{-2} \sum_{k=0}^n F_{nk} L^{n-k} \phi_i L^k \Lambda_i, \]
\[ L^n \phi_{ij} = \rho_j^{-2} \sum_{k=0}^n F_{nk} L^{n-k} \phi_j L^k \Lambda_{ij}. \]

Let us denote the linearized forms of $r_{\nu\nu}$ and $w_{\nu\nu}$ by $\xi_{\nu\nu}$ and $\eta_{\nu\nu}$, respectively. Since $\alpha_{\nu\nu} = \xi_{\nu\nu} - \xi_{\nu\nu}$ and $\beta_{\nu\nu} = \eta_{\nu\nu} - \eta_{\nu\nu}$, for the linearized equations the calculations yield

\[ L^n \xi_{\nu\nu} = L^n \eta_{\nu\nu}. \]
\[ L^n \alpha_{jm} = L^n \xi_{im} - L^n \tilde{\xi}_{jm}, \]  
\[ L^n \beta_{jm} = L^n \eta_{jm} - L^n \tilde{\eta}_{jm}, \]  
\[ \Xi D L^n \Lambda_i = \sum_{k=0}^{n} \binom{n}{k} \left( L^k \xi_{im} L^{n-k} w_{im} + L^k r_{im} L^{n-k} \eta_{jm} \right), \]  
\[ \Xi D L^n \Lambda_{ij} = \sum_{k=0}^{n} \binom{n}{k} \left( L^k \alpha_{jm} L^{n-k} B_{ijm} + L^k A_{ijm} L^{n-k} \beta_{ijm} \right), \]  
\[ L^{n+1} \eta_{jm} = -G(\mathcal{M} + m_i) \sum_{j=0}^{n} \binom{n}{k} \left[ \left( \Xi D L^k \phi_i \right) L^{n-k} r_{im} + L^k \phi_i L^{n-k} \tilde{\xi}_{jm} \right] \]  
\[ \Xi D L^{n+1} \Phi_i = -2 \rho_i^{-2} \tilde{\xi}_{im} r_{im} L^{n+1} \phi_i + \rho_i^{-2} \sum_{k=0}^{n} F_{ik} \left[ \left( \Xi D L^{n-k} \phi_j \right) L^k \Lambda_i + L^{n-k} \phi_i \left( \Xi D L^k \Lambda_i \right) \right], \]  
\[ \Xi D L^{n+1} \Phi_{ij} = -2 \rho_i^{-2} \alpha_{ijm} A_{ijm} L^{n+1} \phi_{ij} + \rho_i^{-2} \sum_{k=0}^{n} F_{ik} \left[ \left( \Xi D L^{n-k} \phi_j \right) L^k \Lambda_{ij} + L^{n-k} \phi_j \left( \Xi D L^k \Lambda_{ij} \right) \right]. \]

**APPENDIX D: SPEED-UP CONSIDERATIONS**

Introducing new variables, the required number of arithmetical operations can be decreased in equations (C1)–(C8) and equations (C9)–(C16). Namely, the calculation of \( L^{n+1} w_{im} \) and \( L^{n+1} \eta_{jm} \) can be written as

\[ L^{n+1} w_{im} = -G(\mathcal{M} + m_i) S^{[n]}_{im} - G \sum_{j=1, j \neq i}^{K} m_j \left( S^{[n]}_{ijm} + S^{[n]}_{jim} \right), \]  
\[ L^{n+1} \eta_{jm} = -G(\mathcal{M} + m_i) \Sigma^{[n]}_{jm} - G \sum_{j=1, j \neq i}^{K} m_j \left( \Sigma^{[n]}_{ijm} + \Sigma^{[n]}_{jim} \right), \]

where the new variables are

\[ S^{[n]}_{im} = \sum_{k=0}^{n} \binom{n}{k} L^k \phi_i L^{n-k} r_{im}, \]  
\[ S^{[n]}_{ijm} = \sum_{k=0}^{n} \binom{n}{k} L^k \phi_{ij} L^{n-k} A_{ijm}, \]  
\[ \Sigma^{[n]}_{im} = \sum_{k=0}^{n} \binom{n}{k} \left[ \left( \Xi D L^k \phi_i \right) L^{n-k} r_{im} + L^k \phi_i L^{n-k} \tilde{\xi}_{im} \right], \]  
\[ \Sigma^{[n]}_{ijm} = \sum_{k=0}^{n} \binom{n}{k} \left[ \left( \Xi D L^k \phi_j \right) L^{n-k} A_{ijm} + L^k \phi_j L^{n-k} \alpha_{ijm} \right]. \]

The implementation of the above relations can increase the speed of the calculations by 20–30 per cent, depending on the number of the bodies.

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