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CONTENTS

ON THE ACCURACY OF STÖRMER/VERLET METHOD AS NUMERICAL INTEGRATOR OF THE *N*-BODY PROBLEM

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Abstract. The Newton-Störmer/Verlet-leapfrog method (S/V) is a symplectic and symmetric one of order two, which, when applied to separable Hamiltonian dynamical systems, becomes explicit and conserves quadratic first integrals, e.g., the angular momentum in the *N*-body problem. As for high accuracy long-time computations required by dynamical systems coming from astronomy, the order two is too low, we consider composed S/V methods up to order 10. Beyond all these remarkable qualities, our numerical experiments on the outer as well as inner Solar system (*N*-body problem for *N* larger than 5) show that, in practice, the conservation of the Hamiltonian of the flow, up to a prescribed order, still remains an open task. Specifically, the order at which the Hamiltonian is conserved seems to be quasi independent of the order of the composed method in spite of the fact that the compensated summation, as a specific technique to reduce the round-off errors, was used. In order to clear up this aspect we perform a round-off error analysis of S/V method as a one-step method applied to an arbitrary vector field. Despite of the fact that we succeeded in improving the classical round-off error estimates, numerical experiments lead to the opinion that the accumulation of round-off errors bears the main responsibility for the lack of accuracy in long time energy conservation.

Key words: *N*-body problem – composed Störmer/Verlet method.

1. INTRODUCTION

There exist a large class of symplectic numerical methods aimed at solving numerically Cauchy problems that rule the motion of a family of N bodies in a gravitational field. They are the core of the monograph of Hairer et al. (2002) devoted to geometric numerical integration schemes and structure-preserving algorithms for ordinary differential equations. From all these methods, due to its properties, the S/V scheme seems to be the most attractive. A paper by the same authors, Hairer et al. (2003), completes their own monograph and provides a deeper analysis of that. As a discrete dynamical system, with special emphasis on its numerical stability, the method

is considered in the monograph of Stuart and Humphries (1996). For the concept of symplecticity we refer to the monograph of Sanz-Serna and Calvo (1996) and for the constructive aspects of symplectic integrators to the papers of Zhang and Skeel (1996) and Yosida (1990, 1993).

In its original formulation the S/V method is a *two-step method* (e.g, Henrici 1962).

Corresponding to the second order differential system

$$\begin{cases} \dot{q} = p, \\ \dot{p} = f(q), \end{cases} \tag{1}$$

it reads

$$\begin{cases} q_{n+1} = q_n + h(p_n + (h/2)f(q_n)) \ , \\ p_{n+1} = p_n + \dfrac{h}{2}(f(q_n) + f(q_{n+1})) \ , \qquad n = 0,\ 1,\ 2,... \end{cases} \tag{2}$$

Whenever the system (1) is a separable Hamiltonian one, the scheme (2) is explicit. We are particularly interested in such a case, beyond the accuracy of solution itself, in the long-term conservation of total energy.

Within the framework of *backward error analysis* Benetin and Giorgilli (1994) and Hairer et al. (2003) prove independently that the Hamiltonian is approximately preserved over very long times. For general Hamiltonians $H(p,q)$, they showed that the total energy along the solution (p_n, q_n) of the S/V method satisfies

$$\left|H(p_n,q_n) - H(p_0,q_0)\right| \le Ch^2 + C_N h^N t, \quad 0 \le t = nh \le h^{-N}, \tag{3}$$

for arbitrary positive integer N. The constants C and C_N are independent of t and h, but C_N depends on bounds of derivatives of H up to order $N+1$ in a region that contains the numerical solution value (p_n, q_n). As far as our knowledge goes, a similar result for the composed S/V method is not available.

On the other hand, our numerical experiments, carried out using the MATLAB codes from the paper of Hairer and Hairer (2003), on a PC led us to some intriguing conclusions. Namely, in some mildly long periods of computations, i.e., 1 million days, the orbits of planets remain (qualitatively) in correct positions. No spiral outwards and inwards are observed (see Fig. 1), when composed S/V methods of orders 6, 8 and 10 are used in outer (Jupiter to Pluto) as well as inner Solar system. With the long-time energy conservation, the situation is entirely different. The Hamiltonian oscillates with the period of the most important planet (Jupiter) and only the first significant decimal digit is conserved (see Fig. 2). This situation repeats almost identically for orders 6, 8

and 10 of the method. A significant improvement is observed passing from order 4 to 6, but further, in contrast with the orbits, almost nothing is gain by increasing the order of the method. The smallest planet (Pluto) exhibits the worst behavior, i.e., its normed Hamiltonian (H/H_0) varies periodically up to 6/10 (see Fig. 3). Unfortunately, these numerical results seem to be less optimistic than the theoretical results quoted above.

We guess that an important perturbing factor in this process of energy-conserving over long times is the rounding off. Thus, in order to reveal the contribution of such errors in S/V method we obtain in Section 3 some upper bounds of these errors. This is the main theoretical result of our paper. Roughly speaking, this states that the round-off error at the $(n+1)$th step of S/V method is bounded by $(n+1)e^{T\Lambda}\varepsilon$, where T is the length of the interval of integration, Λ is a constant that depends on the Lipschitz constant L of the vector field f and step size h, and ε is the machine rounding-off constant, defined as the smallest positive number that satisfies the inequality $1+\varepsilon>1$ in the computer arithmetic. For the machine in use $\varepsilon=10^{-16}$. Our theoretical result is better than Henrici's (1962, p. 332) classical result, which contains T^2 in the above bound. That result was obtained in a detailed analysis of general multi-step methods for second order differential systems. However, due to the persistence of round-off errors in numerical integrators, their reduction was an active research area. From the early sixties, it is well known (e.g., Wilkinson 1960) that in floating-point arithmetic the underflow is one of major sources of round-off errors. But underflow appears frequently in the sum of two quantities that have a large difference in magnitudes, as well as in many situations involving the summation of a large quantity of "small" numbers. The first instance was observed in our computations where the increments, i.e., the second terms in the right-hand sides of (2) are of order 10^{-12} with respect to left-hand side terms. Fortunately, it is possible, to a large extent, to overcome the worst effects of rounding errors. An important technique, and historically the first, is the so called *compensated summation* or Gill-Møller algorithm. A modern survey of that, with further references, is available in the paper of Higham (1993). Particular applications to initial value problems for ordinary differential equations are considered in the monograph of Butcher (2003). Fukushima (2001) considers the reduction of round-off errors in symplectic integrators. He recommends the *quadruple-precision computations* (see also Dekker 1971) and eventually observes that all reductions of round-off errors depend weakly on the order of symplectic integrators. This is also our main conclusion for the particular case of S/V method.

Quinn and Tremaine (1990) infer that the dominant source of error in long-term integration of Solar system is the rounding-off. It leads to a fractional energy error of order $n\varepsilon$, where n and ε have the same significance. They suggest the so called *optimal floating point arithmetic.* As the last two techniques mentioned increase considerable the CPU times and ask important computing resources we confine ourselves to the compensated summation.

The paper is organized as follows. In Section 2 we introduce the governing equations and review the S/V method. In Section 3 we prove our main theoretical result, i.e., a bound for round-off error in S/V process, valid for an arbitrary Lipschitzian vector field. In Section 4 we report our numerical experiments on the N-body problem for $5 \le N \le 9$.

2. GOVERNING EQUATIONS

When we treat each planet as a point of mass m_i with position r_i in a heliocentric frame, the planetary orbits satisfy the following Newtonian system

$$\frac{\mathrm{d}^2 r_i}{\mathrm{d}t^2} = -\frac{G\left(M_S + m_i\right) r_i}{\left|r_i^3\right|} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{G m_j \left(r_j - r_i\right)}{\left|r_j - r_i\right|^3} - \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{G m_j}{\left|r_j^3\right|} r_j \,. \tag{4}$$

Here M_S and G stand for the mass of the Sun and the Newtonian gravitational constant, respectively. The accuracy of any numerical scheme will depend on the accuracy of planetary masses and initial conditions $r_i(t_0)$, $\dot{r}_i(t_0)$. Both masses and initial conditions were taken from DE 102 ephemeris (see Appendix B from Quinn et al. 1991). Because the main goal of our paper is the accuracy of S/V method and its composes, we do not want to get involved into the accuracy of physical parameters. Due to the same reason, we do not use the Jacobi coordinates, mapping methods (see Wisdom and Holman 1991; Sussman and Wisdom 1992), time re-parameterization (see Huang and Leimkuhler 1997), or other physical refinements of the physical model (see also Applegate et al. 1986).

The Hamiltonian corresponding to the system (4) reads

$$H = \frac{1}{2}\sum_{i=1}^{N} m_i p_i^2 - 3G\sum_{i=1}^{N} \frac{\left(M_S + m_i\right)}{\left|q_i\right|} - G\sum_{\substack{j=1 \\ i\neq j}}^{N} m_j \left(\frac{3}{\left|q_i - q_j\right|} - \frac{r_i r_j}{\left|q_j\right|^3} \right). \tag{5}$$

Here each p_i and q_i has to be thought of as a vector with three components and $\dot{p}_i = q_i\left(r_{i1}, r_{i2}, r_{i3}\right)$. The system (4) along with the initial conditions is solved numerically using composed S/V method of orders 4 to 10. It is well known that this method is symplectic, explicit (just in case of separate Hamiltonian (5)) and neglecting the computer round-off is time reversible (see also Gladman et al. 1991, for the shortcomings of symplectic integrators).

It is important to observe that, for an accurate integration with S/V methods, the time step tends to be limited by stability restrictions rather than accuracy restrictions.

Implicit symplectic methods, like implicit midpoint or symplectic Runge-Kutta, have less severe stability restrictions, but the cost of solving large nonlinear systems with dense Jacobian matrices is probably too high to make them worthwhile.

3. BOUNDS FOR THE ROUND-OFF ERRORS

Consider that the vector field f in (1) is Lipschitzian of constant L. In order to see how the round-off errors propagate during the numerical integration process we consider two sequences (p_n, q_n) and $(\tilde{p}_n, \tilde{q}_n)$ defined, respectively, by the systems:

$$\begin{cases} q_{n+1} = q_n + h\left(p_n + \dfrac{h}{2} f(q_n)\right), \\ p_{n+1} = p_n + \dfrac{h}{2}\left(f(q_n) + f(q_{n+1})\right), \end{cases} \tag{6a}$$

$$\begin{cases} \tilde{q}_{n+1} = \tilde{q}_n + h\left(\tilde{p}_n + \dfrac{h}{2} f(\tilde{q}_n)\right) + \varepsilon_n^1, \\ \tilde{p}_{n+1} = \tilde{p}_n + \dfrac{h}{2}\left(f(\tilde{q}_n) + f(\tilde{q}_{n+1})\right) + \varepsilon_n^2. \end{cases} \tag{6b}$$

Assume that $|\varepsilon_n^1| \le \varepsilon$ and $|\varepsilon_n^2| \le \varepsilon$, ε being the machine rounding-off constant. We proceed by subtracting, term by term, the first and respectively the second equation from (6a) and (6b) and then use the fact that f is Lipschitz of constant L. We obtain the inequalities:

$$\|\tilde{q}_{n+1} - q_{n+1}\| \le \left(1 + \frac{h^2}{2} L\right)\|\tilde{q}_n - q_n\| + h\|\tilde{p}_n - p_n\| + \varepsilon, \tag{7a}$$

and

$$\|\tilde{p}_{n+1} - p_{n+1}\| \le \frac{h}{2} L\left(2 + \frac{h^2}{2} L\right)\|\tilde{q}_n - q_n\| + \left(1 + \frac{h^2}{2} L\right)\|\tilde{p}_n - p_n\| + \left(1 + \frac{h}{2} L\right)\varepsilon. \tag{7b}$$

The norm is an arbitrary one in the Euclidean space $\mathbf{R}^N$. In order to simplify the writing we introduce the following notations:

$$\alpha_{n+1} := \|\tilde{q}_{n+1} - q_{n+1}\|, \quad \beta_{n+1} := \|\tilde{p}_{n+1} - p_{n+1}\|,$$

$$a := 1 + \frac{h^2}{2} L, \quad b := h, \quad c := \frac{hL}{2}\left(2 + \frac{h^2 L}{2}\right), \quad d := \begin{pmatrix} 1 \\ 1 + \dfrac{hL}{2} \end{pmatrix}, \quad A := \begin{pmatrix} a & b \\ c & a \end{pmatrix}.$$

With these, the inequalities (7) can be written formally

$$\begin{pmatrix}\alpha_{n+1}\\ \beta_{n+1}\end{pmatrix} \le A^{n+1}\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix} + \left(I_2 + A + A^2 + \cdots + A^n\right)\cdot d\cdot\varepsilon. \tag{8}$$

In order to compute the powers of the matrix **A**, we decompose it in the form $\mathbf{A} = \mathbf{S}\cdot\mathbf{D}\cdot\mathbf{S}^{-1}$,

where

$$\mathbf{S} = \begin{pmatrix}\sqrt{b/c} & -\sqrt{b/c}\\ 1 & 1\end{pmatrix}, \quad \mathbf{D} = \begin{pmatrix}a+\sqrt{bc} & 0\\ 0 & a-\sqrt{bc}\end{pmatrix}.$$

By making use of the elementary inequality, $1 + x \le \mathrm{e}^x$, after a quite tedious algebra, the Euclidean norm of $(\alpha_n \quad \beta_n)^{\mathrm{T}}$, becomes

$$\left\|\begin{pmatrix}\alpha_{n+1}\\ \beta_{n+1}\end{pmatrix}\right\| \le \left[2\left\|\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix}\right\| + 2(n+1)\cdot\sqrt{1+\left(1+\frac{hL}{2}\right)^2}\cdot\varepsilon\right]\cdot \mathrm{e}^{T\Lambda}, \tag{9}$$

where $\Lambda = hL/2 + \sqrt{L + (hL/2)^2}$.

For the norm $\|\cdot\|_\infty$ and $n = 0, 1, 2, \ldots$, we get

$$\max\left(\alpha_{n+1}, \beta_{n+1}\right) \le$$

$$\le \left(1 + \sqrt{L + \left(\frac{hL}{2}\right)^2}\right)\cdot\left[\max\left(\alpha_0, \beta_0\right) + (n+1)\max\left(1,\ 1+\frac{hL}{2}\right)\cdot\varepsilon\right]\cdot \mathrm{e}^{T\Lambda}. \tag{10}$$

For positive as well as for negative step size h the constant Λ remains positive but the second max in the estimation (10) becomes respectively $1 + hL/2$ or 1. However, these estimates improve by a factor T the classical bounds of Henrici (1962). The one-step formulation of S/V method is responsible for this improvement.

4. LONG-TIME ENERGY CONSERVATION. NUMERICAL EXPERIMENTS

The Hamiltonian system (4) was solved numerically by various orders of S/V scheme. The initial data are those given by Quinn et al. (1991, Appendix A).

The trajectories for the outer Solar system (N = 5) are depicted in Fig. 1. A similar figure was obtained for the inner and outer Solar system (N = 9).

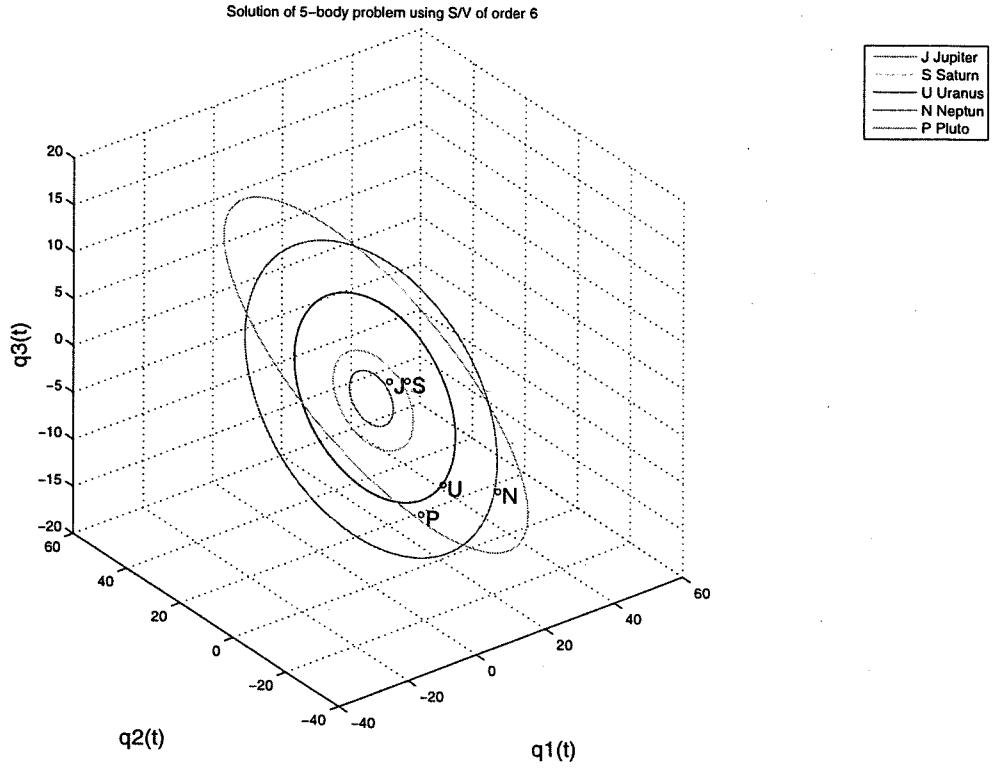

Fig. 1 – The orbits of planets corresponding to S/V of order six.
Step size equals 10 days and $T = 1$ million days.

The *numerical oscillations* of the Hamiltonian of the four giant planets are depicted in Fig. 2, whereas those for Pluto are displayed in Fig. 3. The oscillations of the individual Hamiltonians of the remaining four planets follow closely (remain in the same limits) the oscillations of the whole system. It is worth noting at this point that mass variations of Pluto from $1/(1.3 \cdot 10^8)$ to $1/(3 \cdot 10^7)$ have no effect on the numerical results. However, the worst approximation for Hamiltonian was encountered for this planet (compare Figs. 2 and 3).

The theoretical bounds (9) and (10) are quite difficult to verify numerically due to the lack of accuracy in the numerical evaluation of Lipschitz constant L. In this situation we solved the 5-body problem of the outer Solar system in two distinct hypotheses. Namely, we computed (p_n, q_n) from (6a), using single precision computations and $(\tilde{p}_n, \tilde{q}_n)$ from (6b), using double precision. The evolution of the quantities α_n and β_n, i.e., *error*(q), *error*(p), are visible in Fig. 4. It is very clear that round-off errors cumulate as time proceeds.

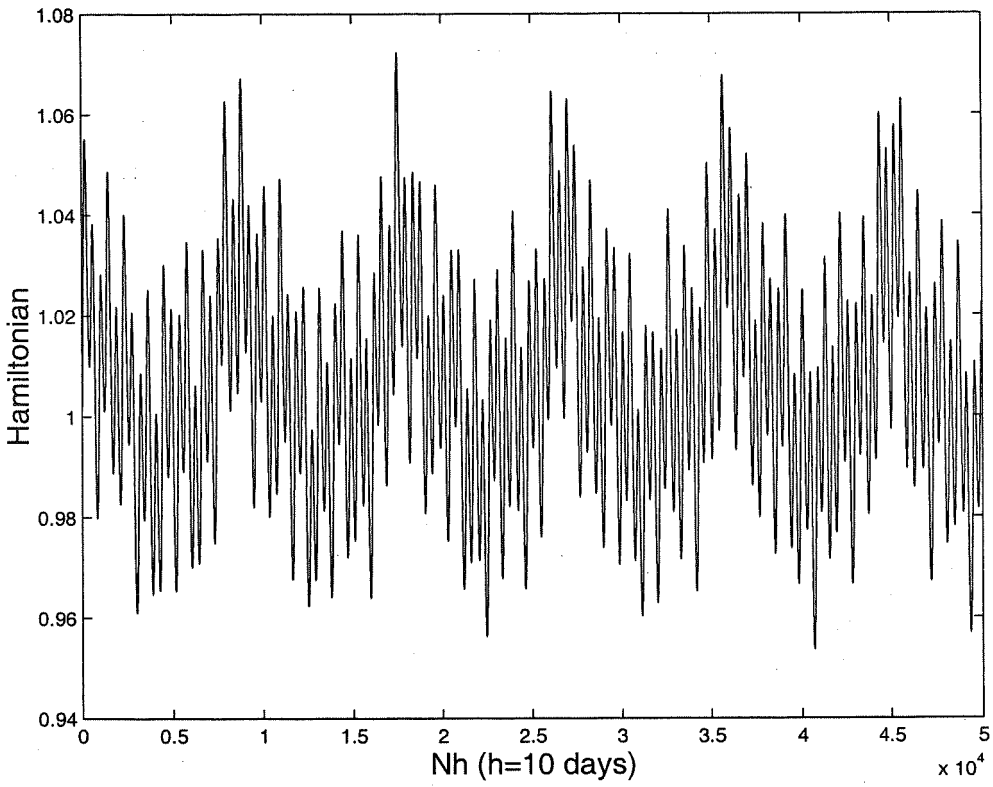

Fig. 2 – The Hamiltonian for the outer Solar system ($N = 4$).

5. CONCLUDING REMARKS

The above numerical experiments, as well as a lot of other experiments performed on a perturbed Kepler problem (the Schwarzschild potential) or the Kepler problem with large eccentricity, i.e., eccentricity = 0.9, show clearly the superiority of high-order composed S/V methods over nonsymplectic high-order Runge-Kutta methods or other usual multi-step methods, such as Adams-Bashforth PECE solver from Matlab. The fact that these S/V methods are explicit, in case of separable Hamiltonians, ensures high-speed computations and reduces CPU times. However, with respect to the preservation of Hamiltonians the situation gets worse and the problem of reduction of round-off errors is not completely solved. Our comparison of single and double precision computations suggests that quadruple precision computations could improve considerably the long-term conservation of the total energy of the system.

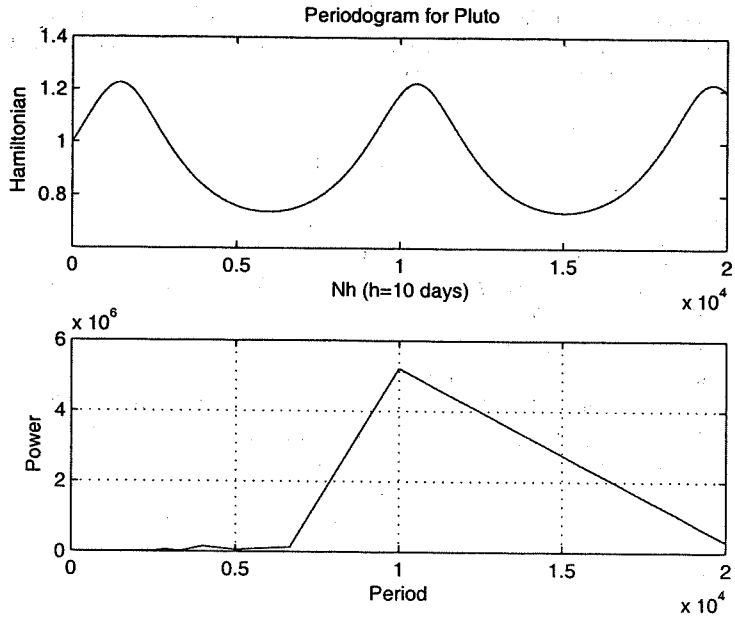

Fig. 3 – The Hamiltonian and the power spectrum for Pluto.

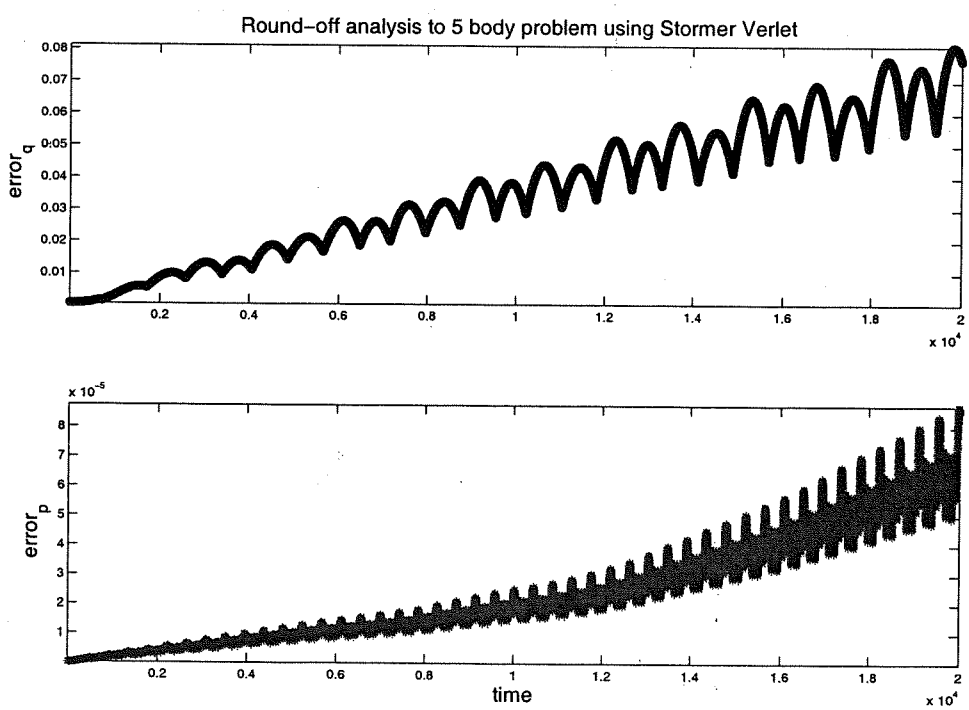

Fig. 4 – The round-off error analysis for the components q and p.

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