

Symplectic test particle encounters: a comparison of methods

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ABSTRACT

A new symplectic method for handling encounters of test particles with massive bodies is presented. The new method is compared with several popular methods (RMVS3, SYMBA, and MERCURY). The new method compares favourably.

Key words: methods: numerical – celestial mechanics.

1 INTRODUCTION

Most modern integration algorithms used in Solar system dynamics are symplectic. The symplectic algorithms split the Hamiltonian into separate efficiently solvable parts, and interleave the solutions of these parts to approximate the solution of the full problem. The splitting can be accomplished by introducing Dirac delta functions (Wisdom 1982; Wisdom & Holman 1991) or through the algebra of Lie series (Kinoshita, Yoshida & Nakai 1990; Yoshida 1993). Each has its advantages. For instance, the delta function approach naturally leads to the symplectic corrector (Tittlemore & Wisdom 1988; Wisdom, Holman & Touma 1996). The Lie series approach is algebraically simple. In this paper, I introduce a new symplectic method for evolving test particles in the field of fully interacting systems of massive bodies. The test particle may have close encounters with the massive bodies, but the massive bodies are assumed not to have close encounters. Example applications include the evolution of asteroids, meteoroids, and Kuiper belt objects.

The method of Wisdom & Holman (1991) is applicable to n -body problems wherein there is a dominant central mass. The method of Wisdom & Holman (1991) does not handle close encounters among the bodies because the averaging principle upon which it is based is not applicable. So a number of algorithms and associated codes have been presented that modify the Wisdom & Holman method to handle close encounters. The most popular codes include RMVS3 (Levison & Duncan 1994), SYMBA (Duncan, Levison & Lee 1998), and MERCURY (Chambers 1999). Wisdom & Holman (1991) used Jacobi coordinates to effect the elimination of the centre of mass, whereas Touma & Wisdom (1993a,b) used canonical heliocentric coordinates. RMVS3 is a straightforward Wisdom & Holman method using Jacobi coordinates, patched together with a non-symplectic method for handling encounters. The RMVS3 program is distributed in the SWIFT package. Duncan et al. (1998) use ‘democratic heliocentric variables’, which are just the canonical heliocentric coordinates with a slightly different splitting. SYMBA handles close encounters by recursively subdividing the step in a symplectic manner. MERCURY

solves the problem of close encounters by introducing a symplectic transition to an ordinary (non-symplectic) integration method that handles the close encounters. MERCURY also uses the democratic heliocentric coordinates. The democratic heliocentric coordinates have the disadvantage that integrators based on them do not perform well for ‘close encounters with the Sun’ (Levison & Duncan 2000). There exists a ‘modified SYMBA’ that addresses this problem by switching to a non-symplectic method for such encounters. The Wisdom & Holman (1991) method also has an instability if a step-size is not small enough to resolve the pericentre (Rauch & Holman 1999; Wisdom 2015).

The focus here is on the evolution of test particles that may have close encounters with massive bodies that do not themselves have close encounters. All of the above-mentioned programs can handle this case, except the ‘modified SYMBA’, which does not integrate test particles. I emphasize that MERCURY and SYMBA are designed to handle close encounters of the massive bodies as well, but that is not the focus here.

2 A NEW TEST PARTICLE ENCOUNTER METHOD

I introduce a new method for handling close encounters of test particles with massive bodies, based on the original Wisdom & Holman (1991) method. I assume that there is a dominant central mass. The method of Wisdom & Holman (1991) is used for the evolution of the massive bodies, which are here assumed not to have close encounters. However, test particles may have encounters with the massive particles. I use a switching function to handle these close encounters, as in Chambers (1999). However, the switching function used here is different from the one advocated by Chambers (1999): The one used here has higher order contact (more derivatives are continuous) and is active in a different range of radii. Also, I use Jacobi coordinates, rather than the democratic heliocentric coordinates used by Chambers (1999). This avoids the instability documented by Levison & Duncan (2000).

The Hamiltonian for the massive particles can be written (Wisdom & Holman 1991) as

$$H = H_K + H_I, \quad (1)$$

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with the Kepler Hamiltonian

$$H_K = \sum_{i=1}^{n-1} \left(\frac{p_i'^2}{2m_i'} - \frac{\mu_i}{r_i'} \right) \quad (2)$$

and the interaction Hamiltonian

$$H_I = \sum_{i=1}^{n-1} \left(\frac{\mu_i}{r_i'} - \frac{Gm_i m_0}{r_{i0}} \right) - \sum_{0 < i < j} \frac{Gm_i m_j}{r_{ij}}, \quad (3)$$

where n is the number of bodies, including the central body. Denoting Jacobi coordinates with a prime, the first Jacobi coordinate is the center of mass, with components \mathbf{x}'_0 . The remaining $n-1$ Jacobi coordinates are ($0 < i < n$)

$$\mathbf{x}'_i = \mathbf{x}_i - \mathbf{X}_{i-1}, \quad (4)$$

where \mathbf{X}_i denotes the centre of mass of bodies with indices up to i :

$$\mathbf{X}_i = \frac{1}{\eta_i} \sum_{j=0}^i m_j \mathbf{x}_j, \quad (5)$$

with

$$\eta_i = \sum_{j=0}^i m_j. \quad (6)$$

The coordinates of particle i are \mathbf{x}_i . The momenta conjugates to \mathbf{x}'_i are $\mathbf{p}'_i = m'_i \mathbf{v}'_i$, with $m'_i = \eta_{i-1} m_i / \eta_i$, and $m'_0 = \eta_{n-1}$ is the total mass. The magnitude of \mathbf{x}'_i is r'_i ; the distance between particles i and j is r_{ij} .

I allow for slightly different splittings from the one used in Wisdom & Holman (1991). Wisdom & Holman (1991) set $\mu_i = Gm_i m_0$; this choice leads to the usual disturbing function. Two other choices make sense: With $\mu_i = (m_0 + m_i) m'_i$, Kepler's two-body period law is satisfied by the unperturbed orbits, and with $\mu_i = \eta_i m'_i$, the unperturbed period of body i gives Kepler's period law with the sum of the masses with lower indices interacting with the body with index i . With the latter choice, for instance, Jupiter's unperturbed period is determined by its interaction with the sum of the masses of the Sun and the inner planets. I make this choice here.

The Hamiltonian governing the motion of test particles is conveniently obtained by setting the index of the test particle to be 1 and assuming the mass m_1 so small as to not affect the motion of the massive bodies. The Hamiltonian governing the motion of test particles is given by

$$H^T = H_K^T + H_I^T, \quad (7)$$

where

$$H_K^T = \frac{p_1'^2}{2m_1'} - \frac{Gm_1 m_0}{r_1'}, \quad (8)$$

and

$$H_I^T = \sum_{j>1} H_j^T, \quad (9)$$

with

$$H_j^T = - \left(\frac{Gm_j m_1}{r_{1j}} - \frac{Gm_j m_1 \mathbf{x}'_1 \cdot \mathbf{x}_{j0}}{r_{j0}^3} \right). \quad (10)$$

Note that if m_1 is infinitesimal, then $m'_1 = m_1$. If r_{1j} becomes small, then H_j^T can become comparable to H_K^T , and it is no longer convenient to approximate the motion in terms of Keplerian motion about

the central body plus interactions. I introduce a switching function to regroup the terms. Define

$$H_A^T = H_K^T + \sum_{j>1} H_j^T (1 - K_{R_j}(r_{1j})), \quad (11)$$

and

$$H_B^T = \sum_{j>1} (H_j^T K_{R_j}(r_{1j})). \quad (12)$$

The full test particle Hamiltonian is

$$H^T = H_A^T + H_B^T. \quad (13)$$

The function K is equal to 1 if r_{1j} is large compared to the Hill radius R_j of planet j , and it is 0 if r_{1j} is small compared to the Hill radius. If $K = 1$, the terms are grouped as before; if $K = 0$ for some j , then H_j^T is moved from H_B^T to H_A^T . I choose K to smoothly transition between 0 and 1, and so in the transition region there is a contribution from H_j^T to both H_A^T and H_B^T . I choose the function K as follows. First, define the function F over the interval 0–1 to be

$$F(x) = x^3 / (1 - 3x + 3x^2). \quad (14)$$

For $x < 0$, I take $F(x) = 0$ and for $x > 1$, I take $F(x) = 1$. Defined in this way, F and its first two derivatives are continuous at $x = 0$ and 1. In terms of F , define the switching function K

$$K_R(r) = F[(r - h_1 R)/(h_2 R)], \quad (15)$$

where h_1 and h_2 are constants, and R is a Hill radius. The Hill radius R_j for each planet j is also a constant that is set at the beginning of the evolution. If K is 1, then H_A^T is a Kepler Hamiltonian. I use the method of Wisdom & Hernandez (2015) to advance the orbit if $r > h_3 R$; otherwise, I use numerical integration. The method of Wisdom & Hernandez (2015) uses the Gauss f and g functions written in terms of universal variables to advance any orbit, whether bound or unbound. If K is not 1, then H_A^T is no longer a Kepler Hamiltonian, and it must be solved by some other method besides a Kepler advance. The Hamiltonian H_B^T does not depend on the momenta so it is easily solved to give a 'kick' to the momenta, regardless of the value of K . In these tests, I use $h_1 = h_2 = 1.5$ and $h_3 = 4.0$, and the Bulirsch–Stoer method to perform the numerical integrations.

To be explicit, the test particle kick, the solution of H_B^T , is

$$\Delta \mathbf{v}'_1 = -\Delta t \sum_j Gm_j (\mathbf{x}_{1j} b_j + \mathbf{x}_{j0} c_j), \quad (16)$$

where

$$b_j = \frac{K_{R_j}(r_{1j})}{r_{1j}^3} - \frac{DK_{R_j}(r_{1j})}{r_{1j}} \left(\frac{1}{r_{1j}} - \frac{\mathbf{x}'_1 \cdot \mathbf{x}_{j0}}{r_{j0}^3} \right) \\ c_j = \frac{K_{R_j}(r_{1j})}{r_{j0}^3}, \quad (17)$$

where DK_R is the derivative of K_R with respect to its argument, and Δt is the stepsize. The DK_R term arises from the application of the product rule since both H_j^T and the argument of K_R depend on the coordinate x_1 .

During an encounter, the solution of H_A^T is obtained by numerical integration. The equation of motion of the test particle is

$$\ddot{\mathbf{x}}'_1 = -\frac{Gm_0 \mathbf{x}'_1}{r_{01}^3} - \sum_{j=2}^n Gm_j (\mathbf{x}_{1j} b'_j + \mathbf{x}_{j0} c'_j), \quad (18)$$

with

$$b'_j = \frac{1 - K_{R_j}(r_{1j})}{r_{1j}^3} + \frac{DK_{R_j}(r_{1j})}{r_{1j}} \left(\frac{1}{r_{1j}} - \frac{\mathbf{x}'_1 \cdot \mathbf{x}_{j0}}{r_{j0}^3} \right),$$

$$c'_j = \frac{1 - K_{R_j}(r_{1j})}{r_{j0}^3}. \quad (19)$$

The equations of motion of the massive bodies are Keplerian:

$$\ddot{\mathbf{x}}'_i = -\frac{G\eta_i \mathbf{x}'_i}{(r'_i)^3}. \quad (20)$$

3 UNDERSTANDING MERCURY

In the algorithm described in the previous section, there are terms involving the switching function K_R , but also, from the product rule, terms involving DK_R , the derivative of the switching function with respect to its argument. Though the details are different in Chambers (1999), the full Hamiltonian still contains products of Hamiltonian-shaped functions multiplied by switching functions. The derivation of the corresponding kicks and equations of motion should therefore contain, by the product rule, terms involving the derivative of the switching function. But the terms involving the derivative of the switching function are missing in the Chambers (1999) algorithm and code. Thus, there is an error in the derivation of the algorithm used in MERCURY: The Hamiltonian describing the algorithm does not correspond to the algorithm.

Let us consider the situation further. In equation (9) of Chambers (1999), two parts of the full Hamiltonian are displayed:

$$H_A = \sum_{i=1}^N \left(\frac{p_i^2}{2m_i} - \frac{Gm_\odot m_i}{r_{i\odot}} \right) - \sum_{i=1}^N \sum_{j=i+1}^N \frac{Gm_i m_j}{r_{ij}} [1 - K(r_{ij})], \quad (21)$$

$$H_B = - \sum_{i=1}^N \sum_{j=i+1}^N \frac{Gm_i m_j}{r_{ij}} K(r_{ij}). \quad (22)$$

In the resulting step-by-step description of the integration algorithm, it is stated in step (i) that ‘Each body receives an acceleration (but not the Sun), weighted by a factor $K(r_{ij})$ ’. Then, again in step (iii), ‘the close encounter terms weighted by $(1 - K)$ are integrated numerically’. So in the stated algorithm there are no terms that involve DK , the derivative of the switching function. It is easy to check that in the MERCURY code this is in fact the case. So the Hamiltonian in Chambers (1999) does not correspond to the algorithm displayed in Chambers (1999) and in the MERCURY code.

Instead of equations (21) and (22), consider a pair of Hamiltonians of the form

$$H'_A = \sum_{i=1}^N \left(\frac{p_i^2}{2m_i} - \frac{Gm_\odot m_i}{r_{i\odot}} \right) - \sum_{i=1}^N \sum_{j=i+1}^N Gm_i m_j \left(\frac{1}{r_{ij}} - \Phi(r_{ij}) \right), \quad (23)$$

$$H'_B = - \sum_{i=1}^N \sum_{j=i+1}^N Gm_i m_j \Phi(r_{ij}). \quad (24)$$

The sum of H'_A and H'_B is independent of Φ for an arbitrary Φ , and the remaining terms are appropriate pieces of the full Hamiltonian.

So this appears to be a valid splitting. In order to be consistent with the MERCURY algorithm, Φ must satisfy

$$D\Phi(r_{ij}) \frac{x_{ij}}{r_{ij}} = -\frac{x_{ij}}{r_{ij}^3} K(r_{ij}). \quad (25)$$

The function of one argument Φ can be obtained by integration:

$$\Phi(r) = - \int_\infty^r \frac{K(\rho)}{\rho^2} d\rho, \quad (26)$$

where ρ is the variable of integration.

However, there is another requirement on the splitting. For a practical algorithm, when r is larger than the encounter distance (a few Hill radii), the Hamiltonian H'_A must equal a sum of Kepler Hamiltonians. Thus, in equation (23), the term involving $1/r_{ij}$ must cancel the term involving $\Phi(r_{ij})$. This is satisfied as follows. The switching function K has the property that it becomes 1 for a large argument. To be specific, let us denote the radius beyond which K is 1 by r_* . For $r > r_*$, the Φ integral is then

$$\Phi(r) = \int_r^\infty \frac{1}{\rho^2} d\rho = \frac{1}{r}, \quad (27)$$

and, for $r < r_*$,

$$\Phi(r) = \int_r^{r_*} \frac{K(\rho)}{\rho^2} d\rho + \frac{1}{r_*}. \quad (28)$$

The fact that $\Phi(r) = 1/r$ for $r > r_*$ means that the required cancellation occurs, and H_A is indeed a sum of Kepler Hamiltonians.

So the MERCURY algorithm and code are derived from an effective Hamiltonian, even though it is not the Hamiltonian described in Chambers (1999).

Hernandez (2016) presented evidence that the MERCURY code was not numerically symplectic. One might have suspected that since there are missing terms in the MERCURY algorithm, those involving the derivative of the switching function, that this might be responsible for the reported lack of symplecticity. However, since the algorithm is after all derived from an effective Hamiltonian, this is not the explanation of the reported lack of symplecticity.

4 COMPARISONS

The focus here is on the evolution of test particles perturbed by a system of massive planets that are not undergoing close encounters. The key issue is how well do the codes handle encounters of the test particles with the massive planets. An appropriate test is therefore the planar circular restricted three-body problem, wherein errors in the Jacobi constant can be used as a proxy for an integration error. None of the codes are specialized for this problem so it is a fair test. I study a chaotic exchange orbit because it repeatedly has strong encounters with the secondary body (even temporarily orbiting it).

Here I use a single planet (‘Jupiter’) and the Sun on a mutually circular orbit. I take the mass ratio for this system to be $\mu = m_J/(m_J + m_S) = 0.01$, where m_J is the mass of Jupiter and m_S is the mass of the Sun. The semimajor axis of Jupiter is 5.2 au; its orbital eccentricity is zero. It is started with longitude zero. The test particle has heliocentric coordinates (4.42, 0, 0) (in au), and heliocentric velocities (0, 0.0072, 0) (in au d⁻¹). The gravitational constant is $G = 0.000\,295\,912\,208\,232\,212\,84$ (in units of au, d, m_S). This is a chaotic exchange orbit that spends time orbiting each massive body.

A segment of the trajectory that is studied is shown in Fig. 1. The chaotic trajectory repeatedly visits each of the massive bodies. The eccentricity of the trajectory for a longer segment is shown in Fig. 2. The eccentricity explores a wide range of values, and the trajectory even becomes hyperbolic with respect to the Sun.

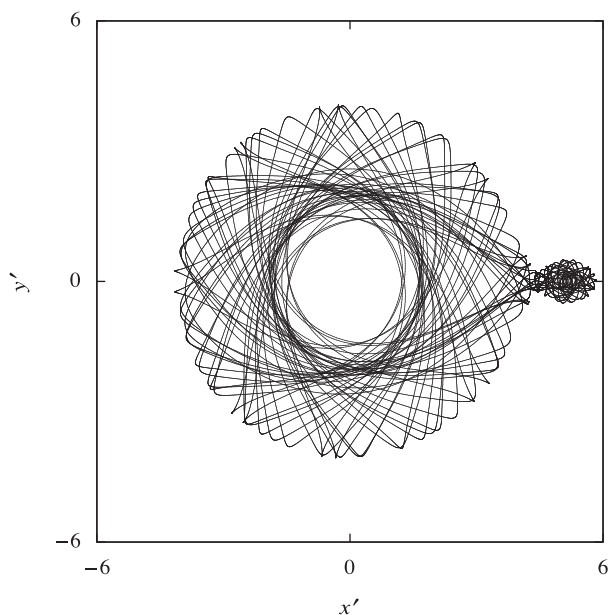


Figure 1. A segment of the trajectory in the frame rotating with Jupiter. Points are plotted once every 4 d for a total of about 500 yr.

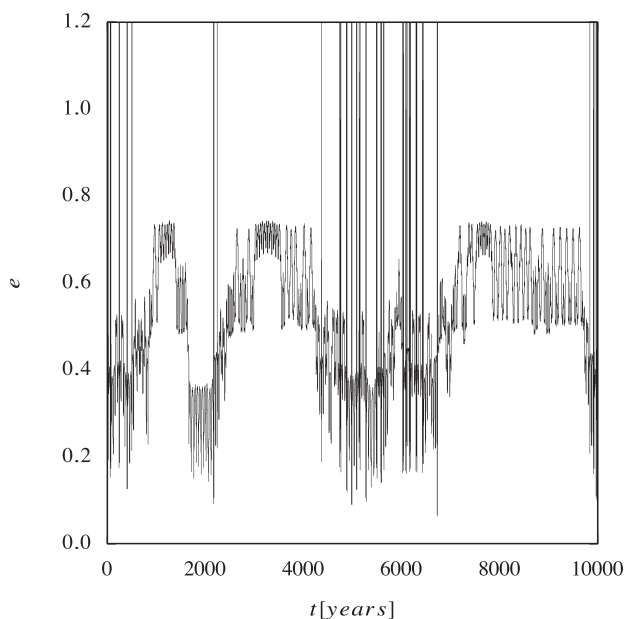


Figure 2. The eccentricity of the trajectory versus time. Points are plotted once every 4 d for a total of about 10 000 yr. This orbit explores many eccentricities, and, yes, the orbit is often hyperbolic with respect to the Sun ($e > 1$).

In the first set of tests, the stepsize was fixed at 40 d. Both *MERCURY* and *SYMBA* fail for this stepsize. This is probably a reflection of the fact that they use ‘democratic heliocentric’ coordinates. The method presented here and the *rmvs3* method exhibit typical relative errors in the Jacobi constant of the order of 10^{-4} (see Figs 3 and 4). The results for the *rmvs3* method exhibit spikes in the Jacobi constant errors.

For the method presented here, the symplectic corrector (Wisdom et al. 1996) can be used to reduce the apparent error (see Fig. 5). The fact that the corrected error exhibits an irregular behaviour (and

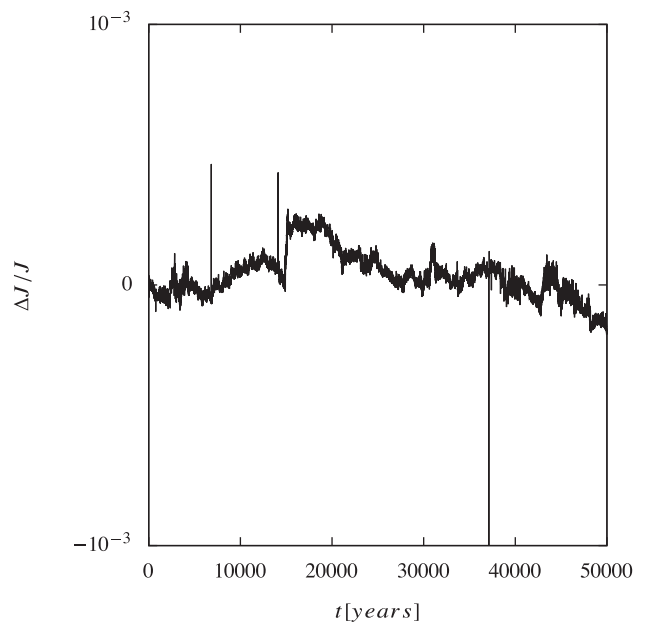


Figure 3. Relative error in the Jacobi constant for 50 000 yr using *rmvs3* with a stepsize of 40 d.

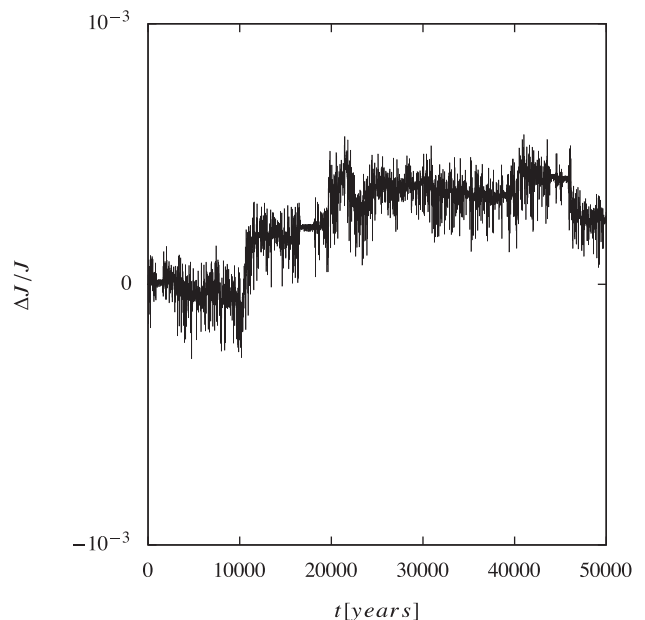


Figure 4. Relative error in the Jacobi constant for 50 000 yr using the method presented here with a stepsize of 40 d.

this behaviour is similar to that of *rmvs3*) suggests to me that the stepsize is too large for these two methods.

In the next set of tests, the stepsize was fixed at 8 d, a factor of 5 smaller than for the previous tests. For *rmvs3* (Fig. 6), *SYMBA* (Fig. 7), and *MERCURY* (Fig. 8), the errors are all of the order of 10^{-5} , but they all have large spiky errors. *SYMBA* may even display a slight secular (linear) error. The errors for the new method are presented in Fig. 9. The errors are smaller than for the other methods, and do not exhibit spikes. Again, this error can be reduced by applying the corrector. The corrected error is of the order of 10^{-6} (see Fig. 10).

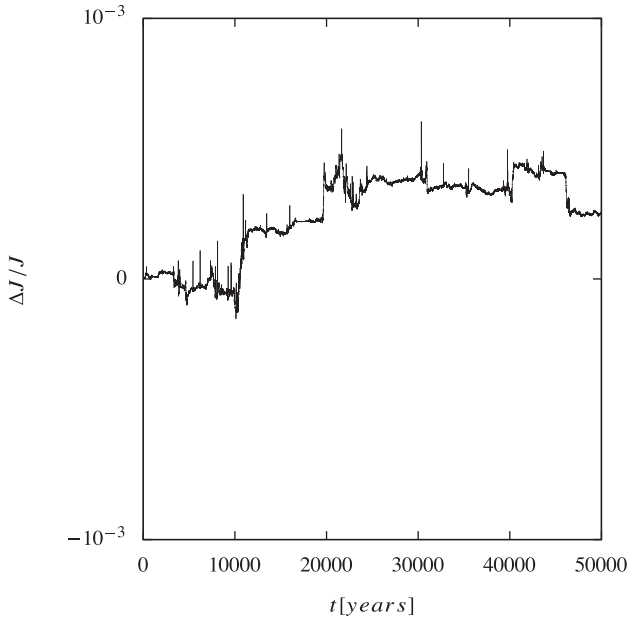


Figure 5. Relative error in the Jacobi constant for 50 000 yr using the method presented here with a stepsize of 40 d. The corrector has been applied.

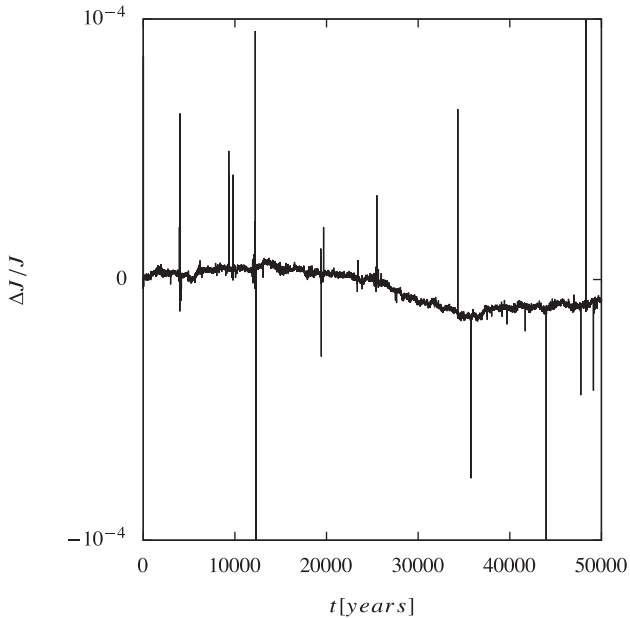


Figure 6. Relative error in the Jacobi constant for 50 000 yr using RMVS3 with a stepsize of 8 d.

5 SUMMARY

I have presented a new symplectic method for handling close encounters between test particles and massive particles. The method is a straightforward generalization of the method of Wisdom & Holman (1991). It uses a switching function to shift large terms during a close encounter.

The performance of the new method has been compared to that of three commonly used integration codes: RMVS3 (Levison & Duncan 1994), SYMBA (Duncan et al. 1998), and MERCURY (Chambers 1999). Both SYMBA and MERCURY are more general than the application here in that they are designed to handle close encounters of massive

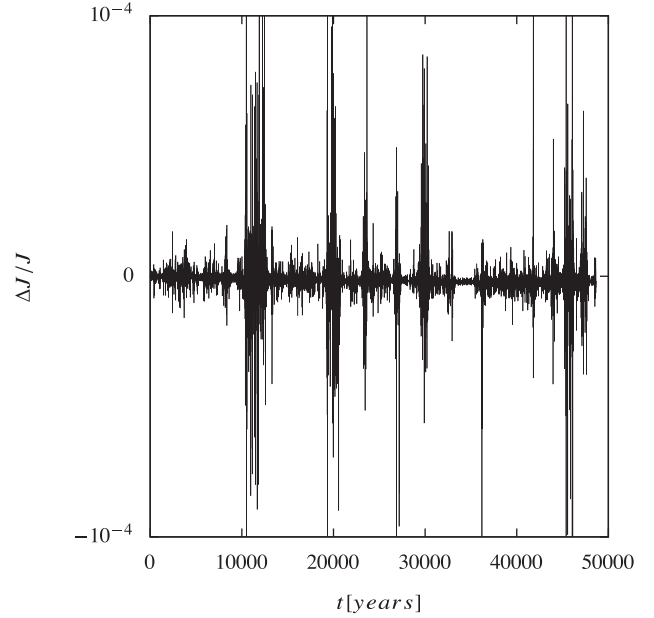


Figure 7. Relative error in the Jacobi constant for 50 000 yr using SYMBA with a stepsize of 8 d. The data for the run were kindly provided by Hal Levison. Note that there may be a slight secular drift downwards.

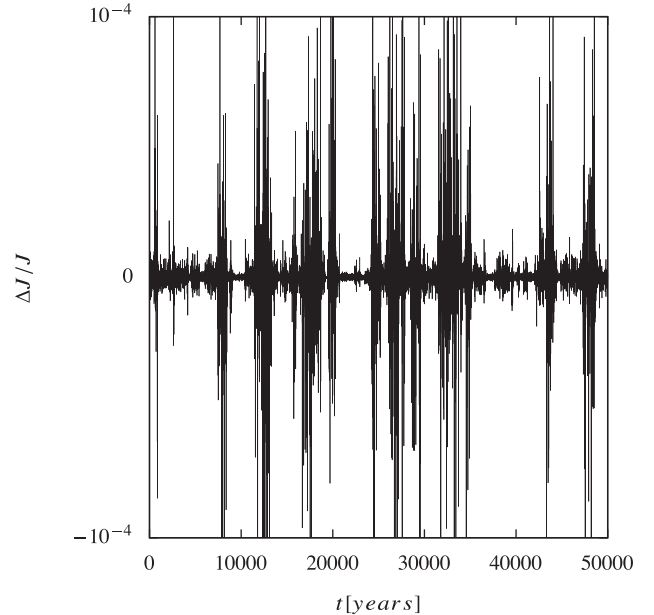


Figure 8. Relative error in the Jacobi constant for 50 000 yr using MERCURY with a stepsize of 8 d. The data for the run were kindly provided by David Hernandez.

bodies as well as close encounters of test particles with massive bodies. In these test particle tests, the performance of both SYMBA and MERCURY is surprisingly poor. They both fail at a large stepsize, and produce noisy results at a smaller stepsize. The performance of RMVS3 is comparable to that of the new method at a large stepsize, but there are indications that the stepsize should be smaller. For a smaller stepsize, the new method produces clean results that can be corrected, whereas RMVS3 exhibits less clean results with troublesome spikes in the Jacobi constant errors. Altogether, the new method performs favourably compared to the other methods.

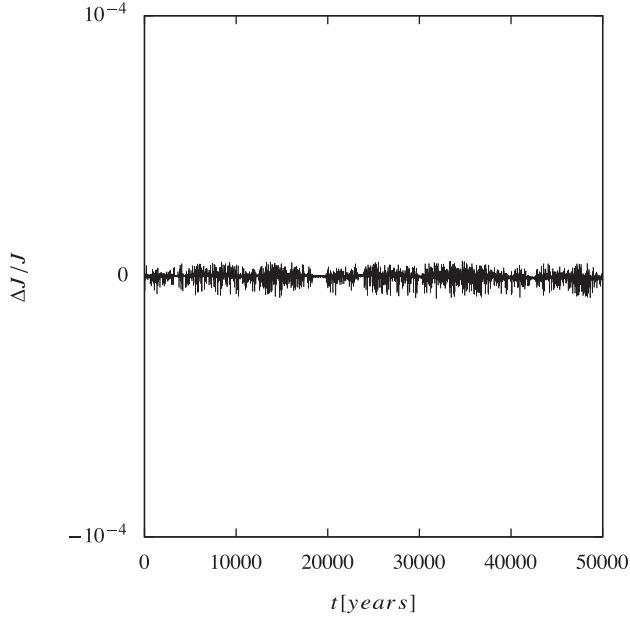


Figure 9. Relative error in the Jacobi constant for 50 000 yr using the method presented here with a stepsize of 8 d.

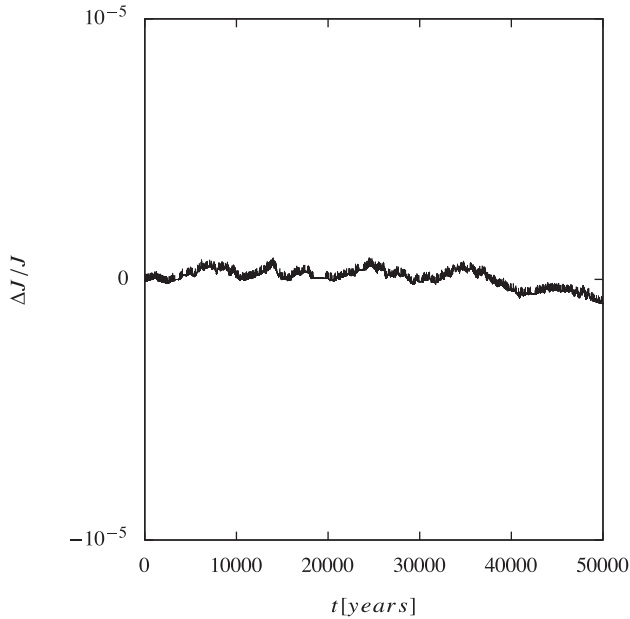


Figure 10. Relative error in the Jacobi constant for 50 000 years using the method presented here with a stepsize of 8 d. The corrector has been applied. Note the change in scale.

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