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ASTEROID MEAN ELEMENTS: HIGHER ORDER AND ITERATIVE THEORIES

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ABSTRACT

Mean orbital elements are obtained from osculating ones by removing the short periodic perturbations. Large catalogues of asteroid mean elements need to be computed, as a first step in the computation of proper elements, used to study asteroid families. The algorithms for this purpose available so far are only accurate to first order in the masses of the perturbing planets; the mean elements have satisfactory accuracy for most of the asteroid belt, but degraded accuracy in the neighbourhoods of the main mean motion resonances, especially the $2:1$. We investigate a number of algorithms capable of improving this approximation; they belong to the two classes of Breiter-type methods and iterative methods. The former are obtained by applying some higher order numerical integration scheme, such as Runge-Kutta, to the differential equation whose solution is a transformation removing the fast angular variables from the equations; they can be used to compute a full second order theory, however, only if the full second order determining function is explicitly computed, and this is computationally too cumbersome for a complicated problem such as the N-body. The latter are fixed point iterative schemes, with the first order theory as an iteration step, used to compute the inverse map from mean to osculating elements; formally the method is first order, but because they implement a fixed frequency perturbation theory, they are more accurate than conventional single iteration methods; a similar method is already in use in our computation of proper from mean elements. Many of these methods are tested on a sample of asteroid orbits taken from the Themis family, up to the edge of the $2:1$ resonance, and the dispersion of the values of the computed mean semimajor axis over $100,000$ years is used as quality control. The results of these tests indicate that the iterative methods are superior, in this specific application, to the Breiter methods, in accuracy and reliability. This is understood as the result of the cancellations occurring between second order perturbation terms: the incomplete second order theory, resulting from the use of a Breiter method with the first order determining function only, can be less accurate than complete, fixed frequency theories of the first order. We have therefore computed new catalogues of asteroid mean and proper elements, incorporating an iterative algorithm in both steps (osculating to mean and mean to proper elements). This new data set, significantly more reliable even in the previously degraded regions of Themis and Cybele, is in the public domain.

Keywords: Asteroids, mean elements, Lie series, short periodic perturbations, mean motion resonances, analytical theories, iterative methods, Runge-Kutta, Themis family.

1 INTRODUCTION

To compute accurate mean elements for a large number of asteroids is an essential step in the procedure to compute proper elements, and therefore to identify asteroid families, to assess their age, to study the dynamical structure of asteroid belt, and the chaotic phenomena of diffusion over very long time spans.

In our previous work, which has been published in Milani and Knežević (1990, 1992, 1994; hereinafter referred to as Paper I, II, III, respectively), mean elements have been computed with a fully analytical theory, of the first order in the mass of the perturbing planets Jupiter and Saturn.

For the purpose of producing large catalogues of mean and proper elements, to identify most asteroid families, the accuracy of the algorithm used in the mean elements computations was satisfactory; see e.g. Tables I and III-IV in Paper III. However, there are regions of the asteroid main belt where the accuracy of the mean elements is known to be degraded, mostly in the neighbourhood of some mean motion resonances with Jupiter; see e.g. Table II in Paper III.

In this paper we report on an attempt to improve upon the accuracy, and especially upon the reliability, of our mean elements computations. This is important because the study of asteroid families, and of dynamical phenomena like stable chaos, needs to be performed without excluding any region populated by asteroids.

We have explored two possible approaches to obtain more accurate and reliable mean elements. One approach is based upon ideas introduced recently by Breiter (1997a). It consists of the use of a numerical integration scheme, not to solve the differential equations of motion, but to solve the differential equations with the determining function playing the rôle of the Hamiltonian, whose solution is a canonical transformation simplifying the equations of motion; see Section 2.2. From this point of view, the conventional first order computation is equivalent to solve this auxiliary differential equation by the Euler method of numerical integration. If a higher order numerical integration method, such as a Runge-Kutta scheme, is used, this allows to include in the computation part of the second order effects, even when only the first order portion of the determining function is available. In other words, this allows to compute the second order portion while performing transformation to symplify the first order part of the equations; for formal definitions, see Sections 2.1 and 2.2. As it is the case for the N-body problem, the second order determining function would contain a very large number of terms, and the question is whether the part of the second order effects accounted for in this way is sufficient to achieve the desired accuracy.

The other approach is similar to the one we have already used in the computation of proper elements from the mean ones, namely the use of iterative methods. They amount, at convergence of the iterations, to the computation of the inverse map, which is a perturbation theory with fixed frequencies. A purely analytical, explicit computation without iterations would on the contrary be a perturbation theory with fixed initial conditions and variable frequencies, and this is known to be an inconsistent way to take into account

higher order effects, due to the divergence of the perturbative series (see e.g. Milani, 1988). The algorithm we propose uses the analytical first order solution as one iteration step, to be repeated until a fixed point equation is solved within the required convergence control; see Section 2.3. As in the case of the proper elements (see Papers I and II), the question is whether this convergence occurs.

This paper is organised as follows. In Section 2 we present, in a general setting, the higher order and iterative methods we were interested in. In Section 3 we present the specific problem of the computation of asteroid mean elements, we describe the tests of many different algorithms on a sample of asteroids in the neighbourhood of the $2:1$ resonance, and we discuss the test results in terms of the dispersion of the mean semimajor axis (which should be almost constant in the hypothetical perfect computation). In Section 4 we draw the conclusions on which algorithm should be used, why it is the best, and where in the asteroid belt it results in significant improvements.

2 SECOND ORDER PERTURBATION THEORIES

To describe the possible strategies to compute perturbative theories complete to higher order in the small parameter, we shall begin with a general discussion, without reference to a specific problem. The general problem to be solved to higher order is defined by some Hamilton function $H(X,Y)$ of vector coordinates X and momenta Y:

$$\begin{cases} \dfrac{dX}{dt} = \dfrac{\partial H}{\partial Y} \\ \dfrac{dY}{dt} = -\dfrac{\partial H}{\partial X} \end{cases} .$$

The goal is to perform a canonical transformation such that in the new variables X', Y' the differential equations are simpler, the simplest possible being the trivially integrable system with Hamiltonian $H' = H'(Y')$ depending only upon the new momenta.

This can be achieved in different ways, which are more or less equivalent up to the first order. On the contrary, the algorithms to push the solution to either second or higher order are very different from each other and, at least from the computational point of view, are not equivalent. The Lie series method appears to be the most efficient, for many specific problems, to define the transformation reducing the complexity of the Hamiltonian. However, even once the Lie series transformation has been defined, there are many different procedures to actually compute it for specific initial conditions. In the rest of this Section we will describe some of the possible choices for these computational procedures.

2.1 LIE SERIES TRANSFORMATIONS

The *Lie transform* of a function H, with *determining function* W, is defined by the expansion in formal power series (see Hori, 1966; Message, 1976; for the specific form of the algorithm used here, see Milani and Knežević, 1990):

$$H' = T_W H = H - \{H, W\} + \tfrac{1}{2}\{\{H, W\}, W\} + \dots \tag{2.1}$$

where $\{.,.\}$ is the Poisson bracket. The series behaves well only when the transformation, defined by the flow of the dynamical system with Hamiltonian W, is close to the identity, and this results in a smallness requirement for W; thus we assume that W is of positive order in some *small parameter* ε:

$$W = \varepsilon W_1 + \varepsilon^2 W_2 + \dots \tag{2.2}$$

and expanding the Lie series (2.1) in powers of the small parameter we get:

$$H' = H - \varepsilon\{H, W_1\} + \varepsilon^2[-\{H, W_2\} + \tfrac{1}{2}\{\{H, W_1\}, W_1\}] + \dots \ ; \tag{2.3}$$

H itself contains an order zero part and an order 1 part in the same small parameter ε

$$H = H_0 + \varepsilon H_1 \ ; \tag{2.4}$$

as a matter of principle, H could also contain higher order portions $\epsilon^2 H_2 + \ldots$, but this is not the case for the asteroid problem in heliocentric coordinates. Then the result of (2.1) is reordered by powers of ε:

$$\begin{aligned} H' =& T_W H = H_0 + \varepsilon[H_1 - \{H_0, W_1\}] + \\ &+ \varepsilon^2[-\{H_0, W_2\} - \{H_1, W_1\} + \frac{1}{2}\{\{H_0, W_1\}, W_1\}] + \ldots \ . \end{aligned} \tag{2.5}$$

The main purpose of a Lie series transformation, given by formulas such as (2.5), is to "solve" the problem, that is to transform the Hamiltonian (2.4) into a simpler one, whose solution can be explicitly computed. Let us assume that the coordinate system is such that the first approximation problem defined by the order zero Hamiltonian H_0 is already solved, i.e. a function of the momenta Y only:

$$H = H_0(Y) + \varepsilon H_1(X, Y) \ . \tag{2.6}$$

Then by the Arnold-Jost theorem (Arnold, 1976, Chap. 10), under suitable conditions of compactness, the coordinates X are angle variables, and H_1 can be expanded in a Fourier series. The Lie series (2.5) can be seen as a set of recursive equations constraining both the determining function W and the transformed Hamiltonian H': if H' is also expanded in powers of ε, that is $H' = H'_0 + \varepsilon H'_1 + \varepsilon^2 H'_2 + \ldots$:

$$\begin{aligned} H'_0(X', Y') &= H_0(Y') \\ H'_1(X', Y') &= H_1(X', Y') - \{H_0, W_1\}(X', Y') \\ H'_2(X', Y') &= -\{H_0, W_2\} - \{H_1, W_1\} + \tfrac{1}{2}\{\{H_0, W_1\}, W_1\} \ . \end{aligned} \tag{2.7}$$

To find the possible solutions of (2.7) we define the linear operator $\mathcal{L}$ acting on any function F as the Poisson bracket with the zero order Hamiltonian:

$$\mathcal{L}F = \{H_0, F\} \ ; \tag{2.8}$$

it defines a decomposition of the function space (of formal series) into a direct sum of the kernel (null space) of the operator $\mathcal{L}$ and of the image of $\mathcal{L}$:

$$F = \tilde{F} + \overline{F} \quad ; \quad \tilde{F} \in Im\,\mathcal{L} \ ; \ \overline{F} \in Ker\,\mathcal{L} \ . \tag{2.9}$$

Then the existence of solutions of the recursive equations (2.7) can be discussed by decomposing $H_1 = \overline{H_1} + \tilde{H}_1$: the equation

$$H'_1 = \overline{H_1} + \tilde{H}_1 - \mathcal{L}W_1 \tag{2.10}$$

has solution with $W_1 \in Im\,\mathcal{L}$ provided

$$H_1' = \overline{H_1} \ . \tag{2.11}$$

The second order equation:

$$H_2' = -\tfrac{1}{2}\{H_1 + \overline{H_1}, W_1\} - \mathcal{L}W_2 \tag{2.12}$$

gives the definition of H_2', and the equation for W_2 by using the decomposition (2.9):

$$H_2' = -\tfrac{1}{2}\overline{\{\tilde{H}_1, W_1\}} \tag{2.13}$$

$$\mathcal{L}W_2 = -\{\overline{H_1}, W_1\} - \tfrac{1}{2}\{\tilde{H}_1, W_1\} + \tfrac{1}{2}\overline{\{\tilde{H}_1, W_1\}} \tag{2.14}$$

and the solution $W_2 \in Im\,\mathcal{L}$ exists and is unique, thus H' and W are uniquely determined up to order 2, with:

$$W \in Im\,\mathcal{L} \quad ; \quad H' \in Ker\,\mathcal{L} \ . \tag{2.15}$$

It is interesting to remark that the two equations (2.13) and (2.14) are independent from each other, which means that to compute H' to order 2 the computation of W can stop at order 1; however, the computation of the map F_W to order 2 requires the use of W_2, e.g. for Y':

$$Y' = Y + \varepsilon\frac{\partial W_1}{\partial X} + \varepsilon^2\frac{\partial W_2}{\partial X} + \tfrac{1}{2}\varepsilon^2\{-\frac{\partial W_1}{\partial X}, W_1\} + \ldots \tag{2.16}$$

In practice, $\tilde{H}_1$ contains a large number of terms, e.g. 378 terms in our mean elements theory (Knežević 1992, Paper II), and so does W_1, because W_1 is obtained by term by term integration solving (2.10)-(2.11), that is $\mathcal{L}W_1 = \tilde{H}_1$. Thus W_2, if obtained by term by term integration to solve (2.14), would have a much larger number of terms, and is a very difficult to compute in an efficient way. As a result, this was never done in practice for asteroid orbits. Then the problem arises if it would be useful to use a reduced computation:

$$Y' = Y + \varepsilon\frac{\partial W_1}{\partial X} + \tfrac{1}{2}\varepsilon^2\{-\frac{\partial W_1}{\partial X}, W_1\} + \ldots \tag{2.17}$$

without the need to compute W_2; this means compute to second order the transformation defined by the first order formalism. We need to stress that this is by no means the same as computing to second order the transformation defined by the first AND the second order determining function as in (2.16). Nevertheless, computing (2.17) many more terms are included with respect to the first order transformation

$$Y' = Y + \varepsilon\frac{\partial W_1}{\partial X} + \ldots \tag{2.18}$$

and one may wonder if (2.17) allows some improvement in accuracy with respect to (2.18). This naive assumption, that computing more terms is better, turns out not to be correct, as we shall see in Section 3.

Another important issue is which transformation has to be computed: either from Y to Y', or from Y' to Y (see Paper I, Section 3.3). From the general theory we know that the perturbative series can be convergent only when computed with fixed frequencies (Poincaré, 1893, page 105), and indeed the so called KAM theory (Arnold, 1963) proves that in this case convergence can occur. If the transformed Hamiltonian H' depends only upon Y', then it is integrable with frequencies depending only upon the momenta Y'; thus the reverse map can be computed by a convergent series, defined by the determining function $-W(X', Y')$, of which the first order part is

$$Y = Y' - \varepsilon \frac{\partial W_1}{\partial X'} + \dots \tag{2.19}$$

and a second order computation would be

$$Y = Y' - \varepsilon \frac{\partial W_1}{\partial X'} - \varepsilon^2 \frac{\partial W_2}{\partial X'} + \tfrac{1}{2}\varepsilon^2 \{-\frac{\partial W_1}{\partial X'}, W_1\} + \dots \ . \tag{2.20}$$

On the contrary, the map from Y to Y' can not be defined by the perturbative series in a convergent way (unless the original problem was integrable, which is not the case for the N-body problem). The problem is, in the computation of mean elements Y' we have the osculating elements Y for input, and we have to compute the map in the "wrong" way.

2.2 THE METHOD OF BREITER

The new idea introduced by Breiter (1997a) can be summarized in this way: the equations such as (2.17) for a Lie series transformation can be understood as the integral flow at time 1 of the Hamilton equations with the determining function εW_1 as Hamiltonian. Then the Lie series method, which essentially amounts to a solution of the differential equation by a power series in the small parameter ε, can be replaced by any numerical integration method applied to the same ordinary differential equation.

From this point of view, the conventional first order perturbation theory (2.18) corresponds to the Euler method

$$y(t+h) = y(t) + hf[y(t)] \quad \text{solution of} \quad \frac{dy}{dt} = f[y] \tag{2.21}$$

applied to the Hamilton equations defined by εW_1, with the stepsize $h = 1$; note that the size of the truncation error contains a power of h, which in this case does not matter, but also a power of the perturbation parameter ε contained in the norm of the right hand side of the differential equation. Euler method being of the first order, the error is of the order of $h^2\varepsilon^2 = \varepsilon^2$.

Thus to compute a transformation equivalent to (2.17), that is to compute to second order in the parameter ε the first order transformation defined by εW_1, it is enough to use

a second order numerical integration algorithm. Breiter suggests to use simply the order 2 explicit Runge-Kutta method:

$$y(t+h) = y(t) + \frac{h}{2}\left\{f[y(t)] + f\left[y(t) + hf[y(t)]\right]\right\} . \tag{2.22}$$

He also points out that any other single step numerical integration scheme could be used, e.g. any other Runge-Kutta method; moreover, the single step of stepsize $h = 1$ could be replaced by two steps of stepsize $h = 1/2$, three steps of stepsize $h = 1/3$ and so on, selecting a short enough step to achieve the desired accuracy, as it is usual in numerical integrations.

As emphasized by Breiter, this argument applies only once the analytical expression of the determining function W_1 has been deduced, e.g. from the equation (2.10). The same algorithm could be applied to the second order transformation defined by $\varepsilon W_1 + \varepsilon^2 W_2$, but this is possible only once the analytical expression of W_2 is known. To achieve this, either the Lie series technique, or some equivalent algorithm, needs to be used to deduce W_2, e.g. from (2.14), before this method can be used to full second order, as in Breiter (1997b). The same argument applies to the extension to an even higher order.

2.3 THE ITERATIVE METHOD

Iterative methods have been introduced in Paper I, thus in the present paper we shall only briefly summarize the argument. The explicit reverse map (2.19)–(2.20), which has the advantage that the perturbation series are computed with fixed frequencies, could be interpreted as an equation defining in an implicit way Y' as a function of Y. To solve this implicit function problem, we can convert it in a fixed point problem, by adding to the set of variables the vector of frequencies:

$$\nu' = \frac{\partial H'(Y')}{\partial Y'} . \tag{2.23}$$

The determining function W_1 for the first order map (2.19) is obtained by solving $\mathcal{L}W_1 = \tilde{H}_1$. This can be done term by term in the expansion of the perturbation H_1 in Fourier series of the angles X', and results in the coefficient of each Fourier term of H_1 being divided by a *divisor*, which is an integer combination of the frequencies ν_i'. Thus $W_1 = W_1(Y', X', \nu')$:

$$\begin{cases} \nu' = \dfrac{\partial H'(Y')}{\partial Y'} \\ Y' = Y + \varepsilon \dfrac{\partial W_1(X', Y', \nu')}{\partial X'} \\ X' = X - \varepsilon \dfrac{\partial W_1(X', Y', \nu')}{\partial Y'} . \end{cases} \tag{2.24}$$

For fixed initial conditions, that is fixed X, Y, the right hand side of the equation (2.24) is a function of X', Y', ν', and the values of X', Y', ν' corresponding to X, Y are obtained as a fixed point of the map defined by the right hand side. The last two equations of (2.24) can be seen as an implicit Euler method, the right hand side being computed on the arrival point, not on the starting point.

For ε small enough, this map is a contraction (with respect to some suitable metric in a function space) and has a unique fixed point, which can be obtained by iteration, starting from any reasonable first approximation.

One possible procedure is to use the unperturbed frequencies and one Euler step (2.18) to obtain a first approximation X'_1, Y'_1:

$$\begin{cases} \nu_1 = \dfrac{\partial H_0(Y)}{\partial Y} \\ Y'_1 = Y + \varepsilon \dfrac{\partial W_1(X, Y, \nu)}{\partial Y} \\ X'_1 = X - \varepsilon \dfrac{\partial W_1(X, Y, \nu)}{\partial X} \end{cases} \tag{2.25}$$

then proceed with fixed point iterations:

$$\begin{cases} \nu'_{n+1} = \dfrac{\partial H'(Y'_n)}{\partial Y'_n} \\ Y'_{n+1} = Y + \varepsilon \dfrac{\partial W_1(X'_n, Y'_n, \nu'_n)}{\partial X'_n} \\ X'_{n+1} = X - \varepsilon \dfrac{\partial W_1(X'_n, Y'_n, \nu'_n)}{\partial Y'_n} \end{cases} \tag{2.26}$$

until satisfactory convergence is achieved, that is until the changes from one iteration to the next become smaller than the required accuracy.

The same procedure could be applied to the second order reverse map (2.20), but again this would require an explicit knowledge of the analytical expression of W_2, and this is unpractical for the mean elements theory.

2.4 THE REVERSIBLE SYMPLECTIC METHOD

There are two properties of single step numerical integration methods especially relevant for their use in the context of the method of Breiter.

The first property is that, when the numerical integration method is applied to a Hamilton system of differential equations, the map defined by the discrete step approximation is canonical (in exact arithmetic, neglecting rounding off). The numerical methods with this property are called *symplectic*.

The second property is that, when one step in the numerical solution of a differential equation is performed with stepsize h, and then it is followed by a step with the same method and stepsize $-h$, the numerical approximation returns exactly to the initial conditions (in exact arithmetic, neglecting rounding off). The numerical methods with this property are called *reversible*.

In general the Runge-Kutta schemes do not have these properties. However, there is a special class of Runge-Kutta methods, the ones based upon the Gauss-Legendre quadrature formula, which have the following three properties:

- the Runge-Kutta-Gauss methods are the only ones with s intermediate steps which are of order $2s$, that is the local truncation error is infinitesimal of the order of h^{2s+1} for $h \to 0$ (Butcher, 1987, page 219).
- the Runge-Kutta-Gauss methods have the symplectic property (Sanz-Serna, 1988).
- the Runge-Kutta-Gauss methods are reversible (Butcher, 1987, page 224).

The Runge-Kutta- Gauss methods are, however, implicit, that is some iterative procedure is involved in the computation of each step. There are no explicit Runge-Kutta methods with the symplectic property (Sanz-Serna, 1988; Cooper 1987). Moreover, no explicit Runge-Kutta scheme with s intermediate steps has order larger than s. Thus the price of the more involved computational procedure for an implicit method is justified by better accuracy and by the symplectic property.

For the definition of the Runge-Kutta-Gauss methods see e.g. Butcher (1987, pages 209–220); for an elementary introduction to the subject, see Milani and Mazzini (1997, Section 4.4).

The property of being symplectic is especially attractive for a numerical integration scheme used in the context of the Breiter method because the differential equation to be solved is indeed Hamiltonian with εW_1 as Hamilton function. The property of being reversible is even more attractive, because this means that it is not necessary to distinguish whether the equation being solved is the one for Y' as a function of Y, rather than the one for Y as a function of Y': a reversible method performs with the same accuracy in both directions. Finally, if the method is of order $2s$ with s intermediate steps, only 1 intermediate step is required for a computation exact to order ε^2.

The Runge-Kutta-Gauss method with 1 intermediate step and of order 2 is as follows, for the differential equation $dy/dt = f[y]$:

$$\begin{cases} z = y(t) + \dfrac{h}{2}\, f[z] \\ y(t+h) = y(t) + h\, f[z]\ . \end{cases} \tag{2.27}$$

A fixed point iteration is required to solve the first of the (2.27); the iteration can be started with $z_1 = y(t)$, then $z_2 = y(t) + h/2\ f[z_1]$ and so on, until satisfactory convergence; then the value of $f[z_n]$ at the last point is used to compute the second of the (2.27).

If too many iterations are required for convergence, the computational load can be decreased by resorting to the method of Aitken (Danby, 1988, page 157) to accelerate the convergence of the fixed point iterations.

When this numerical integration scheme is applied within the Breiter method, and to the transformation equations defined by the determining function εW_1, then the following two equations are simultaneously satisfied to order 2 in ε:

$$\begin{cases} Y' = Y + \varepsilon \dfrac{\partial W_1}{\partial X} + \frac{1}{2}\varepsilon^2 \{-\dfrac{\partial W_1}{\partial X}, W_1\} + \dots \\ Y = Y' - \varepsilon \dfrac{\partial W_1}{\partial X'} + \frac{1}{2}\varepsilon^2 \{-\dfrac{\partial W_1}{\partial X'}, W_1\} + \dots \ . \end{cases} \tag{2.28}$$

The properties of this scheme (Runge-Kutta-Gauss-Breiter method) are very interesting, but again we need to stress that this does not allow to compute in full the perturbative effects to second order in ε, unless the contribution by $\varepsilon^2 W_2$ is added, and this requires the explicit analytical expression of W_2.

It is also possible to use the Runge-Kutta-Gauss method of order 4 with 2 intermediate steps. However, it has little use to compute to order 4 the transformation defined by the determining function εW_1, which is of order 1. To compute in full the transformation to order 4 we would need to compute also W_2, W_3 and W_4, and this is not practical for a problem with many terms, such as the asteroid problems.

3 GENERATION OF ASTEROID MEAN ELEMENTS

The discussion of Section 2 refers to the elimination of all the terms containing any of the angle variables X from the Hamiltonian. In practice this is possible only under the condition that the unperturbed Hamiltonian H_0 is non degenerate, which is equivalent to the condition that the linear system for the coefficients of the Fourier series of W_1 resulting from $\mathcal{L}W_1 = \tilde{H}_1$ has always formal solutions.

In the case of the N-body problem, $H_0(Y)$ is the Hamiltonian of the 2-body problem, and it does not depend upon all the momenta Y, but only upon the canonical variable L corresponding to the semimajor axis of the asteroid, and upon L_p which is an auxiliary variable used to control the mean motion of the perturbing planet (see Paper I, Section 2.3). Therefore only the angular variables conjugate to L, L_p, namely the mean anomalies ℓ, ℓ_p (of the asteroid and of the planet, respectively), can be removed from H_1'; in this way the *mean elements* X', Y' are obtained. The slow angles $\omega, \Omega, \omega_p, \Omega_p$ still appear in H_1', and a second elimination step is required to compute *proper elements*, a new set of variables in which the Hamiltonian has been reduced to an integrable one, function of the momenta only.

In the computation of proper elements, presented in Papers I, II and III, we have used an iterative first order method to compute the proper elements from the mean ones. However, the mean elements have been computed from the osculating ones by a first order, non iterative method, of the Euler type, as defined in Section 2.2. In the present Section we are going to discuss the use of more advanced methods to compute mean elements.

To put the problem in the context of Breiter method, the differential equation to be solved numerically is the Hamiltonian system defined by a determining function

$$W_1 = W_1(\ell, \ell_p, \omega, \omega_p, \Omega, \Omega_p, L, L_p, G, G_p, \Pi, \Pi_p, n, n_p) \tag{2.29}$$

where G, G_p, Π, Π_p are the Delaunay momenta conjugate to $\omega, \omega_p, \Omega, \Omega_p$, and the dependency upon the frequencies (as discussed in Section 2.3) is represented by the mean motions n, n_p only. We have introduced an approximation, by which the secular frequencies of the slow angles $\omega, \omega_p, \Omega, \Omega_p$ are neglected in the computation of the divisors appearing in W_1. This approximation is legitimate because W_1 contains only Fourier terms including the fast variables ℓ, ℓ_p, thus all the divisors contain some multiples of n and/or n_p. Excluding the immediate neighbourhoods of mean motion resonances, where the integer combination of n, n' could be small, the contribution of the secular frequencies to the divisors is not important.

The small parameter ε is simply the mass of the perturbing planet divided by the central mass (which is roughly the mass of the Sun, possibly summed to the mass of Jupiter, depending upon the system of units used). In the first order formulas, the contribution of several perturbing planets can just be added together; in our computation of mean elements, we take into account Jupiter and Saturn. It is easy to check that the short periodic perturbations on the orbit of these two planets are small enough, thus a 2-body approximation (e.g. with constant n') can be used for the planets; for the asteroids, the

2-body formulae give just a zero order approximation, to be improved in the computation. This results in an explicit analytical expression for W_1 as a Fourier series (Yuasa, 1973; Knežević 1988, 1992).

3.1 THE METHODS TESTED

We have tested 9 different algorithms of the Breiter and/or iterative class on the same problem, namely the computation of mean elements for a number of difficult cases, that is for asteroids close to the very strong 2 : 1 mean motion resonance. The algorithms tested are listed below.

EULER Breiter method with Euler numerical integration algorithm; this is in fact the traditional first order perturbation theory, which we had already used in the previous papers.

RKG2 Breiter method with Runge-Kutta-Gauss numerical integration of order 2; this is the symplectic and reversible method of Section 2.4.

RK2 Breiter method with explicit Runge-Kutta of order 2 (and 2 intermediate steps), that is the method used by Breiter (1997a) himself.

EULER+REV Iterative method, with Euler method as starter, that is to compute the initial point of the iteration, as described in Section 2.3.

RKG2+REV Iterative method, but with a Breiter method with Runge-Kutta-Gauss of order 2 as starter.

RKG+REV Iterative method, but with a Breiter method with explicit Runge-Kutta of order 2 as starter.

RKG2AI Breiter method with Runge-Kutta-Gauss numerical integration of order 2; convergence accelerated with Aitken method, thus the right hand side is computed only 3 times.

RKG2AI/2 The same as RKG2AI, but with two half steps of length $h = 1/2$ instead of a single step of length $h = 1$ as in all other cases.

RKG4 Breiter method with Runge-Kutta-Gauss numerical integration of order 4, with 2 intermediate steps.

It has to be noted that some of these methods gave essentially identical results, thus the results are bundled together in the Table 1 of Section 3.3.

3.2 THE TEST CASES

The quality of the asteroid mean elements, as computed in our previous papers I, II and III, has been tested by means of accurate numerical integrations. Therefore it is well known in which regions of the asteroid belt the accuracy is degraded; it is also well understood that this mostly occurs near the strongest mean motion resonances. We have therefore selected for testing the new algorithms the region just inside the 2 : 1 resonance, in particular the portion of the proper elements space occupied by the Themis family, which corresponds to low inclination and moderate eccentricity. A better computation of mean elements, and therefore also of proper elements, for the Themis family members would help in understanding the structure of this family, which has a peculiar shape in proper elements space, in particular on the side neighbouring the resonance (Paper II, Figure 6; Morbidelli et al., 1995, Figure 6).

The selected test cases have been chosen to cover a wide range in values of the semimajor axis, up to the very edge of the resonance. We have numerically computed for $100,000$ years, with our standard public domain software *ORBIT9* for long term numerical integration, the orbits of 10 asteroids belonging to the Themis family. The test procedure is as follows: the output of the numerical integration has been stored once every 100 years, that is 1001 data points per asteroid; for each data point the mean elements have been computed with each of the 9 algorithms listed in Section 3.1. Smoothed orbital elements, from which all the oscillations with periods between 2 and 200 years have been removed, are also produced by online digital filtering (Carpino et al., 1987).

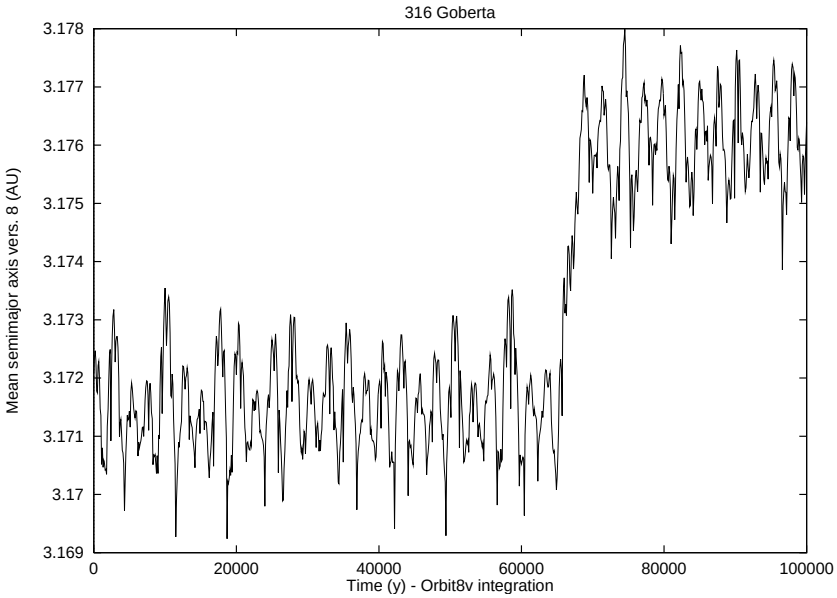

Fig. 1: The mean semimajor axis of *(316) Goberta* shows an abrupt change, indicating the switch between two different dynamical states. This behaviour is typical of stable chaos, and therefore this asteroid is not suitable as a test case.

The quality of the results is measured by the dispersion of values of the mean semimajor axis, which should be nearly constant if the computations had been perfect; more exactly we use the root mean square of the deviation from the long term average, and also the excursion, that is difference between maximum and minimum value over the entire set of data points. The filtered data are in most cases more stable than the analytically computed mean elements: secular changes on the semimajor axis are due to second order perturbations; because of the latter, the average value of the filtered semimajor axis is slightly different from the average value of the mean semimajor axis (Milani et al., 1987); these second order effects are anyway of the order of a few 10^{-4} AU, smaller than the accuracy in the computation of the mean semimajor axis, as it is clear from Table 1.

The filtered data are used as a check, to guard against chaotic behaviours which can degrade the stability of the mean elements, whatever the algorithm to compute them; these phenomena are discussed in Milani et al. (1997). Out of the sample of 10 Themis family members, *(316) Goberta* exhibited a typical "stable chaos" behaviour, with transition between different dynamical states (Figure 1). In this case the excursion of the values of the mean semimajor axis ($\Delta a = 8.7 \times 10^{-3}$ AU) and the RMS ($\sigma_a = 2.3 \times 10^{-3}$ AU) can not be significantly reduced: they measure a real diffusion phenomenon, and not the accuracy of our algorithms. The resonances involved are the same affecting *(490) Veritas*, e.g. with small divisors containing $10n - 21n_p$ (Milani et al., 1997). Thus this asteroid has not been used for the tests of our mean elements, and the results about it are not given.

3.3 RESULTS

For all selected asteroids we have computed the mean elements by using in turn each of the methods listed in Section 3.1. We performed other checks and comparisons, in particular we also computed proper elements to estimate the impact of the improved mean elements on the stability of the proper elements. These tests generated a wealth of data; thus we present and discuss only the most representative and the most significant results. Out of the nine methods, we are giving in Table 1 the results for only five (plus the digital filtering output for comparison), because some of the methods either gave results of lower accuracy and/or reliability, or gave results essentially equal to those of some others.

To illustrate our results, we have chosen the asteroid *(2114) Wallenquist* as the most representative of the results achieved. Its orbit is quite close to the resonance, thus the short periodic perturbations to be removed are quite large (Figure 2), and nevertheless suitable higher order and iterative methods can achieve a satisfactory accuracy (standard deviation less than 0.001 AU). Even closer to the resonance, as in the case of *(1229) Tilia*, the almost resonant perturbations are so large, and their period so long, that even digital filtering failed to remove them accurately, because the input frequency we used was too high. Farther from the resonance, the improvements resulting from the use of more advanced methods are less important. Thus we shall show the time series of the mean elements of *(2114) Wallenquist*, as obtained with different methods, starting from EULER, that is the method we had used in the past (Figure 3).

In addition to the time versus mean semimajor axis plot, we give the computed mean a versus the osculating one: a representation which clearly shows the relationship between the closeness to the resonance and the accuracy of the computation. The osculating semimajor axis changes by a large amount, ranging in this case from 3.18 to more than 3.24 AU, bringing the orbit in the resonance region (the nominal resonance being at 3.28 AU).

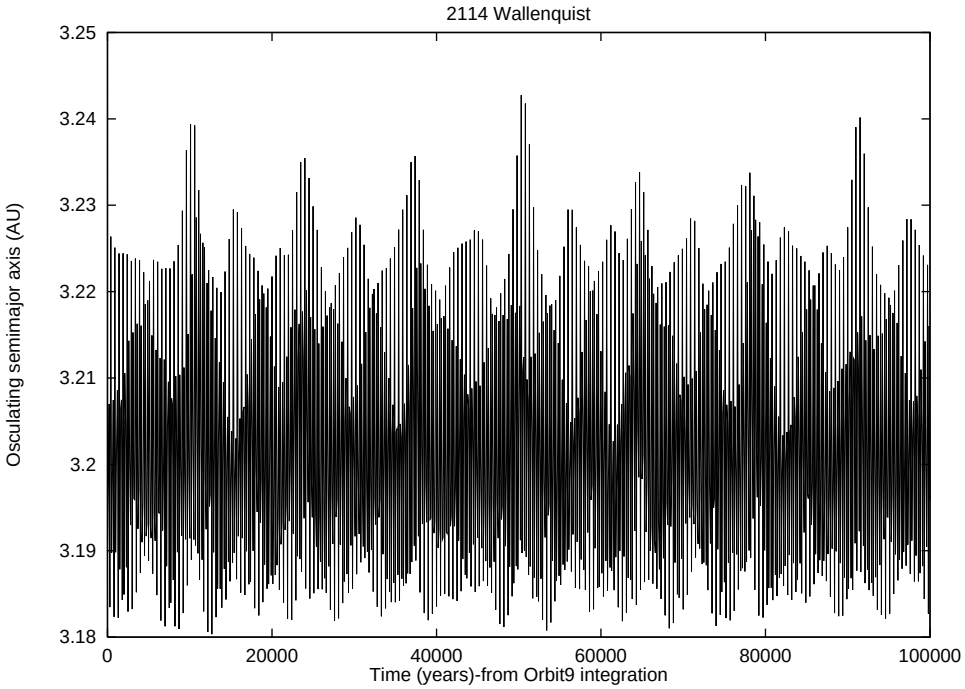

Fig. 2: Osculating semimajor axis of the asteroid *2114 Wallenquist*, obtained by numerical integration over a time span of $100,000$ years and sampled every 100 years. The apparently regular variations, with comparatively large amplitude, show no visible chaotic features. Thus this is a good test case for advanced methods of removal of the short periodic perturbations.

When the osculating orbit is closer to the resonance, the divisors containing the combination $n-2n_p$ are much smaller when n is a function of osculating semimajor axis a than when it is a function of the mean a. Thus the direct map (osculating to mean) contains bigger short periodic terms than the reverse map (mean to osculating). This results in overshooting, that is the short periodic term to be removed is computed at a value larger than the true one. On the other side, when the osculating a is smaller than the mean a, the short periodic terms to be removed are computed at a value smaller than the true one, and the direct map undershoots, resulting again in a computed value of the mean a lower than the true one. The undershooting is less pronounced than the overshooting, because the derivative of the divisor (with respect to a) is much larger near the resonance. Only for osculating a close to mean a the result is accurate. This explains the comparatively large peaks (in the direction opposite to the resonance) in the top Figure 3, and the curvature in the bottom part. As shown in Figures 4 and 5, this diagnostic curvature, typical of Euler method, can be reduced (and even reversed) by the use of more advanced methods.

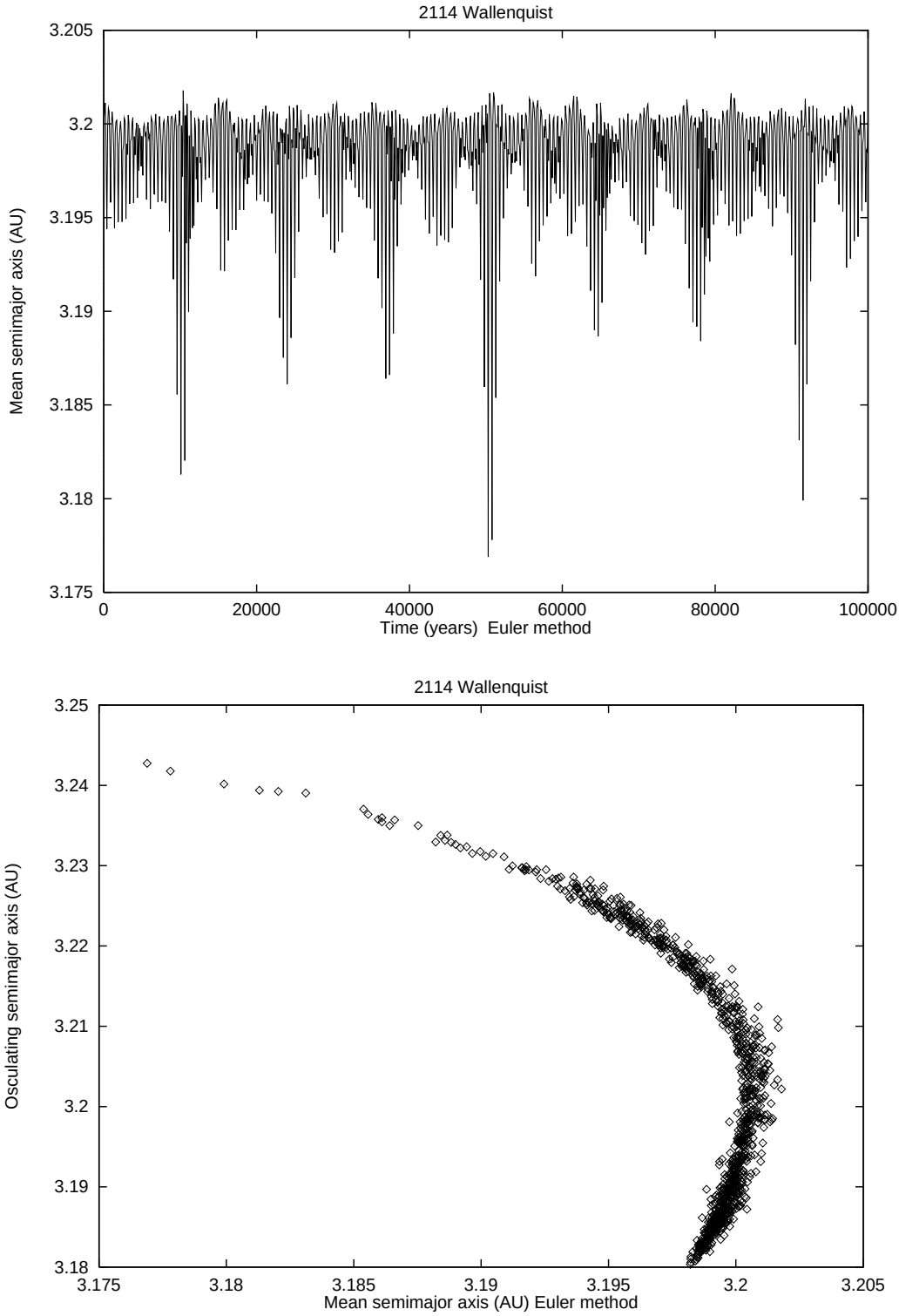

Fig. 3: Top: the mean semimajor axis of *2114 Wallenquist*, obtained by the Euler method. These results are typical of the previous state-of-the-art: the amplitude of the short periodic effects is much reduced, but still significant. Note the peaks in the direction opposite to the resonance. Bottom: the mean semimajor axis versus the osculating value. The curvature indicates that the 2:1 divisor computed with the osculating mean motion is the main source of error.

The Breiter methods, and especially the reversible RKG2, achieve a significant improvement with respect to EULER (see the comparison of the results in Table 1). The reason is the attenuation of the overshooting/undershooting effect due to the use of the osculating value of the small divisor discussed above, as it is graphically evident from Figure 4. The jumps towards lower values of the compute mean semimajor axis, however, are still there, and some curvature remains in the mean/osculating semimajor axis plot. From these results we can conclude that the Breiter type methods indeed result in improved accuracy, although the superiority of RKG2 over RK2, shown by Table 1, indicates that the reversibility (that is, the correct computation of the reverse map) plays also a role.

The iterative methods (EULER+REV, RKG2+REV, RKG+REV) gave almost identical results; this can be understood, since these methods only differ in the starting procedure; when an iterative method is convergent, the fixed point does not depend upon the starting point. The results are the same because convergence was always achieved, although the number of iterations was in some cases large, up to 7 iterations (up to 9 iterations for the asteroid closest to the resonance in our sample, namely *(1229) Tilia*). By using a more sophisticated starter, the number of iterations can be reduced, but typically only by either 1 or 2. Since a more complicated starter has also a computational cost, the conclusion is that the method with the simplest Euler starter is more efficient; thus Table 1 contains only the results of EULER+REV, which are representative of the accuracy of all three iterative methods; Figure 5 illustrates the result for this method, showing the almost complete disappearance of the jumps to lower values; the curvature of the mean/osculating semimajor axis plot has been replaced by a strange shape, reflecting the known complexity of a map defined by an iterative method.

The methods using the Aitken convergence accelerator did not give satisfactory results. The main reason was that we limited the number of iterations to three, hoping that the Aitken extrapolation based upon these would achieve convergence with competitive accuracy. This was not the case for the asteroids closer to the resonance, such as *(1229) Tilia* and *(2114) Wallenquist*; also for others there were some data points where convergence did not occur. The situation was not much improved even using the half step. We conclude that the use of such a small number of iterations decreases the reliability of the result. On the other hand, for the Aitken method to perform another extrapolation, three more iterations are required, and this would become even less efficient than the plain iterative method. Therefore the results for RKG2AI and RKG2AI/2 are not listed in Table 1.

In the Table we give, for each method and for each orbit, the asteroid number, the average value $\overline{a}$, over the entire time span, of the mean semimajor axis, the standard deviation σ_a and the excursion Δa. The two measures of the dispersion of a are given because they provide different insights. The standard deviation measures the average accuracy, which is important for statistical applications such as identification of asteroid families. The excursion measures the reliability of the method, and this is important to understand the shape of the families, as in the already discussed case of the apparent spreading of the Themis family, as the border of the $2:1$ resonance is approached.

TABLE 1.
Results of the accuracy tests

	FILTERED			EULER		
No	$\bar{a}$	σ_a	Δa	$\bar{a}$	σ_a	Δa
24	3.13451	0.00005	0.00027	3.13439	0.00023	0.00220
90	3.14619	7	41	3.14597	30	293
561	3.16794	42	201	3.16772	55	421
1229	3.21494	446	1403	3.20883	460	5025
1340	3.18087	46	209	3.17951	100	884
1489	3.18647	24	108	3.18339	184	1478
1674	3.18430	22	95	3.18359	68	540
1956	3.19963	18	89	3.19868	95	812
2114	3.20294	38	180	3.19853	290	2490
	RKG2			RK2		
No	$\bar{a}$	σ_a	Δa	$\bar{a}$	σ_a	Δa
24	3.13429	0.00016	0.00131	3.13428	0.00016	0.00130
90	3.14587	20	183	3.14586	21	180
561	3.16753	48	328	3.16751	49	327
1229	3.21018	125	978	3.20980	196	1959
1340	3.17955	63	405	3.17951	66	447
1489	3.18393	68	490	3.18386	81	595
1674	3.18341	46	346	3.18338	49	353
1956	3.19839	60	434	3.19834	68	476
2114	3.19937	90	667	3.19920	120	979
	EULER+REV			RKG4		
No	$\bar{a}$	σ_a	Δa	$\bar{a}$	σ_a	Δa
24	3.13419	0.00020	0.00134	3.13429	0.00016	0.00132
90	3.14577	24	145	3.14587	20	184
561	3.16735	53	318	3.16753	48	327
1229	3.21098	131	616	3.21010	147	1222
1340	3.17960	66	358	3.17955	63	427
1489	3.18436	74	418	3.18392	74	537
1674	3.18327	53	308	3.18342	45	349
1956	3.19818	71	356	3.19840	59	448
2114	3.19996	98	484	3.19933	102	793

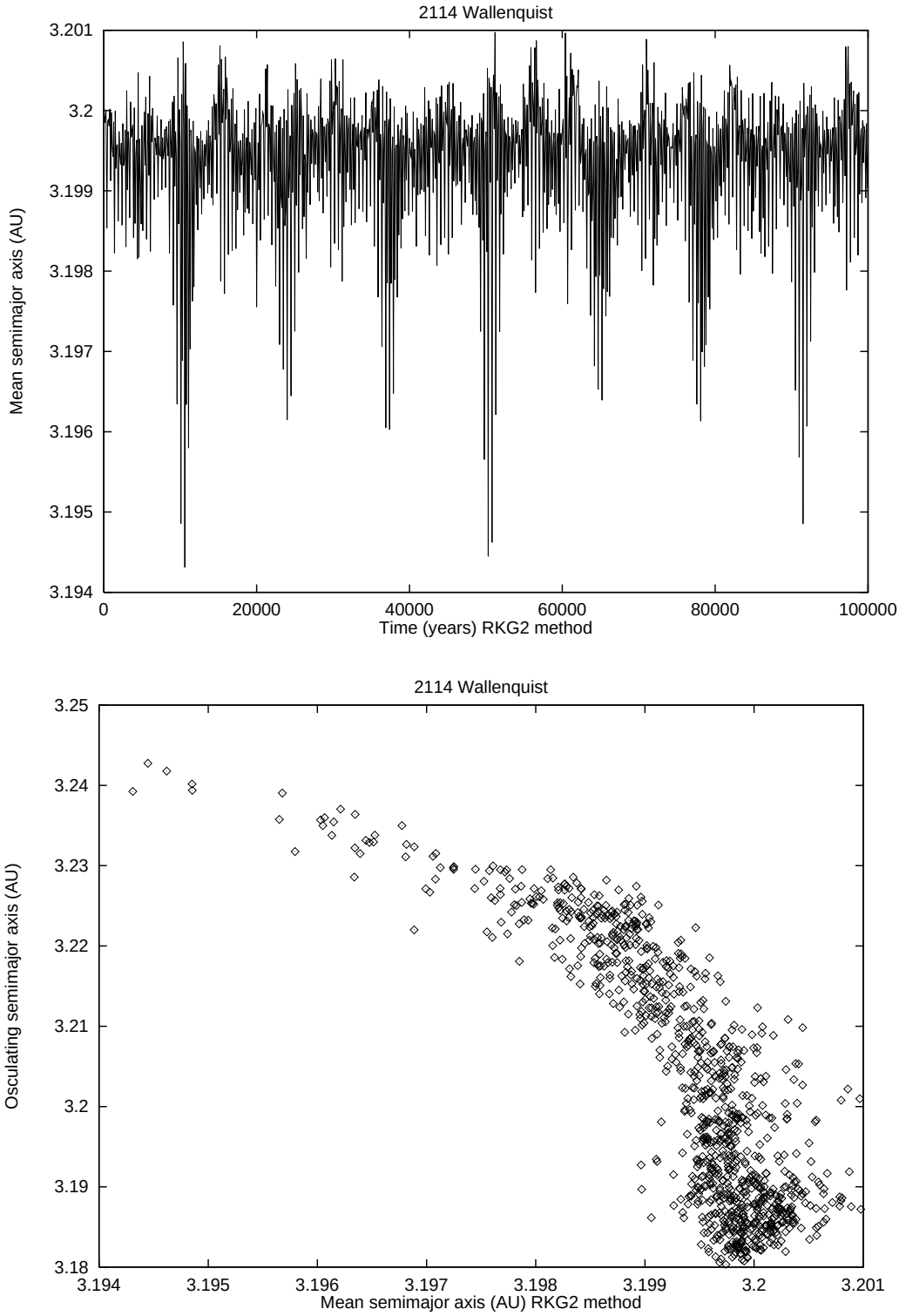

Fig. 4: Top: the mean semimajor axis of the asteroid *2114 Wallenquist*, obtained by the Runge-Kutta-Gauss method of order 2. Bottom: the mean semimajor axis versus the osculating value. The curvature of the figure indicates that the 2:1 divisor is still a significant source of error, although the effect is much less pronounced than in Figure 3.

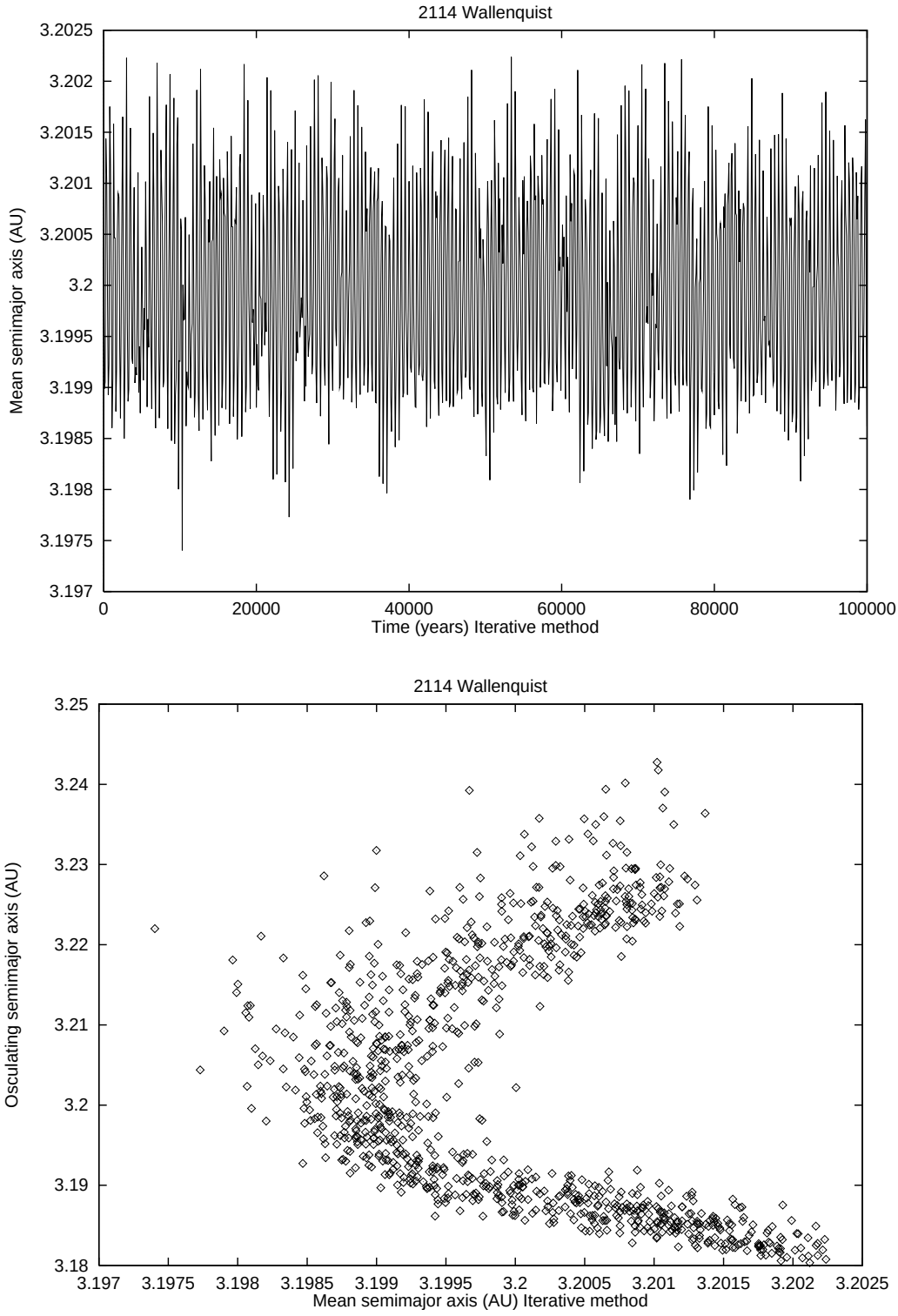

Fig. 5: Top: the mean semimajor axis of the asteroid *2114 Wallenquist*, obtained by the iterative theory. Bottom: the mean semimajor axis versus the osculating value. These results are better than those of Figure 4, mostly because the curvature has been reversed by the iterations.

Taking into account all the above considerations, the comparison of the data in Table 1 clearly suggests that, among the methods tested, the iterative EULER+REV method provides the best results. Both measures of the quality of the results are quite favourable for this method; moreover, the results are well balanced in the sense that low σ_a corresponds to low Δa, even in the most difficult cases (closest to the resonance).

This conclusion is also favourable from another, more practical, point of view. The EULER+REV method has been quite simple to implement, with moderate changes to the previous well tested software; it is also efficient enough, given the speed of the current computers, for the purpose of computing large catalogues of mean elements.

4 CONCLUSIONS

The results of the tests presented in Section 3 indicate that a more accurate and reliable algorithm to compute mean elements has been found, and that it can be used with satisfactory accuracy much closer to the strongest mean motion resonances than the previous methods. This algorithm is the iterative one, with the simplest starter (Euler method). This is basically the same method we have been using for the computation of proper elements. As can be seen from Table 1, the improvement is especially significant in the excursion; this means that a single computation for a given asteroid is more reliable, and this is important to study the shape of asteroid families closer to the resonance.

The main questions we would like to address in the conclusions are: why and where? That is, why the iterative methods are superior to nominally higher order methods? And where in the asteroid belt is the superiority of the new algorithm relevant?

We would like to understand why the iterative methods, which compute the reverse map for a purely first order theory, that is (2.19), are more accurate than methods which account, at least in part, for effects of the second order (in the planetary masses). The explanation can not have to do with the argument on the superiority of the reverse map, discussed in Section 2.1. As a matter of fact, the RKG2 method computes exactly (to second order) both the direct and the inverse map (2.28).

We are led to conclude that the lower reliability (as measured by the excursion) of the RKG2 method is due to the difference between (2.20) and the second of (2.28), that is to the absence of the portion of the second order effects resulting from $\varepsilon^2 W_2$. Adding the second order effects of εW_1, without the former ones, results in a larger error, at least for orbits very close to the resonance, than ignoring all second order effects altogether.

This result indicates that some cancellation effect is taking place in the second order part of (2.20); that is most of the terms in $-\varepsilon^2 \partial W_2/\partial X'$ and the terms in $\varepsilon^2/2\,\{-\partial W_1/\partial X', W_1\}$ cancel out, giving a result closer to the first order one of (2.19). The conclusion is that there is no point in an effort to compute second order effects, unless the computation can be complete. For a complicated problem such as the computation of the short period perturbations, with hundreds of terms in the first order, and hundred of

thousands in the second order, this means that there is no way to do a useful second order computation unless some sophisticated computer algebra system is used.

This does not mean that the methods of the class proposed by Breiter (1997a) are not useful, but only that they should be applied under different circumstances, e.g. when an explicit computation of W_2 is possible, as in Breiter (1997b).

The results of this paper are also relevant for the computation of proper elements. On one hand, the availability of better mean elements allows to improve the reliability also of the proper elements, especially in the regions of the asteroid belt neighbouring the principal mean motion resonances. On the other hand, our algorithm to compute proper elements has always been, since Paper I, iterative (with Euler starter), that is conceptually the same we are now adopting for mean elements. This means that, as far as the computation of proper elements is concerned, there is little, if any, room for improvement. Indeed, we have tested the RKG2 algorithm for the map mean elements to proper elements, and found no improvement, even a small increase in the proportion of divergent cases.

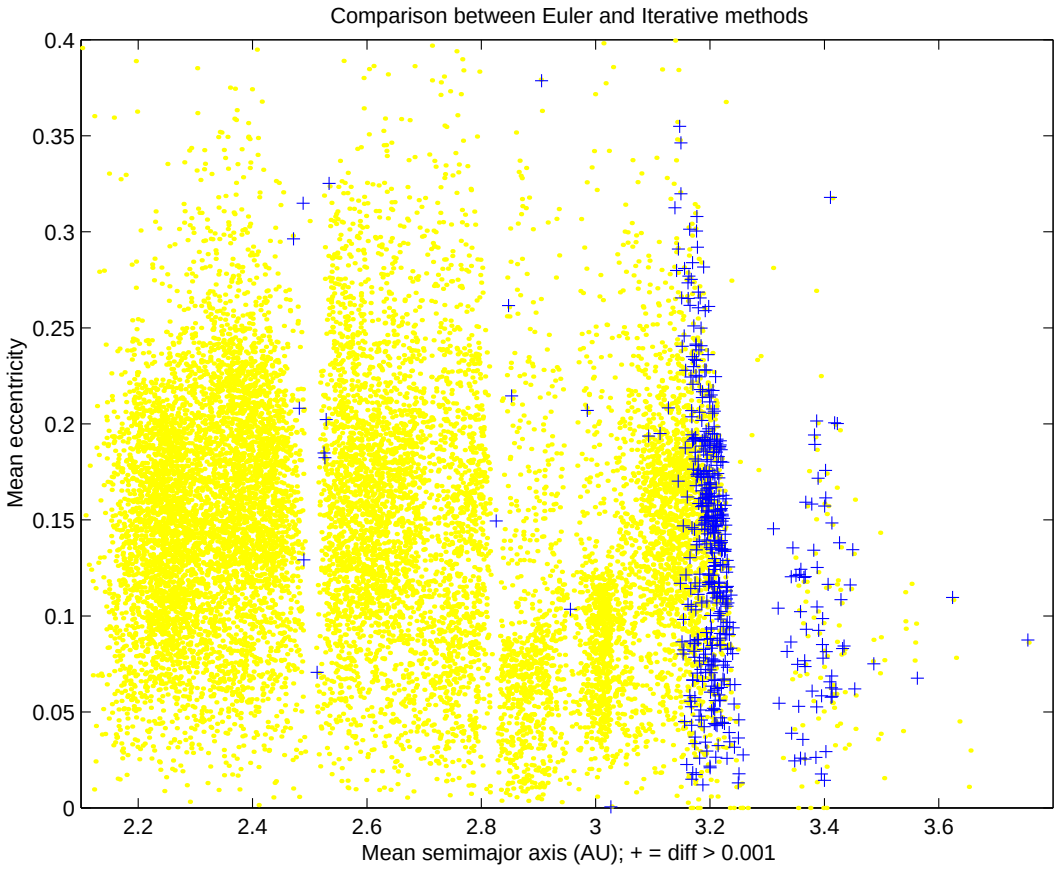

Fig. 6: The mean semimajor axis and mean eccentricity computed for 13345 asteroids with well determined orbits (observed at more than one opposition). The crosses indicate the cases with difference between Euler and iterative method exceeding 0.001 AU in the mean semimajor axis.

The second question can be answered by monitoring in which regions of the asteroid belt the changes, between the mean elements computed with the conventional EULER and those obtained by the use of iterative methods, are larger than some significant level, e.g. 0.001 AU in semimajor axis. The result of this check is shown in Figure 6, where it is easy to appreciate that there are many significant changes in the neighbourhood of the 2 : 1 resonance, and a number besides the 3 : 1 and the 5 : 2 resonances; very few other cases appear near the 7 : 3 and the 5 : 3 resonance. The mean elements for all the rest of the asteroid belt are only marginally affected.

The conclusion is that the improvements introduced in our new proper elements version 8, due to the use of the iterative algorithm to compute mean elements, without changes to the algorithm to compute proper elements, have only local significance; no important change is introduced for most asteroids and most families. In the Introduction of Paper III, we had anticipated that there is very little room left for improvements in our analytical theories, apart from local improvements, and indeed this appears to be the case.

On the other hand, the new version of the proper elements contains proper elements for more asteroids, and especially more asteroids with reliable osculating elements (e.g. having been observed at more than one opposition), thus they can allow a better study of all the asteroid families because of the larger sample. They will also allow better results where the improvement in mean elements is significant, e.g. for the analysis of the Themis family and of the Cybele region, on both sides of the 2 : 1 resonance. To obtain a copy of the new version mean and proper elements, you can use anonymous ftp with the URL:

`ftp://ftp.dm.unipi.it/pub/propel/`

and get e.g. the compressed archive file `vers8.tar.Z`.

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