Uniform formulation for orbit computation: the intermediate elements

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Abstract

We present a new method for computing orbits in the perturbed two-body problem: the position and velocity vectors of the propagated object in Cartesian coordinates are replaced by eight orbital elements, i.e. constants of the unperturbed motion. The proposed elements are uniformly valid for any value of the total energy. Their definition stems from the idea of applying Sundman's time transformation in the framework of the projective decomposition of motion, which is the starting point of the Burdet–Ferrándiz linearisation, combined with Stumpff's functions. In analogy with Deprit's ideal elements, the formulation relies on a special reference frame that evolves slowly under the action of external perturbations. We call it the *intermediate* frame, hence the name of the elements. Two of them are related to the radial motion, and the next four, given by Euler parameters, fix the orientation of the intermediate frame. The total energy and a time element complete the state vector. All the necessary formulae for extending the method to orbit determination and uncertainty propagation are provided. For example, the partial derivatives of the position and velocity with respect to the intermediate elements are obtained explicitly together with the inverse partial derivatives. Numerical tests are included to assess the performance of the proposed special perturbation method when propagating the orbit of comets C/2003 T4 (LINEAR) and C/1985 K1 (Machholz).

1 Introduction

Stumpff (1947, 1962) devised a method to represent the solution of the two-body problem at any time t from the position ($\mathbf{r}_0$) and velocity ($\dot{\mathbf{r}}_0$) at some reference epoch t_0 (see also Stumpff, 1959, vol. 1, chap. V). His formulation is very attractive because it is the same for all types of orbits including those that are rectilinear. For this reason, the coordinates of $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ are commonly referred to as *universal variables* (or elements). Stumpff introduced a new independent

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variable, here denoted by χ, through the time transformation (he assumed $\mu = 1$)

$$\frac{\mathrm{d}t}{\mathrm{d}\chi} = \frac{r}{\sqrt{\mu}}, \quad \mu = k^2(m+M), \tag{1}$$

where k^2 is the gravitational constant and M, m are the masses of the two bodies. Equation (1) together with the Keplerian energy integral produce a third-order linear differential equation with constant coefficients for the orbital distance r and the Lagrangian functions. Then, a unique solution for any type of conic section can be written in terms of the constants of the motion $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ and *Stumpff's functions* c_n (see Eq. 12). Inserting the solution $r(\chi)$ in the right-hand side of Eq. (1) and integrating with the initial condition $\chi(t_0) = 0$, he obtained the generalised form of Kepler's equation, from which the value of χ corresponding to t can be determined by an iterative algorithm.

Samuel Herrick was among the first to get interested in Stumpff's work. Since the mid 1940s, he devoted his efforts to improving orbit computation for near parabolic and near rectilinear motion (Herrick, 1945, 1953). His universal formulae of the two-body problem (Herrick 1960, sect. 6P; Herrick 1965) are simpler and more convenient than those proposed by Stumpff. The same formulation was presented by Wong (1962) and a similar version by Battin (1964, sect. 2.8). Herrick's method relying on universal variables, which is nowadays regarded as the classic solution, uses a universal anomaly defined by the differential relation (1). Herrick (1965) showed alternative forms of the universal variables, by introducing two arbitrary parameters. One of them allows for a more general definition of the universal anomaly, given by $\psi = \chi/\sqrt{\beta}$. Among the six different choices for β that are considered, two deserves special attention: if we set $\beta = (t - t_0)^2/r_0^2$ then Stumpff's form is obtained; the choice $\beta = \mu$, proposed by Goodyear (1965, 1966), makes the term $\sqrt{\mu}$ disappear from the formulation, so repulsive forces can be taken into account.

The derivations of Pitkin (1965)[1], Sconzo (1967), and Everhart and Pitkin (1983) put in result the regularising role of the universal anomaly. By applying the time transformation (1) and taking advantage of the conservation of the energy, a third-order linear differential equation with constant coefficients can be obtained for the position vector $\mathbf{r}$ (see Battin, 1999, sect. 4.5). In particular, following more closely Stumpff's original approach, Sconzo (1967) showed that Stumpff's functions can be introduced in a straightforward way if the solution is represented via Taylor series.

The universal elements $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ can also describe rectilinear orbits, but the formulae that relate them to $\mathbf{r}$, $\dot{\mathbf{r}}$ lose their meaning when the radial distance becomes zero, that is, when the body collides with the centre of attraction. In order to mitigate the loss of accuracy that occurs close to the singularity, Pitkin (1965) suggested replacing $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ by $\mathbf{r}_0/\sqrt{r_0}$, $r_0\dot{\mathbf{r}}_0/\sqrt{\mu}$, respectively.

The variation of parameters equations for the universal variables $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ were first given by Wong (1962) and later by Herrick (1965, 1971, sect. 16J) and

[1] Pitkin (1965) calls universal variables the functions $U_n = \chi^n c_n$, which will be defined in Eq. (11) and named *universal functions*.

Pitkin (1966) in a more suitable form for computer programming. The latter presented some numerical tests with low-thrust trajectories.

This special perturbation method has two drawbacks from the perspective of numerical integration. First, the variable χ must be obtained at each step by solving the universal Kepler equation with an iterative method. Moreover, the time derivatives of $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ contain secular terms in the variable χ. To solve this second problem, Born et al (1974) allowed t_0 to vary in a prescribed way instead of keeping it constant throughout the propagation as in Herrick's variation of parameters method. However, one additional differential equation is required to compute χ, and the time derivatives of both t_0 and χ are affected by secular terms. In fact, their elimination is not possible without compromising the universality of the formulation (see Battin, 1999, sect. 10.7).[2]

There are other notable sets of elements that are universal, i.e. well defined for any motion with the only possible exception of the case $r = 0$. They are related to the regularisations due to Sperling (1961), Kustaanheimo and Stiefel (1965, hereafter KS), and to the linearisation method shown by Burdet (1969).

The *natural* elements were derived by Burdet (1968) from Sperling's regularisation. Sperling (1961) found that it is possible to write a second-order linear differential equation not only for the orbital radius r but also for the position vector $\mathbf{r}$ if the eccentricity vector and the energy integral are both embedded in the equation of motion resulting from the change of independent variable (1). The solutions $r(\chi)$, $\mathbf{r}(\chi)$, $t(\chi)$ are then expressed in terms of the natural elements and the special functions c_n (Eq. 12) originally introduced by Stumpff. The new formulation is universal, and it is valid even for $r = 0$. Burdet derived also the formulae for computing the variation of the natural elements with respect to the anomaly χ.

The general solution of the KS regularised equations in terms of Stumpff's functions was presented by Deprit (1968). The elements that appear in the solution are uniformly valid for all values of the Keplerian energy and are regular at collision. The same elements had already been introduced by Broucke (1966), who also obtained explicit expressions of their derivatives by the method of variation of parameters. Scheifele (1970), Stiefel and Scheifele (1971, pp. 250–254) applied the theory of Hamilton–Jacobi to the KS Hamiltonian system to obtain two sets of ten canonical elements that are regular and uniform with respect to the total energy. An element linked to the physical time was naturally introduced following this approach. Bond (1974) developed a special perturbation method that is based on a set of elements very similar to the one called Type II in Scheifele (1970). An alternative formulation in which mixed-secular terms are eliminated from the derivative of the time element was also presented.

The idea behind the transformation applied by Burdet (1969) dates back to the eighteenth century (see Deprit et al, 1994). The inverse of the orbital

[2]The secular terms are completely removed if, in addition to properly prescribing the variation of t_0, we include in the state vector the difference between the true anomalies of the current position at time t and of the departure point at time t_0. The drawback of this approach is that the formulation becomes singular when the angular momentum vanishes, and therefore, it is not universal.

distance (ρ) and the radial unit vector ($\mathbf{e}_r = \rho\,\mathbf{r}$) are chosen as new coordinates to represent the position. Then, the system of differential equations for ρ, $\mathbf{e}_r$ is linear if the independent variable is changed according to the relation

$$\kappa \mathrm{d}t = r^2 \mathrm{d}\phi, \quad \kappa > 0, \tag{2}$$

where κ is a constant (at least of the Kepler problem). Burdet chose $\kappa = 1$, so that the frequency of oscillation of both ρ and $\mathbf{e}_r$ along Keplerian motion is given by the angular momentum of the particle divided by its mass (h).[3] The solution of the new system is written in a unified way for $h > 0$ and $h = 0$ by means of functions that are analogous to those used by Stumpff and of the *focal* elements. Their differential equations are derived together with that of a time element.

Chelnokov (1992) formally established the connection between KS variables and the Euler parameters, already pointed out by Broucke and Lass (1975). These quantities represent a reference frame that has one axis aligned with the position vector and rotates with angular velocity always parallel to the angular momentum vector. By changing time according to Eq. (2), the four Euler parameters satisfy the equations of an harmonic oscillator with frequency $1/2$ for $\kappa = h$. This fact opened the way for generating new orbital elements, as shown by Chelnokov (1993) and more recently by Roa and Kasdin (2017). We observe that the elements proposed by these authors are universal if $\kappa = 1$, but they are not regular.

Although against the spirit of universal variables, we consider formulations based on orbital elements that allow a uniform transition through elliptic, parabolic, and hyperbolic motion as long as the angular momentum is not zero. Milanković's vectorial elements describe the geometry of any orbit, and their definition is not related to a particular reference frame (Milanković, 1939; Allan and Ward, 1963). Orbit propagation with these quantities is possible thanks to appending to the state vector an angle that locates the position of the particle with respect to a preferably non-singular direction on the osculating plane. The true longitude is suitable for this purpose (Roy and Moran, 1973; Rosengren and Scheeres, 2014), but it loses its meaning when $h = 0$. Parameters related to an orbital reference frame[4] at epoch are doomed to fail in describing rectilinear orbits. This is evident from the expression of the transverse unit vector, $\mathbf{e}_{t,0} = [r_0\dot{\mathbf{r}}_0 - (\mathbf{r}_0 \cdot \dot{\mathbf{r}}_0)\mathbf{e}_{r,0}]/h$, where $\mathbf{e}_{r,0} = \mathbf{r}_0/r_0$. As noted by Herrick (1965), a proper scaling of $\mathbf{e}_{t,0}$ can avoid the problem, and for example, $\mathbf{e}_{r,0}$, $h\mathbf{e}_{t,0}$ recover their universal nature. The modified equinoctial elements (Walker et al, 1985) also fail at $h = 0$ because they are related to an orbital reference frame (Broucke and Cefola, 1972).

By setting κ equal to h in Burdet's linearisation,[5] the angle ϕ becomes the

[3] This result for ρ with $\kappa = h$ is called Binet's formula, after Jacques Binet (1786–1856), and it was already known to Isaac Newton (1642–1726).

[4] With the adjective *orbital*, we mean that the reference frame is defined by the osculating plane of motion, and more specifically that one axis has the same direction of the angular momentum vector.

[5] This method is known in the literature as Burdet–Ferrándiz regularisation. Ferrándiz

true anomaly in the unperturbed case, and the oscillation frequencies of ρ, $\mathbf{e}_r$ are equal to 1. This fact brings a considerable advantage: the new elements do not exhibit secular terms in their derivatives unlike the original focal elements. Even more interesting is that three of them fix the shape of the osculating ellipse and the remaining six define the orientation of an orbital reference frame, which is called *ideal* after Hansen (1857, see p. 66 for the definition of the ideal coordinates). In the light of this geometric interpretation, a reduction of the dimension of the system from nine to seven is achieved by taking the Euler parameters that describe the rotation of the ideal frame. The choice $\kappa = h$ introduces a singularity when the value of h is zero which was not present in Burdet's variables. Deprit (1975) and Vitins (1978) developed seven elements of this kind by following two different approaches. A review of several references about this subject can be found in the introduction of Baù et al (2015), where the concept of Hansen ideal frames and the connection between the ideal elements and Burdet's linearisation are discussed in detail. The method named *Dromo* (Peláez et al, 2007) revived the interest in ideal elements for orbit propagation, especially because the authors showed that it can be much more accurate and faster than Cowell's method (Battin, 1999, p. 447). Dromo is based on seven quantities almost equivalent to Deprit's and Vitins' and on a fictitious time which is represented by the anomaly ϕ (Eq. 2, wherein $\kappa = h$). For an extensive presentation of Dromo, we refer to Urrutxua et al (2016) and Roa (2017, chap. 4), who also mention the important updates that have been recently proposed to improve its numerical performance.

A propagator similar to Dromo but working only for negative values of the total energy was devised by Baù et al (2014, 2015). The basic idea behind this method is to search for a linearisation of the equations of motion starting from the *projective* coordinates $(r, \mathbf{e}_r)$, as in the Burdet–Ferrándiz regularisation, and choosing a time transformation of Sundman's type instead of Eq. (2). In the unperturbed motion, the independent variable is the eccentric anomaly and the differential equation of the radial distance r is linear with constant coefficients (a well-known result, see Bohlin, 1911). The solution can be written so that the two constants of integration are the projections of the eccentricity vector along a pair of fixed orthogonal axes which lie on the orbital plane. Based on these two directions, the authors defined a reference frame, named *intermediate*, and introduced four Euler parameters to represent its orientation in space. The six integrals of the Kepler problem obtained in this way constitute the state vector together with the semi-major axis, and a time element. The special perturbation method generated from the new elements can exhibit a substantial advantage with respect to Dromo. Numerical investigations conducted by Amato et al (2017, 2019) show its excellent behaviour in the propagation of both asteroids and artificial satellites of the Earth. An analogous formulation was derived independently by Roa and Peláez (2015) and Baù et al (2016) for positive values of the Keplerian and total energy, respectively.

(1988) achieved the same linearisation in the framework of the Hamiltonian formalism (see Deprit et al, 1994).

The methods proposed by Baù et al (2015, 2016), Roa and Peláez (2015) cannot be used, in general, to propagate a body that presents transitions from elliptic to hyperbolic motion or vice versa. We also expect that they loose accuracy when the energy is close to zero. Therefore, we tried to find a unique formulation that includes those in Baù et al (2015, 2016) and Roa and Peláez (2015) and is able to deal with cases in which the Keplerian or the total energy changes sign during the motion. In the present paper we achieve such goal by switching to a regularising time variable and taking advantage of Stumpff's functions as shown in Section 2. Eight uniform elements arise from our procedure: they are non-singular for any value of the total energy and are not defined when the angular momentum is zero. The new quantities are called *intermediate elements* because there exists an intermediate frame that plays a key role in their definition. This frame establishes the orientation of the osculating plane and of a departure direction on it, from which the position of the particle is reckoned. In Section 2, we also obtain the first-order differential equations that govern the variations of the new elements with respect to the fictitious time. Numerical tests assessing the performance of the new method for orbit propagation are shown in Section 4.

In our derivation, particular attention is paid to the appearance of secular terms with respect to the independent variable when the total energy is negative. In order to better understand their origin, we introduce an arbitrary quantity β in the time transformation (Eq. 6). Secular terms can only be eliminated from the time derivatives of the new elements by selecting β in a proper way, at the cost of losing the uniform character of the proposed special perturbation method. An alternative formulation which is completely free of secular terms and that is still uniform is derived in Appendix A after Conclusions (in Section 5).

In some applications, orbit propagation is part of a more complicated procedure known as orbit determination: given a set of observations at different epochs relative to the same celestial body, we want to determine its position and velocity and the associated uncertainties at some prescribed epoch. An essential ingredient in orbit determination is the *state-transition matrix* (STM). Its elements are the partial derivatives of position and velocity with respect to their initial values and obey the *variational equation.* Sitarski (1967) presented a solution of the two-body variational equation which is independent of the type of the orbit. Crawford (1969) started from Sitarski's result to write a simpler expression of the two-body STM. Herrick (1965) and Goodyear (1965, 1966) derived a closed-form solution for the partial derivatives in terms of Stumpff's functions (a simpler presentation than Herrick's is available in Battin, 1999, sect. 9.7). Improvements to Goodyear's STM were proposed by Shepperd (1985) and Der (1997): the former suggested a new scheme for solving Kepler's equation, which is a preliminary step necessary to compute the STM; the latter found a way to remove the secular terms contained in the universal functions U_4 and U_5 (see Eq. 11).

Section 3 deals with the use of our formulation for orbit determination and uncertainty propagation. The delicate aspect of computing the STM for the rectangular coordinates at a certain time from the STM of the intermediate elements at the corresponding fictitious time is addressed. Appendix C reports the expressions of the derivatives that appear in the variational equations of the intermediate elements.

2 The intermediate elements

Consider the perturbed Kepler problem. The evolution of the position $\mathbf{r}$ of a particle of mass m with respect to a body of mass M (here referred to as the central body) is described by Newton's second law

$$\ddot{\mathbf{r}} = -\frac{\mu}{r^3}\mathbf{r} + \mathbf{F}, \tag{3}$$

where $\mu = G(m + M)$, with G the gravitational constant, $r = |\mathbf{r}|$ and $\mathbf{F}$ is the vector sum of the perturbing forces acting on m. We assume that

$$\mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t) = \mathbf{P}(\mathbf{r}, \dot{\mathbf{r}}, t) - \nabla\mathscr{U}(\mathbf{r}, t), \tag{4}$$

where $\nabla\mathscr{U}$ is the gradient of the disturbing potential $\mathscr{U}$ and $\mathbf{P}$ is the sum of the perturbing forces that are not related to the gradient of a potential energy. We will refer to *unperturbed motion* when both $\mathbf{F} = \mathbf{0}$ and $\mathscr{U} = 0$.

For future use, let us introduce the local vertical, local horizontal (LVLH) reference frame $\{O, \mathbf{e}_r, \mathbf{e}_\nu, \mathbf{e}_z\}$, where O denotes the location of the centre of mass of the central body, and

$$\mathbf{e}_r = \frac{\mathbf{r}}{r}, \qquad \mathbf{e}_\nu = \mathbf{e}_z \times \mathbf{e}_r, \qquad \mathbf{e}_z = \frac{\mathbf{r} \times \dot{\mathbf{r}}}{|\mathbf{r} \times \dot{\mathbf{r}}|}. \tag{5}$$

In this section, we develop a set of eight orbital elements that can be used to represent the position and velocity of the particle at a given epoch. We first derive the elements that describe the motion *on* the orbital plane and next those that describe the evolution *of* the orbital plane.

2.1 Motion *on* the orbital plane

Let us introduce the polar coordinates (r, ν) on the osculating plane of motion, where ν is the angle measured from a reference axis Ox to the position vector $\mathbf{r}$. The definition of ν and therefore of Ox is given in the end of this section. Then, we can introduce the *intermediate* reference frame $\{O, \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$, where $\mathbf{e}_x$ obeys the relations $\mathbf{e}_x \cdot \mathbf{e}_r = \cos\nu$, $\mathbf{e}_x \times \mathbf{e}_r = \sin\nu\, \mathbf{e}_z$ (see Figure 1), and $\mathbf{e}_y = \mathbf{e}_z \times \mathbf{e}_x$.

The independent variable is changed from the physical time t to a fictitious time χ by the transformation

$$\beta \mathrm{d}t = r\, \mathrm{d}\chi, \tag{6}$$

where $\beta \in \mathbb{R}^+$ is an arbitrary constant along any solution of the Kepler problem. The introduction of the parameter β has been suggested in the past, for example,

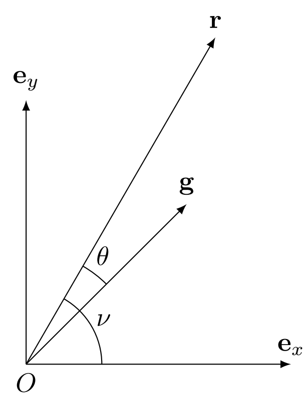

Figure 1: Orientation of the position vector $\mathbf{r}$ and the generalised eccentricity vector $\mathbf{g}$ with respect to the unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$ of the intermediate frame. All vectors lie on the osculating orbital plane at some epoch t.

by Herrick (1965). We will make a specific choice for β in Section 2.6. The orbital radius obeys the second-order differential equation

$$\beta^2 r'' = 2\mathscr{E} r + \mu + r(rF_r - 2\mathscr{U}) - \beta r' \beta', \tag{7}$$

where prime denotes differentiation with respect to χ, F_r is the radial component of the perturbing force $\mathbf{F}$, and $\mathscr{E}$ is the specific total energy. Equation (7) is obtained from (3) and (6). The quantity $\mathscr{E}$ is defined as

$$\mathscr{E} = \frac{1}{2}\left(\dot{r}^2 + \frac{h^2}{r^2}\right) - \frac{\mu}{r} + \mathscr{U}, \tag{8}$$

where $h = |\mathbf{r} \times \dot{\mathbf{r}}|$ is the specific angular momentum. From (7), one finds that the following relation holds for the Kepler problem

$$\sigma'' = -\alpha\sigma, \tag{9}$$

where $\sigma = r'$, and

$$\alpha = -\frac{2\mathscr{E}}{\beta^2}. \tag{10}$$

Let us introduce the *universal functions* (Battin, 1999, sect. 4.5):

$$U_n(\chi; \alpha) = \chi^n c_n(\chi; \alpha), \quad n \in \mathbb{N}, \tag{11}$$

where

$$c_n(\chi; \alpha) = \sum_{k=0}^{\infty} (-1)^k \frac{(\alpha\chi^2)^k}{(n+2k)!}. \tag{12}$$

The series $c_n(\chi;\alpha)$, known as Stumpff's functions, converge absolutely for all values of χ, α, and uniformly in any bounded domain of χ, α. The solution of Eq. (9) can be written as

$$\sigma = a_1 U_0(\chi;\alpha) + a_2 U_1(\chi;\alpha). \tag{13}$$

Then, the orbital radius adopts the form

$$r = a_0 + a_1 U_1(\chi;\alpha) + a_2 U_2(\chi;\alpha). \tag{14}$$

The constants of integration a_0, a_1, a_2 are determined from the initial values of r, σ. If we assume that $\chi = 0$ at the initial time, we obtain

$$a_0 = r(0) = r_0, \qquad a_1 = \sigma(0) = \sigma_0. \tag{15}$$

By evaluating the equation $\beta^2 r'' = 2\mathscr{E} r + \mu$ at $\chi = 0$, we also find

$$a_2 = \frac{\mu + 2\mathscr{E} r_0}{\beta^2}. \tag{16}$$

Using (15), (16) in (13), (14), and noting that $U_0 + \alpha U_2 = 1$, we can write

$$r = r_0 U_0(\chi;\alpha) + \sigma_0 U_1(\chi;\alpha) + \frac{\mu}{\beta^2} U_2(\chi;\alpha), \tag{17}$$

$$\sigma = \sigma_0 U_0(\chi;\alpha) + \frac{\mu}{\beta^2}(1 - \lambda r_0) U_1(\chi;\alpha), \tag{18}$$

where

$$\lambda = \frac{-2\mathscr{E}}{\mu}. \tag{19}$$

The quantities r_0, σ_0 will not be constant if perturbations are present ($\mathbf{F} \neq \mathbf{0}$). Moreover, the time evolution of r_0, σ_0 will depend on the specific choice of β, that is on the choice of independent variable (see Eq. 6).

Before dealing with the polar angle ν, we define

$$g = \sqrt{1 - \lambda p}, \qquad \mu p = h^2 + 2r^2 \mathscr{U}, \qquad c = \sqrt{\mu p}. \tag{20}$$

Let us call g, p, c the *generalised* eccentricity, semilatus rectum, and angular momentum, respectively. They reduce to their *osculating* counterparts when $\mathscr{U} = 0$. The quantities g, p are functions of r_0, σ_0, β, λ. Their expressions, which can be found from (20) and (8), (17), (18), are

$$g^2 = (1 - \lambda r_0)^2 + \frac{\beta^2}{\mu} \lambda \sigma_0^2, \tag{21}$$

$$p = r_0(2 - \lambda r_0) - \frac{\beta^2}{\mu} \sigma_0^2. \tag{22}$$

Note that g, p take finite values for $\alpha = 0$.

We aim at relating the polar angle ν to the independent variable χ. The angle ν is comprised between the position of the particle and a reference axis that lies on the osculating orbital plane and passes through the central body. Additionally, this axis must remain fixed in space at least when the motion is unperturbed and to be well defined for any value of h different from zero. Possible definitions of the polar angle ν must obey the following condition: when the motion is Keplerian, ν is the true anomaly up to an additive constant angle, that is

$$\dot{\nu} = \frac{c}{r^2}. \tag{23}$$

In our formulation, ν is defined as follows. Assume $\nu(0) = 0$, then from Eqs. (23) and (6) we have

$$\nu = \frac{c}{\beta} \int_0^{\chi} \frac{1}{r(s)} \mathrm{d}s, \tag{24}$$

with $r(s)$ taken from Eq. (17). After solving the integral, we find

$$\beta \tan \frac{\nu}{2} = \frac{c\, U_1\left(\frac{1}{2}\chi; \alpha\right)}{r_0 U_0\left(\frac{1}{2}\chi; \alpha\right) + \sigma_0 U_1\left(\frac{1}{2}\chi; \alpha\right)}. \tag{25}$$

The above formula, called by Sperling (1961) the Gaussian equation, defines ν as a function of χ.

2.2 Particularisations for positive, negative, and zero values of α

Equations (17), (25) are here particularised to the cases $\alpha > 0$, $\alpha < 0$, $\alpha = 0$, which correspond to negative, positive, and zero total energy, respectively. For this purpose, we need to provide the definition of the generalised true anomaly θ. Given the generalised eccentricity vector

$$\mathbf{g} = \mathbf{w} \times (\mathbf{r} \times \mathbf{w}) - \mathbf{e}_r, \tag{26}$$

where

$$\mathbf{w} = \dot{r}\, \mathbf{e}_r + \frac{c}{r}\, \mathbf{e}_\nu, \tag{27}$$

we have that θ is the angle measured from $\mathbf{g}$ to $\mathbf{r}$ counterclockwise as seen from $\mathbf{e}_z$ (see Figure 1). Therefore, from (26) and noting that $|\mathbf{g}| = g$, with g given in (20), we have ($c \neq 0$)

$$g \cos\theta = \frac{c^2}{r} - 1, \qquad g \sin\theta = c\, \dot{r}. \tag{28}$$

2.2.1 The case $\alpha > 0$

After substituting into Eq. (17) the expressions taken by U_0, U_1, U_2 for $\alpha > 0$ we have

$$r = \frac{1}{\lambda}[1 - \wp_1 \cos(\sqrt{\alpha}\chi) - \wp_2 \sin(\sqrt{\alpha}\chi)], \tag{29}$$

where

$$\wp_1 = 1 - \lambda r_0, \qquad \wp_2 = -\beta\sigma_0\sqrt{\frac{\lambda}{\mu}}. \tag{30}$$

Then, following Baù et al (2015) we can define the generalised eccentric anomaly G from

$$\mu g \cos G = \mu + 2\mathscr{E} r, \qquad \mu g \sin G = r\,\dot{r}\sqrt{-2\mathscr{E}}. \tag{31}$$

By using the first relation in (31) and Eq. (29), we obtain

$$\begin{aligned} \wp_1 &= g\cos(\sqrt{\alpha}\chi - G), \\ \wp_2 &= g\sin(\sqrt{\alpha}\chi - G). \end{aligned} \tag{32}$$

Since $\wp_1 = g\cos G_0$, $\wp_2 = -g\sin G_0$, where G_0 is the value taken by G at $\chi = 0$, we have

$$\sqrt{\alpha}\chi = G - G_0. \tag{33}$$

Equation (25) can be written for $\alpha > 0$ as

$$\tan\frac{\nu}{2} = \frac{\sqrt{1-\wp_1^2-\wp_2^2}\sin\left(\frac{1}{2}\sqrt{\alpha}\chi\right)}{(1-\wp_1)\cos\left(\frac{1}{2}\sqrt{\alpha}\chi\right) - \wp_2\sin\left(\frac{1}{2}\sqrt{\alpha}\chi\right)}, \tag{34}$$

or alternatively as

$$\tan\frac{\nu-\theta}{2} = \sqrt{\frac{1+g}{1-g}}\tan\frac{\sqrt{\alpha}\chi - G}{2}. \tag{35}$$

Thus, the angular difference $\nu - \theta$ is obtained from $\sqrt{\alpha}\chi - G$ by applying the classical relation between the true anomaly and the eccentric anomaly in the two-body problem.

Remark. The method presented in Baù et al (2015), called EDromo, employs $\beta = \sqrt{-2\varepsilon}$, so that $\alpha = 1$ and Eq. (29) becomes

$$r = \frac{1}{\lambda}(1 - \wp_1\cos\chi - \wp_2\sin\chi),$$

where[6]

$$\wp_1 = g\cos(\chi - G), \qquad \wp_2 = g\sin(\chi - G). \tag{36}$$

Interestingly, in EDromo the polar angle is defined as

$$\nu = \theta + \chi - G. \tag{37}$$

This choice seems quite natural looking at the expressions of $\wp_1$, $\wp_2$ given in (36), which suggest to directly take $\chi - G$ as the angle between $\mathbf{g}$ and $\mathbf{e}_x$ (see Figure 1). Finally, it is worth noting that from (37) by using a formula proposed by Broucke and Cefola (1973), Eqs. (31) and the first relation in (20), we get the relation

$$\nu = \chi + 2\arctan\frac{\sigma}{r + \sqrt{p/\lambda}}.$$

[6] In Baù et al (2015) the elements $\wp_1$, $\wp_2$, λ^{-1} are denoted by λ_1, λ_2, λ_3, respectively, and the independent variable χ by φ.

2.2.2 The case $\alpha < 0$

For $\alpha < 0$, Eq. (17) becomes

$$r = -\frac{1}{\lambda}[\wp_1 \cosh(\sqrt{-\alpha}\chi) + \wp_2 \sinh(\sqrt{-\alpha}\chi) - 1], \tag{38}$$

where

$$\wp_1 = 1 - \lambda r_0, \qquad \wp_2 = \beta\sigma_0\sqrt{\frac{-\lambda}{\mu}}. \tag{39}$$

We can define the generalised hyperbolic anomaly F by (see Baù et al, 2016)

$$\mu g \cosh F = \mu + 2\mathscr{E} r, \qquad \mu g \sinh F = r\,\dot{r}\sqrt{2\mathscr{E}}, \tag{40}$$

where g is the generalised eccentricity as in (31). Then, the following relations hold:

$$\begin{aligned} \wp_1 &= g\cosh(F - \sqrt{-\alpha}\chi), \\ \wp_2 &= g\sinh(F - \sqrt{-\alpha}\chi). \end{aligned} \tag{41}$$

Since $\wp_1 = g\cosh F_0$, $\wp_2 = g\sinh F_0$, where F_0 is the value of F for $\chi = 0$, we have

$$\sqrt{-\alpha}\chi = F - F_0. \tag{42}$$

Equation (25) for $\alpha < 0$ can be written as

$$\tan\frac{\nu}{2} = \frac{\sqrt{\wp_1^2 - \wp_2^2 - 1}\sinh\left(\frac{1}{2}\sqrt{-\alpha}\chi\right)}{(\wp_1 - 1)\cosh\left(\frac{1}{2}\sqrt{-\alpha}\chi\right) + \wp_2\sinh\left(\frac{1}{2}\sqrt{-\alpha}\chi\right)}, \tag{43}$$

or alternatively as

$$\tan\frac{\nu - \theta}{2} = \sqrt{\frac{1+g}{g-1}}\tanh\frac{\sqrt{-\alpha}\chi - F}{2}, \tag{44}$$

which is the relation between the true anomaly and the hyperbolic anomaly in the two-body problem.
Remark. The method presented in Baù et al (2016), here called HDromo, employs $\beta = \sqrt{2\varepsilon}$, so that $\alpha = -1$ and Eq. (38) takes the form

$$r = -\frac{1}{\lambda}(\wp_1\cosh\chi + \wp_2\sinh\chi - 1),$$

where[7]

$$\wp_1 = g\cosh(F - \chi), \qquad \wp_2 = g\sinh(F - \chi).$$

[7] In Baù et al (2016) the elements $\wp_1$, $\wp_2$, $-\lambda^{-1}$ are denoted by λ_1, λ_2, λ_3, respectively, and the independent variable χ by φ.

HDromo implements a different definition for ν with respect to that given in Eqs. (43), (44). Let us consider

$$\zeta = \operatorname{gd} 2(F - \chi), \qquad \tan\frac{\zeta}{2} = \tanh(F - \chi),$$

where $\operatorname{gd} x$ is the Gudermannian function (see Battin, 1999, p.165). Then, we obtain for $\wp_1$, $\wp_2$:

$$\wp_1 = \wp\cos\frac{\zeta}{2}, \qquad \wp_2 = \wp\sin\frac{\zeta}{2},$$

where $\wp = \sqrt{{\wp_1}^2 + {\wp_2}^2}$. These expressions invite to set the angle between $\mathbf{g}$ and the reference axis equal to $\zeta/2$, so that

$$\nu = \theta + \frac{\zeta}{2}.$$

2.2.3 The case $\alpha = 0$

For $\alpha = 0$, the equations for the orbital radius and the polar angle reduce to

$$r = r_0 + \sigma_0\chi + \frac{\mu}{2\beta^2}\chi^2, \qquad \beta\tan\frac{\nu}{2} = \frac{c\,\chi}{2r_0 + \sigma_0\chi}. \tag{45}$$

One can find that χ, ν are related to the angle θ, introduced in (28). Indeed,

$$\chi = \frac{c\,\beta}{\mu}\left(\tan\frac{\theta}{2} - \tan\frac{\theta_0}{2}\right), \tag{46}$$

$$\nu = \theta - \theta_0. \tag{47}$$

In fact, the latter relation holds for any α.

2.3 Variation of the elements r_0, σ_0, λ

The quantities r_0, σ_0, λ are attractive candidates for the set of intermediate elements. From their evolution, one obtains r, σ, p, ν as functions of χ once β is defined. Then, from the orientation of the intermediate basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$, we can determine the position and velocity of the particle at any χ. In this section, we deal with the computation of the derivatives of r_0, σ_0, λ with respect to χ, which vanish when the motion is unperturbed. For simplicity, we will adopt the notation

$$U_n = U_n(\chi;\alpha), \qquad \tilde{U}_n = U_n(2\chi;\alpha), \qquad n \in \mathbb{N}. \tag{48}$$

Consider the equations

$$\frac{\mathrm{d}r}{\mathrm{d}\chi} = \sigma, \tag{49}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\chi} = \frac{1}{\beta^2}[2\mathscr{E}r + \mu + r(rF_r - 2\mathscr{U})] - \frac{\sigma\beta'}{\beta}, \tag{50}$$

which stem from differentiating the definition of r, σ given in (17), (18), and regarding r_0, σ_0, λ, β as functions of χ. After some algebraic manipulations, we find

$$\begin{aligned}\beta^2 r_0' &= -r(rF_r - 2\mathscr{U})U_1 - \frac{\mu}{4}\Big(r_0\tilde{U}_2 + \sigma_0\tilde{U}_3 + 2\frac{\mu}{\beta^2}U_2^2\Big)\lambda' \\ &\quad + \chi\sigma_0\beta\beta', \end{aligned} \tag{51}$$

$$\begin{aligned}\beta^2\sigma_0' &= r(rF_r - 2\mathscr{U})U_0 + \frac{\mu}{4}\Big[r_0(2\chi + \tilde{U}_1) + \sigma_0\tilde{U}_2 \\ &\quad + \frac{\mu}{\beta^2}(\tilde{U}_3 - 4U_3)\Big]\lambda' + \Big[\frac{\mu}{\beta^2}(1 - \lambda r_0)\chi - \sigma_0\Big]\beta\beta'. \end{aligned} \tag{52}$$

Moreover, we have

$$\lambda' = -\frac{2}{\mu}\Big(\sigma P_r + \frac{h}{\beta}P_\nu + \frac{r}{\beta}\frac{\partial\mathscr{U}}{\partial t}\Big), \tag{53}$$

where $P_r = \mathbf{P}\cdot\mathbf{e}_r$, $P_\nu = \mathbf{P}\cdot\mathbf{e}_\nu$.

It is worth noting that for $\mathscr{E} < 0$, the expressions of r_0', σ_0' contain some terms in which χ appears explicitly. The presence of these terms can deteriorate the accuracy of r_0, σ_0 computed by numerical integration of Eqs. (51), (52), especially for long propagations. On the other hand, the variational equations of g, p (see 21, 22) are not affected by this disadvantage. Secular terms can be avoided in both r_0' and σ_0' if and only if we select $\beta = k\sqrt{-2\mathscr{E}}$ ($\mathscr{E} < 0$), where k is a nonzero constant, so that the quantity α is conserved along the perturbed motion.[8]

In Appendix A, we show that it is still possible to eliminate the secular terms from the derivatives r_0', σ_0' without having to restrict the domain of $\mathscr{E}$ to negative values, by adequately changing Eq. (7) and imposing that β is constant, i.e. $\beta' = 0$.

2.4 The time element t_0 and its evolution

By integrating the time transformation (6), we obtain Kepler's equation in its universal form

$$\beta(t - t_0) = r_0 U_1(\chi;\alpha) + \sigma_0 U_2(\chi;\alpha) + \frac{\mu}{\beta^2}U_3(\chi;\alpha), \tag{54}$$

where the quantity t_0 is called *time element*.

In the classic formulations by Wong (1962), Herrick (1965), and Pitkin (1966), time is the independent variable and the value of χ corresponding to a given t is obtained by solving the universal Kepler equation. Moreover, the time element t_0 is a constant, also when the motion is perturbed. Born et al (1974) suggested that it may be more convenient to let t_0 vary with time instead of keeping it fixed. In fact, by properly choosing the time derivative of t_0, the

[8] In the method EDromo (Baù et al, 2015), it is $\alpha = 1$ and secular terms are not present in the derivatives of $\wp_1$, $\wp_2$ (see 36).

secular terms that appear in the variational equations of $\mathbf{r}_0$, $\dot{\mathbf{r}}_0$ can be eliminated.[9] The drawback of this approach is that t_0 is added to the state vector thus increasing the dimension of the system.

In our formulation, χ is the independent variable as defined in (6), and Eq. (54) is used to directly compute the physical time t, so t_0 must be known. The variational equation of t_0, which is obtained by differentiation of Eq. (54), becomes

$$\beta^3 t_0' = r(rF_r - 2\mathscr{U})U_2 - \frac{\mu}{4}\Big[r_0(4U_3 - \tilde{U}_3) - 2\sigma_0 U_2^2 - \frac{\mu}{\beta^2}(\tilde{U}_5 - 8U_5)\Big]\lambda' + \chi r_0 \beta\beta'. \quad (55)$$

In the case $\mathscr{E} < 0$, the expression above for t_0' contains terms that are linear in χ.[10] By selecting $\beta = k\sqrt{-2\mathscr{E}}$, where k is a nonzero constant (see Section 2.3), we can eliminate only some of them, because, as expected, those in $\tilde{U}_5 - 8U_5$ survive. However, with this choice of β it is still possible to get rid of the secular terms as follows. Let us use the identity $U_1 + \alpha U_3 = \chi$ to write Kepler's equation as

$$k\sqrt{\lambda\mu}(t - t_1) = \Big(r_0 - \frac{1}{\lambda}\Big)U_1 + \sigma_0 U_2, \quad (56)$$

where

$$t_1 = t_0 + \frac{\chi}{k\sqrt{\lambda^3\mu}}. \quad (57)$$

Then, the variational equation of t_1 is free of secular terms. This quantity, which is a linear function of χ when the motion is unperturbed, is also referred to as *linear* time element. In Baù et al (2015), both t_0 and t_1 are presented for EDromo.

A time element analogous to t_0 was developed also by Burdet (1968) and Bond (1974). In their formulation, the time transformation (6) is applied with β equal to $\sqrt{\mu}$ and 1, respectively. Moreover, the variables r_0, σ_0 are included in the set of elements, even if they are not necessary to describe the motion. The advantage of adding these redundant variables is not clear in Burdet (1968). On the other hand, Bond finds out that substituting in (6) the expression of r given in (17), t_0' is not affected by *mixed* secular terms.[11] They arise instead if the orbital distance is written as a function of the elements related to the Kustaanheimo-Stiefel parameters.

2.5 Motion *of* the orbital plane

The proposed method relies on the existence of the orbital plane, and so it becomes singular when the angular momentum vanishes. We track the evolution

[9] Unfortunately, the secular terms are not completely removed since they are contained in the expression of t_0 (see Battin, 1999, pp. 510, 511).

[10] Note that the terms with χ^3, which stem from $\tilde{U}_5$, U_5, cancel out.

[11] These terms contain the product of a trigonometric function of χ and some power of χ.

of this plane and of a reference direction on it by describing the orientation of the *intermediate* frame $\{O, \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ that we have introduced in Section 2.1.

Let $\{O, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be a reference frame with the origin at O (i.e. the centre of mass of the central body) and the directions of $\mathbf{e}_i$, $i = 1, 2, 3$, fixed in space. In particular, the unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$ generate the fundamental plane (e.g. the plane of the Earth's orbit, or the plane of the Earth's equator). We denote by Ω, I, ω the three classical orbital elements given by the longitude of the ascending node, inclination, and argument of pericentre. Let us consider the quantity $\Psi = \omega + f - \nu$, where f is the true anomaly and ν is the angle defined in Section 2.1. Then, the Euler angles Ω, I, Ψ define the orientation of the basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$.

Following Goldstein (1980, p. 155), we introduce the Euler parameters q_1, q_2, q_3, q_4 related to the Euler angles Ω, I, Ψ by:

$$\begin{aligned} q_1 &= \cos\frac{\Omega+\Psi}{2}\cos\frac{I}{2}, & q_2 &= \cos\frac{\Omega-\Psi}{2}\sin\frac{I}{2}, \\ q_3 &= \sin\frac{\Omega-\Psi}{2}\sin\frac{I}{2}, & q_4 &= \sin\frac{\Omega+\Psi}{2}\cos\frac{I}{2}. \end{aligned} \tag{58}$$

Note that these parameters satisfy the following relation:

$$q_1^2 + q_2^2 + q_3^2 + q_4^2 = 1. \tag{59}$$

Taking the time derivatives of Eqs. (58), we find

$$\begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \\ \dot{q}_4 \end{pmatrix} = \frac{1}{2} \begin{bmatrix} -q_4 & -q_1\tan(I/2) & -q_4 \\ -q_3 & q_2\cot(I/2) & q_3 \\ q_2 & q_3\cot(I/2) & -q_2 \\ q_1 & -q_4\tan(I/2) & q_1 \end{bmatrix} \begin{pmatrix} \dot{\Omega} \\ \dot{I} \\ \dot{\Psi} \end{pmatrix}. \tag{60}$$

Replacing $\dot{\Omega}$, $\dot{I}$, $\dot{\omega} + \dot{f}$ with the expressions available in, for example, Battin (1999, pp. 500, 501), and using Eq. (6), we arrive at

$$\begin{pmatrix} q_1' \\ q_2' \\ q_3' \\ q_4' \end{pmatrix} = \frac{1}{2}\left(\frac{h}{r\beta} - \nu'\right) \begin{pmatrix} -q_4 \\ q_3 \\ -q_2 \\ q_1 \end{pmatrix} - \frac{r^2}{2\beta h} F_z \begin{pmatrix} q_2\cos\nu + q_3\sin\nu \\ -q_1\cos\nu + q_4\sin\nu \\ -q_4\cos\nu - q_1\sin\nu \\ q_3\cos\nu - q_2\sin\nu \end{pmatrix}, \tag{61}$$

where $F_z = \mathbf{F}\cdot\mathbf{e}_z$ and prime denotes the derivative with respect to χ. By differentiating Eq. (25) and simplifying the result, we find the following expression for ν'[12]

[12]We also used the relation

$$\cos^2\frac{\nu}{2} = \frac{\left[r_0 U_0\left(\frac{1}{2}\chi;\alpha\right) + \sigma_0 U_1\left(\frac{1}{2}\chi;\alpha\right)\right]^2}{r r_0},$$

which can be obtained from Eqs. (17), (22), and (25).

$$\beta\nu' = \frac{c}{r} + \frac{r}{cr_0}(rF_r - 2\mathscr{U})(\alpha r_0 U_2 - \sigma_0 U_1) - \frac{\chi c}{\beta r_0}\beta' \\ - \frac{\mu}{2r_0}\left[\frac{r}{c}(r_0 U_1 + \sigma_0 U_2) - \frac{c}{\beta^2}U_3\right]\lambda'. \quad (62)$$

The identities involving the universal functions that we used in the computation of r_0', σ_0', t_0', ν' are reported in Appendix D. For negative values of $\mathscr{E}$, the presence of secular terms in the derivative of ν can be avoided only by setting $\beta = k\sqrt{-2\mathscr{E}}$, where k is a nonzero constant. We observe that the four Euler parameters q_1, q_2, q_3, q_4 are constant when the motion is unperturbed. Therefore, in this case the intermediate frame remains fixed in space.

2.6 The proposed formulation

All that remains to be ready to present our formulation is the definition of the quantity β, which was first introduced in Eq. (6). Several choices are possible in principle; however it seems natural to set β equal to a constant. We take $\beta = 1$ as in the original Sundman (1913, p. 127) transformation,

$$\frac{\mathrm{d}t}{\mathrm{d}\chi} = r. \quad (63)$$

Then, we have $\alpha = \mu\lambda = -2\mathscr{E}$.

The first four intermediate elements are defined as

$$\iota_1 \coloneqq r_0, \quad \iota_2 \coloneqq \sigma_0, \quad \iota_3 \coloneqq \alpha, \quad \iota_4 \coloneqq t_0. \quad (64)$$

The remaining four elements are the Euler parameters that represent the orientation of the intermediate frame:

$$\iota_5 \coloneqq q_1, \quad \iota_6 \coloneqq q_2, \quad \iota_7 \coloneqq q_3, \quad \iota_8 \coloneqq q_4. \quad (65)$$

The Newtonian equation of motion (3) is replaced by the system of first-order differential equations:

$$\iota_1' = -r(rF_r - 2\mathscr{U})U_1 - \frac{\iota_3'}{4}(\iota_1\tilde{U}_2 + \iota_2\tilde{U}_3 + 2\mu U_2^2), \quad (66)$$

$$\iota_2' = r(rF_r - 2\mathscr{U})U_0 + \frac{\iota_3'}{4}[\iota_1(2\chi + \tilde{U}_1) + \iota_2\tilde{U}_2 + \mu(\tilde{U}_3 - 4U_3)], \quad (67)$$

$$\iota_3' = -2\Big(\sigma P_r + hP_\nu + r\,\frac{\partial\mathscr{U}}{\partial t}\Big), \quad (68)$$

$$\iota_4' = r(rF_r - 2\mathscr{U})U_2 - \frac{\iota_3'}{4}[\iota_1(4U_3 - \tilde{U}_3) - 2\iota_2 U_2^2 - \mu(\tilde{U}_5 - 8U_5)], \quad (69)$$

$$\iota_5' = -\frac{N}{2}\iota_8 - \frac{r^2}{2h}F_z(\iota_6\cos\nu + \iota_7\sin\nu), \quad (70)$$

$$\iota_6' = \frac{N}{2}\iota_7 + \frac{r^2}{2h}F_z(\iota_5\cos\nu - \iota_8\sin\nu), \quad (71)$$

$$\iota_7' = -\frac{N}{2}\iota_6 + \frac{r^2}{2h}F_z(\iota_8\cos\nu + \iota_5\sin\nu), \tag{72}$$

$$\iota_8' = \frac{N}{2}\iota_5 - \frac{r^2}{2h}F_z(\iota_7\cos\nu - \iota_6\sin\nu), \tag{73}$$

where

$$N = \frac{h-c}{r} - \frac{r}{c\iota_1}(rF_r - 2\mathscr{U})(\iota_1\iota_3 U_2 - \iota_2 U_1) + \frac{\iota_3'}{2\iota_1}\Big[\frac{r}{c}(\iota_1 U_1 + \iota_2 U_2) - c\,U_3\Big]. \tag{74}$$

We want to propagate the position $\mathbf{r}$ and velocity $\dot{\mathbf{r}}$ from some starting epoch t_* to a different time t by solving the system of Eqs. (66)–(73). The definition of ι_i, $i = 1, ..., 8$, at $\chi(t_*) = 0$ is as follows. For the first four elements, we have

$$\iota_1 = |\mathbf{r}|, \quad \iota_2 = \mathbf{r}\cdot\dot{\mathbf{r}}, \quad \iota_3 = \frac{2\mu}{|\mathbf{r}|} - |\dot{\mathbf{r}}|^2 - 2\mathscr{U}(\mathbf{r}, t_*), \quad \iota_4 = t_*. \tag{75}$$

Since $\nu = 0$ at time $t = t_*$, the intermediate and the LVLH frames coincide and we can compute

$$\mathbf{e}_x = \frac{\mathbf{r}}{|\mathbf{r}|}, \qquad \mathbf{e}_y = \mathbf{e}_z \times \mathbf{e}_x, \qquad \mathbf{e}_z = \frac{\mathbf{r}\times\dot{\mathbf{r}}}{|\mathbf{r}\times\dot{\mathbf{r}}|}. \tag{76}$$

The corresponding Euler parameters are obtained by the formulae (58) where Ψ is the argument of latitude, i.e. $\Psi = \omega + f$. While the sum of Ω and $\omega + f$ is defined for any conic, their difference is not. If $I = 0$, we can take $\Omega = 0$. In Eqs. (75), (76) the quantities $\mathbf{r}$, $\dot{\mathbf{r}}$ are referred to the starting epoch.

We solve the initial value problem given by the differential Eqs. (66)–(73) with the initial conditions computed above by means of a numerical algorithm. At each integration step, the position $\mathbf{r}$, velocity $\dot{\mathbf{r}}$, and time t can be recovered from the intermediate elements and the independent variable. We compute

$$r = \iota_1 U_0(\chi;\iota_3) + \iota_2 U_1(\chi;\iota_3) + \mu U_2(\chi;\iota_3), \tag{77}$$

$$\sigma = \iota_2 U_0(\chi;\iota_3) + (\mu - \iota_1\iota_3)U_1(\chi;\iota_3). \tag{78}$$

The components of $\mathbf{e}_x$, $\mathbf{e}_y$ in the basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, introduced in Section 2.5, are obtained by

$$\mathbf{e}_x = \begin{pmatrix} \iota_5^2 + \iota_6^2 - \iota_7^2 - \iota_8^2 \\ 2\iota_6\iota_7 + 2\iota_5\iota_8 \\ 2\iota_6\iota_8 - 2\iota_5\iota_7 \end{pmatrix}, \qquad \mathbf{e}_y = \begin{pmatrix} 2\iota_6\iota_7 - 2\iota_5\iota_8 \\ \iota_5^2 - \iota_6^2 + \iota_7^2 - \iota_8^2 \\ 2\iota_5\iota_6 + 2\iota_7\iota_8 \end{pmatrix}. \tag{79}$$

Then, we determine the radial and transverse unit vectors as

$$\mathbf{e}_r = \cos\nu\,\mathbf{e}_x + \sin\nu\,\mathbf{e}_y, \tag{80}$$

$$\mathbf{e}_\nu = -\sin\nu\,\mathbf{e}_x + \cos\nu\,\mathbf{e}_y, \tag{81}$$

where

$$\nu = 2\arctan\frac{c\,U_1\left(\frac{1}{2}\chi;\iota_3\right)}{\iota_1 U_0\left(\frac{1}{2}\chi;\iota_3\right) + \iota_2 U_1\left(\frac{1}{2}\chi;\iota_3\right)}. \tag{82}$$

The generalised and osculating angular momentum are given from the relations

$$c^2 = \iota_1(2\mu - \iota_1\iota_3) - \iota_2^2, \qquad h^2 = c^2 - 2r^2\mathscr{U}(\mathbf{r}, t). \tag{83}$$

Finally, the position and velocity read

$$\mathbf{r} = r\mathbf{e}_r, \qquad \dot{\mathbf{r}} = \frac{1}{r}(\sigma\mathbf{e}_r + h\mathbf{e}_\nu), \tag{84}$$

and the physical time is obtained by

$$t = \iota_4 + \iota_1 U_1(\chi; \iota_3) + \iota_2 U_2(\chi; \iota_3) + \mu U_3(\chi; \iota_3). \tag{85}$$

As expected, our method is affected by the following singularities: $r = 0$, $\iota_1 = 0$, $h = 0$, $c = 0$.

Remark. Note that we first compute the potential $\mathscr{U}$ and then the osculating angular momentum h, which means that in the proposed method $\mathscr{U}$ should ideally not depend on the velocity $\dot{\mathbf{r}}$. Such limitation can be overcome if h is regarded as a new state variable. The consequent increase in the dimension of the system (from 8 to 9) is avoided if one uses the modification of the Euler parameters suggested by Lara (2017).

3 Orbit determination and uncertainty propagation

The topic of orbit determination by means of coordinates different from the Cartesian ones and an independent variable which is not the physical time is still quite unexplored. Only very recently, Roa and Peláez (2017b) have shown in the context of relative motion that better numerical performance can be achieved with regularised formulations. Using the results in Shefer (2007) and Roa and Peláez (2017a), we describe in this section how to map the state-transition matrix (STM) of the intermediate elements at some fictitious time χ to the classic STM in Cartesian coordinates at the corresponding time t.

Let us denote by $\boldsymbol{\iota} \in \mathbb{R}^8$ the column vector of the intermediate elements, i.e. $\boldsymbol{\iota} = (\iota_1, \ldots, \iota_8)^T$, so that we can write Eqs. (66)–(73) in the compact form

$$\frac{\mathrm{d}\boldsymbol{\iota}}{\mathrm{d}\chi} = \mathbf{f}(\chi, \boldsymbol{\iota}). \tag{86}$$

For the solution $\boldsymbol{\iota}(\chi, \boldsymbol{\iota}_0)$ of (86) with the initial condition $\boldsymbol{\iota}_0 = \boldsymbol{\iota}(0)$ we introduce the state-transition matrix

$$A(\chi, \boldsymbol{\iota}_0) = \frac{\partial \boldsymbol{\iota}}{\partial \boldsymbol{\iota}_0}(\chi, \boldsymbol{\iota}_0). \tag{87}$$

The matrix A satisfies the Cauchy problem

$$\frac{\partial A}{\partial \chi} = \frac{\partial \mathbf{f}}{\partial \boldsymbol{\iota}}(\boldsymbol{\iota}(\chi, \boldsymbol{\iota}_0))A, \quad A(0, \boldsymbol{\iota}_0) = I_d, \tag{88}$$

where I_d is the 9×9 identity matrix. The solution of the differential equation in (88), which is called variational equation, is computed numerically together with the solution of Eq. (86).

Let $\mathbf{x} \in \mathbb{R}^6$ be the (column) vector with components given by the coordinates of the position $\mathbf{r}$ and velocity $\dot{\mathbf{r}}$ of a space object in a suitable reference frame. Suppose we apply the method known as *differential corrections* (for more details, see Milani and Gronchi, 2010, chap. 5) to determine $\mathbf{x}_0 = \mathbf{x}(t_*)$, from a set of observations collected at times $t_1 < t_2 < \ldots < t_m$.[13] In each iteration of this method, we need the state-transition matrix

$$S(t, \mathbf{x}_0) = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_0}(t, \mathbf{x}_0) \tag{89}$$

at t_i, $i = 1, \ldots, m$. We can calculate $S(t, \mathbf{x}_0)$ from $A(\chi, \boldsymbol{\iota}_0)$ through the formula (we set $\chi = 0$ at $t = t_*$)

$$S = J\, \tilde{A}\, J_0, \tag{90}$$

where

$$J = \frac{\partial \mathbf{x}}{\partial \boldsymbol{\iota}}, \qquad J_0 = \frac{\partial \boldsymbol{\iota}_0}{\partial \mathbf{x}_0}, \qquad \tilde{A} = A - \frac{1}{r}\mathbf{f}\frac{\partial t}{\partial \boldsymbol{\iota}_0}. \tag{91}$$

Starting from a first guess of $\mathbf{x}_0$, the iterative method converges to a nominal solution. Moreover, the associated covariance matrix $\Gamma_{\mathbf{x}_0}$ is known. One may want to propagate $\Gamma_{\mathbf{x}_0}$ to $\Gamma_{\mathbf{x}}$ at time $t \neq t_*$. Linear propagation is in many cases acceptable, and it can be made more efficient if we use orbital elements (Junkins et al, 1996). First, the matrix $\Gamma_{\mathbf{x}_0}$ is transformed to $\Gamma_{\boldsymbol{\iota}_0} = J_0\, \Gamma_{\mathbf{x}_0}\, J_0^T$. Then, the covariance matrix at time t is obtained by

$$\Gamma_{\boldsymbol{\iota}} = \tilde{A}\, \Gamma_{\boldsymbol{\iota}_0}\, \tilde{A}^T. \tag{92}$$

Finally, we apply the conversion $\Gamma_{\mathbf{x}} = J\, \Gamma_{\boldsymbol{\iota}}\, J^T$. The explicit expressions of the Jacobian matrices J, J_0 are given in the following sections, and of the matrix $\partial \mathbf{f} / \partial \boldsymbol{\iota}$ in Appendix C.

3.1 Partial derivatives of position and velocity with respect to intermediate elements

Let us first give the expression of the Jacobian matrix $\partial \mathbf{r} / \partial \boldsymbol{\iota}$. From the first relation in (84) and using Eqs. (80), (81), we have

$$\frac{\partial \mathbf{r}}{\partial \boldsymbol{\iota}} = \mathbf{e}_r \frac{\partial r}{\partial \boldsymbol{\iota}} + r \frac{\partial \mathbf{e}_r}{\partial \boldsymbol{\iota}}, \tag{93}$$

where

$$\frac{\partial \mathbf{e}_r}{\partial \boldsymbol{\iota}} = \mathbf{e}_\nu \frac{\partial \nu}{\partial \boldsymbol{\iota}} + \frac{\partial \mathbf{e}_x}{\partial \boldsymbol{\iota}} \cos\nu + \frac{\partial \mathbf{e}_y}{\partial \boldsymbol{\iota}} \sin\nu. \tag{94}$$

Differentiation of the expressions for r, ν, c in (77), (82), (83) yields

$$\frac{\partial r}{\partial \boldsymbol{\iota}} = \Big(U_0,\, U_1,\, \frac{1}{2}[\iota_2 U_3 + 2\mu U_4 - \chi(t - \iota_4)],\, \mathbf{0}_5\Big),$$

[13] The time t_* is usually chosen as the average of the observation times.

$$
\begin{aligned}
r\iota_1 \frac{\partial \nu}{\partial \boldsymbol{\iota}} &= (\iota_1 U_1 + \iota_2 U_2)\frac{\partial c}{\partial \boldsymbol{\iota}} - c\Big(U_1,\, U_2,\, -\frac{\iota_1 U_3}{2},\, \mathbf{0}_5\Big),\\
\frac{\partial c}{\partial \boldsymbol{\iota}} &= \frac{1}{c}\Big(\mu - \iota_1\iota_3,\, -\iota_2,\, -\frac{\iota_1^2}{2},\, \mathbf{0}_5\Big),
\end{aligned}
$$

where $\mathbf{0}_5 \in \mathbb{R}^5$ is a row vector having null entries. The unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$ are functions only of the four Euler parameters, and

$$
\begin{aligned}
\frac{\partial \mathbf{e}_x}{\partial(\iota_5, \iota_6, \iota_7, \iota_8)} &= 2\begin{pmatrix} \iota_5 & \iota_6 & -\iota_7 & -\iota_8 \\ \iota_8 & \iota_7 & \iota_6 & \iota_5 \\ -\iota_7 & \iota_8 & -\iota_5 & \iota_6 \end{pmatrix},\\
\frac{\partial \mathbf{e}_y}{\partial(\iota_5, \iota_6, \iota_7, \iota_8)} &= 2\begin{pmatrix} -\iota_8 & \iota_7 & \iota_6 & -\iota_5 \\ \iota_5 & -\iota_6 & \iota_7 & -\iota_8 \\ \iota_6 & \iota_5 & \iota_8 & \iota_7 \end{pmatrix}.
\end{aligned}
$$

Then, we deal with the Jacobian matrix $\partial\dot{\mathbf{r}}/\partial\boldsymbol{\iota}$. From the second relation in (84) and Eq. (81), we get

$$
\frac{\partial \dot{\mathbf{r}}}{\partial \boldsymbol{\iota}} = \frac{1}{r}\Big(\mathbf{e}_r \frac{\partial \sigma}{\partial \boldsymbol{\iota}} + \mathbf{e}_\nu \frac{\partial h}{\partial \boldsymbol{\iota}} + \sigma \frac{\partial \mathbf{e}_r}{\partial \boldsymbol{\iota}} + h \frac{\partial \mathbf{e}_\nu}{\partial \boldsymbol{\iota}} - \dot{\mathbf{r}} \frac{\partial r}{\partial \boldsymbol{\iota}}\Big), \tag{95}
$$

where

$$
\frac{\partial \mathbf{e}_\nu}{\partial \boldsymbol{\iota}} = -\mathbf{e}_r \frac{\partial \nu}{\partial \boldsymbol{\iota}} - \frac{\partial \mathbf{e}_x}{\partial \boldsymbol{\iota}} \sin\nu + \frac{\partial \mathbf{e}_y}{\partial \boldsymbol{\iota}} \cos\nu. \tag{96}
$$

Using the expressions of σ, h in (78), (83), we can compute

$$
\begin{aligned}
\frac{\partial \sigma}{\partial \boldsymbol{\iota}} &= \Big(-\iota_3 U_1,\, U_0,\, \frac{1}{2}(\mu U_3 - \iota_1 U_1 - \chi r),\, \mathbf{0}_5\Big),\\
\frac{\partial h}{\partial \boldsymbol{\iota}} &= \frac{1}{h}\Big(\mu - \iota_1\iota_3 - 2rU_0\mathscr{U},\, -\iota_2 - 2rU_1\mathscr{U},\, -\frac{\iota_1^2}{2} - 2r\mathscr{U}\frac{\partial r}{\partial \iota_3},\, \mathbf{0}_5\Big) - \frac{r^2}{h}\frac{\partial \mathscr{U}}{\partial \boldsymbol{\iota}}.
\end{aligned}
$$

The vector $\partial\mathscr{U}/\partial\boldsymbol{\iota}$ is obtained as shown in Eq. (108).
Remark. We observe that when $\mathscr{E} < 0$, secular terms appear only in 6 out of the 48 components of the matrix of the partial derivatives of position and velocity with respect to intermediate elements, denoted by J. As observed, for example, by Broucke and Cefola (1972), this is a remarkable advantage over the universal variables, in which the fundamental matrix contains secular terms in all 36 elements.

3.2 Partial derivatives of intermediate elements with respect to position and velocity at the initial time

All the quantities of this section are referred to the initial time t_* of propagation. For the first four intermediate elements, a straightforward computation from relations (75) yields

$$
\begin{aligned}
\frac{\partial \iota_1}{\partial \mathbf{r}} &= \mathbf{e}_x^T, & \frac{\partial \iota_1}{\partial \dot{\mathbf{r}}} &= \mathbf{0}_3, \\
\frac{\partial \iota_2}{\partial \mathbf{r}} &= \dot{\mathbf{r}}^T, & \frac{\partial \iota_2}{\partial \dot{\mathbf{r}}} &= \mathbf{r}^T, \\
\frac{\partial \iota_3}{\partial \mathbf{r}} &= -2\Big(\frac{\mu}{r^2}\mathbf{e}_x^T + \frac{\partial \mathscr{U}}{\partial \mathbf{r}}\Big), & \frac{\partial \iota_3}{\partial \dot{\mathbf{r}}} &= -2\dot{\mathbf{r}}^T, \\
\frac{\partial \iota_4}{\partial \mathbf{r}} &= \mathbf{0}_3, & \frac{\partial \iota_4}{\partial \dot{\mathbf{r}}} &= \mathbf{0}_3,
\end{aligned}
\tag{97}
$$

where $\mathbf{0}_3 = (0,\, 0,\, 0)$.

At the initial time the intermediate and the LVLH frames coincide (see Eqs. 76). The partial derivatives of the Euler parameters take the following simple expressions which are obtained as shown in Appendix B:

$$
\begin{aligned}
\frac{\partial \iota_5}{\partial \mathbf{r}} &= \frac{1}{2r}[(\iota_7 + \iota_6 \upsilon)\mathbf{e}_z^T - \iota_8\, \mathbf{e}_y^T], \\
\frac{\partial \iota_6}{\partial \mathbf{r}} &= \frac{1}{2r}[(\iota_8 - \iota_5 \upsilon)\mathbf{e}_z^T + \iota_7\, \mathbf{e}_y^T], \\
\frac{\partial \iota_7}{\partial \mathbf{r}} &= -\frac{1}{2r}[(\iota_8 \upsilon + \iota_5)\mathbf{e}_z^T + \iota_6\, \mathbf{e}_y^T], \\
\frac{\partial \iota_8}{\partial \mathbf{r}} &= \frac{1}{2r}[(\iota_7 \upsilon - \iota_6)\mathbf{e}_z^T + \iota_5\, \mathbf{e}_y^T],
\end{aligned}
\tag{98}
$$

where $\upsilon = \sigma/h$, and

$$
\begin{aligned}
\frac{\partial \iota_5}{\partial \dot{\mathbf{r}}} &= -\frac{r}{2h}\iota_6\, \mathbf{e}_z^T, & \frac{\partial \iota_6}{\partial \dot{\mathbf{r}}} &= \frac{r}{2h}\iota_5\, \mathbf{e}_z^T, \\
\frac{\partial \iota_7}{\partial \dot{\mathbf{r}}} &= \frac{r}{2h}\iota_8\, \mathbf{e}_z^T, & \frac{\partial \iota_8}{\partial \dot{\mathbf{r}}} &= -\frac{r}{2h}\iota_7\, \mathbf{e}_z^T.
\end{aligned}
\tag{99}
$$

4 Numerical tests

We present two numerical tests to have a taste of the performance of the intermediate elements compared to other methods existing in the literature. In particular, we choose Cowell's method (Battin, 1999, p. 447), the modified equinoctial elements (Walker et al, 1985), Dromo (Peláez et al, 2007), the natural elements derived by Burdet (1968), and the regular KS-based elements published by Bond (1974). Hereafter, we will refer to them as Cowell, ModEq, Dromo, Nat–Burdet, and KS–Bond, respectively. Some relevant features of these formulations and the intermediate elements are given in Table 1. We use the label "New" to refer to the formulation described in Section 2.6.

Performance is assessed by analysing accuracy and speed of each special perturbation method. The accuracy is measured by propagating the orbit forward

Table 1: Formulations compared in the numerical tests (labels are explained in the text above). The quantities t, r, h are time, the orbital radius, and the osculating angular momentum. Prime denotes the derivative with respect to the independent variable. For each formulation, we specify the adopted independent variable, the dimension of the state vector, the number of orbital elements (i.e. constants of the unperturbed motion) among the state variables, and if a time element is included.

Formulations	Indep. variable	Dim.	Elements	Time el.
Cowell	t	6	0	no
ModEq	t	6	5	no
Dromo	$t' = r^2/h$	8	7	no
Nat–Burdet	$t' = r$	11	11	yes
KS–Bond	$t' = r$	10	10	yes
New	$t' = r$	8	8	yes

until the final time, reversing the integration back to the initial time, and computing the error as the difference between the final state (position and velocity) and the initial one. The speed of a particular integration is determined by the number of times the integrator calls the force function. This metric is preferred over the actual runtime because it is machine and implementation independent. In real scenarios, evaluating the perturbation forces is computationally more expensive than the rest of operations required to calculate the right-hand side of the differential equations. Thus, the additional cost per function call that one has to pay for using a formulation that is more sophisticated than Cowell is usually negligible. The selected integrator is the standard variable step Runge–Kutta 4(5) implemented in Matlab's `ode45` function. Performance curves are generated by changing the relative tolerance from 10^{-6} to 10^{-13}. We note that Nat–Burdet, KS–Bond, and the new elements make use of Stumpff's functions. The series are evaluated via recursive formulae implementing an argument-reduction technique to ensure convergence, as indicated by Danby (1992, sect. 6.9) and Roa and Peláez (2017b, Appendix 1).

4.1 The hyperbolic comet C/2003 T4 (LINEAR)

We consider the orbit of the hyperbolic comet C/2003 T4 (LINEAR), defined by its osculating elements in Table 2. Non-gravitational forces are modelled following Marsden et al (1973): we use the coefficients $A_1 = 1.0592 \times 10^{-7}$ au d^{-2}, $A_2 = 8.1043 \times 10^{-10}$ au d^{-2}, and $A_3 = 3.2073 \times 10^{-9}$ au d^{-2} for the radial, transverse, and normal components, respectively (d stands for day). Although the resulting acceleration is small, obviating this effect results in a non-negligible separation of approximately 0.05 au at the final epoch. Gravitational perturbations are given by the attraction of the outer planets (Jupiter through Neptune). Their positions are retrieved from the DE431 ephemeris.

Table 2: Osculating elements of C/2003 T4 (LINEAR) at epoch JD 2453296.5 (2004 October 18) TDB (Barycentric Dynamical Time). Orbit solution JPL 132. They are the eccentricity (e), perihelion distance (q, in astronomical units), time of perihelion passage (t_p), inclination (I), longitude of the node (Ω), and argument of perihelion (ω). Angles are in degrees.

e	q (au)	t_p (TDB)	I	Ω	ω
1.0005	0.8498	2453464.16	86.7612	93.9029	181.6795

The orbit reported in Table 2 is propagated for 10 years starting on 2000 April 3, that is 5 years before perihelion passage. Figure 2 displays the performance curves for each of the selected formulations. Since external perturbations are weak in this example, using the modified equinoctial elements instead of Cartesian coordinates reduces the number of function calls by approximately a factor of two for the same accuracy. Time is the independent variable also for ModEq, which means that the performance gains with respect to Cowell are only due to the use of slowly varying variables. In Dromo, the fictitious time behaves like the true anomaly when the motion is Keplerian, and it results in this method being four and two times faster than Cowell and ModEq, respectively. The improvement comes from a more efficient step size control, specifically during pericentre passage. The methods Nat–Burdet, KS–Bond, and the intermediate elements presented in this paper all rely on a (first-order) Sundman time transformation. Thus, the independent variable evolves like the hyperbolic anomaly, which naturally optimises the discretisation of hyperbolic orbits. These three formulations exhibit the best performance: they are almost one order of magnitude faster than the integration in Cartesian coordinates in this particular example. Only when the comet is close to perihelion, the step size is slightly reduced, although the reduction is only by a factor of two compared to the two order of magnitude reduction observed when time is the independent variable. The more efficient discretisation of the orbit around perihelion produces the aforementioned improvements in performance.

The positive effect of the analytic step size adaption, observed thanks to introducing a modified time variable, becomes apparent in Fig. 3. This figure compares the evolution of the time step when Cowell's method and the new elements are used to propagate the orbit. Cowell sequentially reduces the step size as the comet approaches the perihelion. This is required to meet the integration tolerance as the velocity increases and the problem becomes more sensitive to small deviations. Conversely, the length of the integration step shows a small variation when the orbit is propagated by the intermediate elements. After the comet passes the closest approach with the Sun and moves away from it along the outgoing asymptote, the step size increases again for Cowell, while the velocity decreases. Finally, we observe that far enough from the perihelion, it becomes comparable to that of the new formulation.

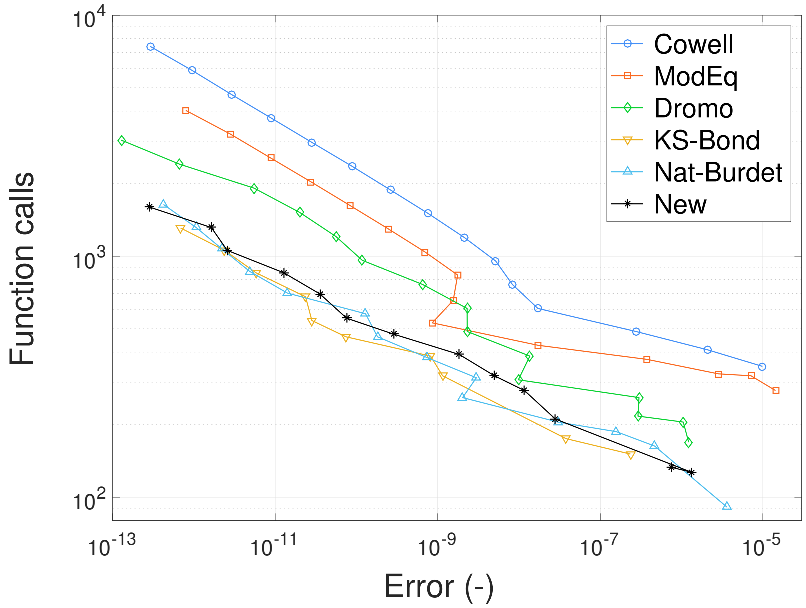

Figure 2: Performance of different propagation methods when integrating the orbit of comet C/2003 T4. The state error is normalised using the heliocentric distance of the comet at the initial time as the unit of length and the unit of time is chosen so that the gravitational parameter is normalised to unity.

4.2 The comet C/1985 K1 (Machholz)

Gravitational perturbations from the outer planets cause the orbit of comet C/1985 K1 to transition between hyperbolic and elliptic repeatedly, as shown in Fig. 4. This behaviour is ideal for testing how a uniform formulation handles different orbital regimes. The orbit is initially hyperbolic (see the osculating orbital elements listed in Table 3), the eccentricity decreases as the comet approaches perihelion temporarily becoming less than unity, then increasing to produce a hyperbolic orbit at perihelion. The orbit is propagated for 20 years, starting 10 years before perihelion.

To propagate the orbit of comet C/1985 K1, we resort to the numerical setup described in Section 4.1 except that non-gravitational forces are not included. Figure 5 compares the performance of the selected formulations. Although Cowell's method does not depend explicitly on the type of orbit, its overall performance is affected by the fact that using the physical time as independent variable results in an inefficient discretisation of the orbit. The orbital elements evolve slowly over time, and consequently, employing the modified equinoctial elements instead of Cartesian coordinates produces a substantial improvement in performance. Next, Dromo replaces the physical time with the true anomaly and the performance gain observed in Fig. 5 relative to ModEq is due to the an-

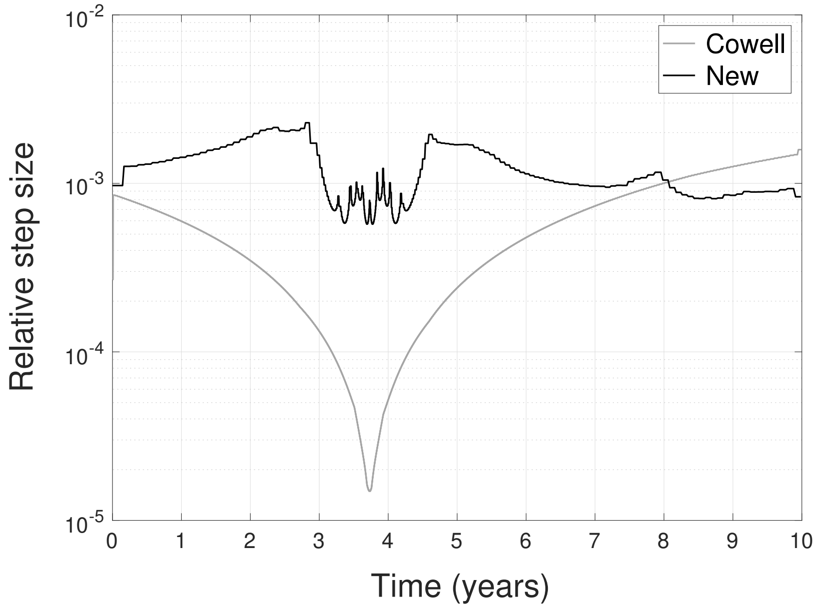

Figure 3: Evolution of the integration step size during the propagation of the orbit of comet C/2003 T4. The close encounter with the Sun causes a strong reduction of the step for Cowell, while it has almost no effect on the new method.

alytic step size adaption implicit in the change of the independent variable. The best behaviour is shown by the formulations relying on the Sundman transformation (63): KS–Bond, Nat–Burdet, and the new elements. The performance of these three formulations is similar, with the intermediate elements being slightly more accurate for small integration tolerances. The new formulation is capable of transitioning between orbital regimes without singularities or accuracy losses.

Table 3: Osculating elements of C/1985 K1 (Machholz) at epoch JD 2442592.7 (1975 June 29) TDB (Barycentric Dynamical Time). Orbit solution from 2008 SAO Comet Catalog. Angles are in degrees.

e	q (au)	t_p (TDB)	I	Ω	ω
1.000026	0.1085	2446245.24	16.0812	198.2520	271.7063

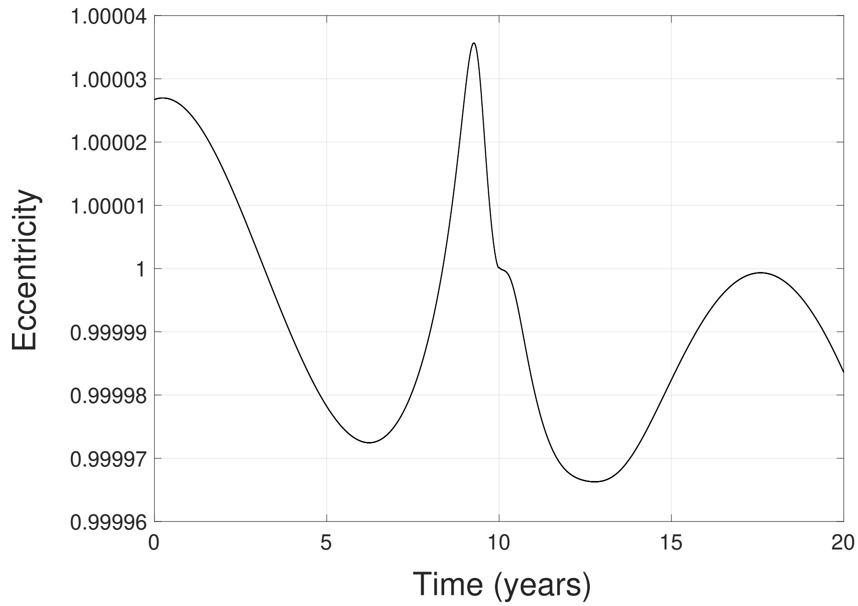

Figure 4: Evolution of the eccentricity of comet C/1985 K1.

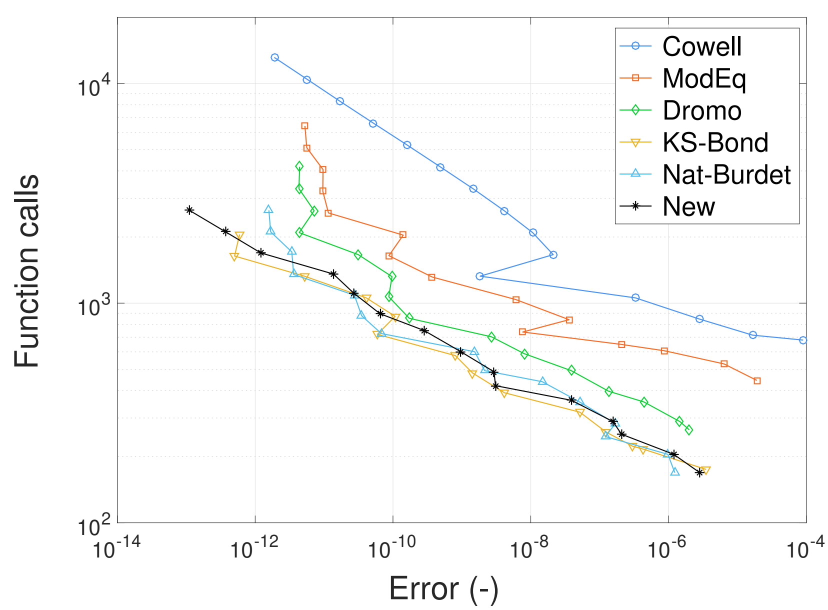

Figure 5: Performance of different propagation methods when integrating the orbit of comet C/1985 K1.

5 Conclusions

Uniform and regular orbital elements for propagating the motion of a celestial body in the perturbed two-body problem have been developed so far only from the KS and Sperling's regularisations. In both methods, the variables from which the elements are generated contain information on the radial distance and the orientation of the radial unit vector. By contrast, if the separate evolution of these two quantities is considered, as in the Burdet–Ferrándiz (BF) regularisation, an intrinsic singularity arises for $r = 0$.

In this work, a formulation that consists of eight orbital elements is presented. We derive them following the spirit of BF decomposition, but we introduce a new time variable χ through a transformation of the Sundman type, instead of using Eq. (2) as in the BF regularisation. First, for the radial displacement r, we find a second-order linear differential equation with constant coefficients (as expected). The two intermediate elements (r_0, σ_0) that stem from its solution correspond to the values of r and its derivative with respect to χ at the epoch t_0. We note that secular terms affect their derivatives for negative values of the total energy, and we identified the reason. This drawback is common to all the universal formulations based on orbital elements (see Introduction) and can be avoided only at the price of losing universality. Then, following a more geometric approach, we define an intermediate reference frame whose evolution keeps track of the orientation of the orbital plane and of a reference direction on it. From such direction, the position of the particle is obtained by a counterclockwise rotation of ν (Eq. 82) about the angular momentum vector. The angle ν is determined by χ, the total energy, r_0, σ_0, and when $\mathscr{U} = 0$, it corresponds to the difference between the true anomalies at times t and t_0 (measured from the pericentre of the osculating conic at time t). The total energy (multiplied by -2), the time element t_0, and four Euler parameters associated with the intermediate frame are the remaining six intermediate elements. The resulting set is uniform, but not universal because it does not work when the angular momentum is zero. An alternative formulation which is completely free of secular terms is also presented.

In addition to a pure theoretical interest in alternative variables for new special perturbation methods, we are concerned with their practical utility. Numerical tests performed by the authors and others corroborate our belief that they can be much more accurate and faster than the classic computation of orbits with Cartesian coordinates. We are aware that the implementation becomes more difficult, because the independent variable is not the physical time and the conversion between position and velocity and the new quantities involves complicated expressions. Therefore, in order to encourage the reader to code the proposed method, we have reported all the necessary formulae for propagating initial conditions and computing orbits from observations by means of the differential corrections method.

Finally, we tested the performance of the intermediate elements by evaluating their accuracy and computational speed with respect to several other methods. For this purpose, we propagated the orbits of the hyperbolic comet (with eccentricity almost equal to 1) C/2003 T4 (LINEAR) and of the comet C/1985 K1 (Machholz) whose eccentricity fluctuates around 1. The new elements and other two universal formulations, which rely on Sundman's time transformation and include a time element, substantially outperform Cowell's method. In the case of C/1985 K1, the intermediate elements reach the highest accuracy with a relatively small computational cost. Finally, we also checked that secular terms do not affect the performance shown by the proposed formulation for propagation times in the order of centuries/thousands of years.

6 Acknowledgements

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A Avoiding secular terms, alternative formulation

When the total energy is negative ($\mathscr{E} < 0$), secular terms that appear in the derivatives of the intermediate elements (Eqs. 66–73) may deteriorate the accuracy of the predicted state in long-term propagations. The proposed formulation can be modified in order to overcome this drawback. The idea is inspired by the regularised methods presented in Stiefel et al (1967, chap. 1).

By setting $\beta = 1$, we can rewrite Eq. (7) as

$$r'' = 2\bar{\mathscr{E}}r + \mu + r(rF_r + 2\mathscr{E}_K - 2\bar{\mathscr{E}}),$$

where $\mathscr{E}_K = \mathscr{E} - \mathscr{U}$ is the Keplerian energy and $\bar{\mathscr{E}}$ is the value taken by $\mathscr{E}$ at the initial time of the propagation. The quantity $\bar{\mathscr{E}}$ is a constant which is fixed by the initial position and velocity of the particle. Let us introduce

$$\bar{\alpha} = -2\bar{\mathscr{E}}, \qquad \alpha = -2\mathscr{E}, \qquad \delta\alpha = \bar{\alpha} - \alpha.$$

The solution of $r'' = 2\bar{\mathscr{E}}r + \mu$ is given by

$$r = r_0 u_0(\chi; \bar{\alpha}) + \sigma_0 u_1(\chi; \bar{\alpha}) + \mu u_2(\chi; \bar{\alpha}), \tag{100}$$

where we have introduced the universal functions (see Eq. 11):

$$u_n(\chi; \bar{\alpha}) = \chi^n \sum_{k=0}^{\infty} (-1)^k \frac{(\bar{\alpha}\chi^2)^k}{(n+2k)!}, \quad n \in \mathbb{N}.$$

The derivatives of u_n with respect to χ do not contain secular terms. Following the same steps as in Sections 2.3 and 2.4, we obtain

$$r_0' = -ru_1(rF_r - 2\mathscr{U} + \delta\alpha),$$
$$\sigma_0' = ru_0(rF_r - 2\mathscr{U} + \delta\alpha),$$
$$t_0' = ru_2(rF_r - 2\mathscr{U} + \delta\alpha).$$

Then, by substituting in Eq. (24) the expression of r in (100) we arrive at the Gaussian equation

$$\tan\frac{\nu}{2} = \frac{c\,u_1\left(\frac{1}{2}\chi;\bar\alpha\right)}{r_0u_0\left(\frac{1}{2}\chi;\bar\alpha\right) + \sigma_0u_1\left(\frac{1}{2}\chi;\bar\alpha\right)}.$$

Differentiation with respect to χ yields

$$\nu' = \frac{2}{d}\Big[\frac{c}{r}(d - r_0) + \frac{r}{c}(rF_r - 2\mathscr{U})(\bar\alpha r_0u_2 - \sigma_0u_1) - \frac{\alpha' r}{2c}(r_0u_1 + \sigma_0u_2)\Big],$$

where

$$d = 2r_0 + r\delta\alpha\, u_2.$$

The expressions of r_0', σ_0', t_0', ν' reported above do not contain secular terms for $\bar{\mathscr{E}} < 0$. Thus, we can select r_0, σ_0, α, t_0 and four Euler parameters exactly as we did in Section 2.6, for the elements of a formulation of the perturbed two-body problem, which will be free of secular terms. The case $d = 0$ does not introduce additional singularities to those affecting the intermediate elements (see Section 2.6).[14] Finally, we note that the same relation as in (83) for c^2 does not hold anymore, and we have to use instead

$$c^2 = r_0(2\mu - r_0\bar\alpha) - \sigma_0^2 + \delta\alpha\, r^2.$$

B Partial derivatives of ι_5, ι_6, ι_7, ι_8 with respect to position and velocity at the initial time

We show a possible way of deriving formulae (98) and (99). We recall that $\mathbf{e}_r$, $\mathbf{e}_\nu$, $\mathbf{e}_z$ are the unit vectors of the LVLH reference frame (see Eqs. 5). From the following relation for the angular momentum vector

$$\mathbf{r} \times \dot{\mathbf{r}} = h\mathbf{e}_z,$$

we obtain

$$h\frac{\partial \mathbf{e}_z}{\partial \mathbf{r}} = V - \mathbf{e}_z\frac{\partial h}{\partial \mathbf{r}}, \qquad h\frac{\partial \mathbf{e}_z}{\partial \dot{\mathbf{r}}} = R - \mathbf{e}_z\frac{\partial h}{\partial \dot{\mathbf{r}}}, \tag{101}$$

where V, R are the skew-symmetric matrices defined by

$$V(1,2) = v_3, \qquad V(1,3) = -v_2, \qquad V(2,3) = v_1,$$

[14] In fact, it can be shown that $rd = 2c^2u_1^2\left(\frac{1}{2}\chi;\bar\alpha\right)/\sin^2\frac{\nu}{2}$.

$$R(1,2) = -r_3, \qquad R(1,3) = r_2, \qquad R(2,3) = -r_1,$$

with $r_i = \mathbf{r} \cdot \mathbf{e}_i$, $v_i = \dot{\mathbf{r}} \cdot \mathbf{e}_i$, $i = 1, 2, 3$, and

$$\frac{\partial h}{\partial \mathbf{r}} = \mathbf{e}_z^T V, \qquad \frac{\partial h}{\partial \dot{\mathbf{r}}} = \mathbf{e}_z^T R.$$

By inserting in Eqs. (101) the expression of $\mathbf{e}_z$ as a function of I, Ω, that is

$$\mathbf{e}_z = \mathbf{e}_1 \sin\Omega \sin I - \mathbf{e}_2 \cos\Omega \sin I + \mathbf{e}_3 \cos I,$$

we find

$$\frac{\partial \Omega}{\partial \mathbf{r}} = -\frac{1}{p \sin I}(\cos L + e\cos\omega)\mathbf{e}_z^T, \qquad \frac{\partial \Omega}{\partial \dot{\mathbf{r}}} = \frac{r \sin L}{h \sin I}\,\mathbf{e}_z^T, \tag{102}$$

$$\frac{\partial I}{\partial \mathbf{r}} = \frac{1}{p}(\sin L + e\sin\omega)\mathbf{e}_z^T, \qquad \frac{\partial I}{\partial \dot{\mathbf{r}}} = \frac{r}{h}\cos L\,\mathbf{e}_z^T, \tag{103}$$

where $L = \omega + f$ is the argument of latitude.

Then, from the relation

$$\cos L = (\mathbf{e}_r \cdot \mathbf{e}_1)\cos\Omega + (\mathbf{e}_r \cdot \mathbf{e}_2)\sin\Omega,$$

we can write

$$\frac{\partial L}{\partial \mathbf{r}} = -\frac{\partial \Omega}{\partial \mathbf{r}}\cos I + \frac{1}{r}\mathbf{e}_\nu^T, \qquad \frac{\partial L}{\partial \dot{\mathbf{r}}} = -\frac{\partial \Omega}{\partial \dot{\mathbf{r}}}\cos I, \tag{104}$$

where we have used

$$\frac{\partial \mathbf{e}_r}{\partial \mathbf{r}} = (I_d - \mathbf{e}_r \mathbf{e}_r^T),$$

and I_d is the 3×3 identity matrix.

The Euler parameters ι_5, ι_6, ι_7, ι_8 at the initial time t_* are written in terms of L, Ω, I by means of Eqs. (58), in which we set $\Psi = L$. Then, these expressions are differentiated with respect to $\mathbf{r}$, $\dot{\mathbf{r}}$, and taking into account (102), (103), and (104), we obtain formulae (98) and (99).

C Partial derivatives of $\iota_1', \ldots, \iota_8'$ with respect to intermediate elements

Let us recall that $\boldsymbol{\iota} = (\iota_1, \ldots, \iota_8)^T$. We define

$$\mathcal{K}_n = (rF_r - 2\mathscr{U})\frac{\partial (ru_n)}{\partial \boldsymbol{\iota}} + ru_nF_r\frac{\partial r}{\partial \boldsymbol{\iota}} - \frac{1}{2}(\sigma P_r + hP_\nu)\frac{\partial b_n}{\partial \boldsymbol{\iota}} + \frac{b_n}{4}\frac{\partial \iota_3'}{\partial \boldsymbol{\iota}} + ru_n\Big(r\frac{\partial F_r}{\partial \boldsymbol{\iota}} - 2\frac{\partial \mathscr{U}}{\partial \boldsymbol{\iota}}\Big), \quad n = 1, 2, 4, 5,$$

where

$$u_1 = -U_1, \quad u_2 = U_0, \quad u_4 = U_2, \quad u_5 = \frac{\iota_2 U_1 - \iota_1 \iota_3 U_2}{c\iota_1},$$

and

$$b_1 = -\iota_1 \tilde{U}_2 - \iota_2 \tilde{U}_3 - 2\mu U_2^2,$$
$$b_2 = \iota_1(2\chi + \tilde{U}_1) + \iota_2 \tilde{U}_2 + \mu(\tilde{U}_3 - 4U_3),$$
$$b_4 = \iota_1(\tilde{U}_3 - 4U_3) + 2\iota_2 U_2^2 + \mu(\tilde{U}_5 - 8U_5),$$
$$b_5 = \frac{1}{2\iota_1}\Big[\frac{r}{c}(\iota_1 U_1 + \iota_2 U_2) - cU_3\Big].$$

The desired derivatives take the form

$$\frac{\partial \iota_n'}{\partial \boldsymbol{\iota}} = \mathcal{K}_n, \quad n = 1, 2, 4, \tag{105}$$

$$\frac{\partial \iota_3'}{\partial \boldsymbol{\iota}} = -2\Big(P_r \frac{\partial \sigma}{\partial \boldsymbol{\iota}} + P_\nu \frac{\partial h}{\partial \boldsymbol{\iota}} + \sigma \frac{\partial P_r}{\partial \boldsymbol{\iota}} + h \frac{\partial P_\nu}{\partial \boldsymbol{\iota}}\Big), \tag{106}$$

$$\begin{aligned}2\frac{\partial \iota_{k+4}'}{\partial \boldsymbol{\iota}} &= \frac{\alpha_k}{r}\Big(\frac{\partial h}{\partial \boldsymbol{\iota}} - \frac{\partial c}{\partial \boldsymbol{\iota}} + \frac{c-h}{r}\frac{\partial r}{\partial \boldsymbol{\iota}} + r\mathcal{K}_5\Big) + \frac{r}{h}\Big(2F_z \frac{\partial r}{\partial \boldsymbol{\iota}} - F_z \frac{r}{h}\frac{\partial h}{\partial \boldsymbol{\iota}} \\ &\quad + r\frac{\partial F_z}{\partial \boldsymbol{\iota}}\Big)(\beta_k c_\nu + \gamma_k s_\nu) + \frac{r^2}{h}F_z\Big[(\gamma_k c_\nu - \beta_k s_\nu)\frac{\partial \nu}{\partial \boldsymbol{\iota}} + \frac{\partial \beta_k}{\partial \boldsymbol{\iota}} c_\nu + \frac{\partial \gamma_k}{\partial \boldsymbol{\iota}} s_\nu\Big] \\ &\quad + N\frac{\partial \alpha_k}{\partial \boldsymbol{\iota}}, \quad k = 1, 2, 3, 4,\end{aligned} \tag{107}$$

where c_ν, s_ν denote $\cos\nu$, $\sin\nu$, respectively, and α_k, β_k, γ_k denote the k-th component of the vectors α, β, γ defined below:

$$\alpha = (-\iota_8,\, \iota_7,\, -\iota_6,\, \iota_5), \qquad \beta = (-\iota_6,\, \iota_5,\, \iota_8,\, -\iota_7), \qquad \gamma = (-\iota_7,\, -\iota_8,\, \iota_5,\, \iota_6).$$

The partial derivatives of r, σ, c, h, ν are reported in Section 3.1. Moreover, we need the following relations:

$$\frac{\partial b_1}{\partial \boldsymbol{\iota}} = -\Big(\tilde{U}_2,\, \tilde{U}_3,\, \iota_1\tilde{U}_4 + \frac{3}{2}\iota_2\tilde{U}_5 + 4\mu U_2 U_4 - \chi(\iota_1\tilde{U}_3 + \iota_2\tilde{U}_4 + 2\mu U_2 U_3),\, \mathbf{0}_5\Big),$$

$$\frac{\partial b_2}{\partial \boldsymbol{\iota}} = \Big(2\chi + \tilde{U}_1,\, \tilde{U}_2,\, \frac{1}{2}\iota_1\tilde{U}_3 + \iota_2\tilde{U}_4 + \frac{3}{2}\mu(\tilde{U}_5 - 4U_5) + \chi(b_1 - 2\mu U_4),\, \mathbf{0}_5\Big),$$

$$\begin{aligned}\frac{\partial b_4}{\partial \boldsymbol{\iota}} &= \Big(\tilde{U}_3 - 4U_3,\, 2U_2^2,\, \frac{3}{2}\iota_1(\tilde{U}_5 - 4U_5) + 4\iota_2 U_2 U_4 + \frac{5}{2}\mu(\tilde{U}_7 - 8U_7) \\ &\qquad - \chi[\iota_1(\tilde{U}_4 - 2U_4) + 2\iota_2 U_2 U_3 + \mu(\tilde{U}_6 - 4U_6)],\, \mathbf{0}_5\Big),\end{aligned}$$

$$\begin{aligned}2\iota_1 c\frac{\partial b_5}{\partial \boldsymbol{\iota}} &= (\iota_1 U_1 + \iota_2 U_2)\Big(\frac{\partial r}{\partial \boldsymbol{\iota}} - \frac{r}{c}\frac{\partial c}{\partial \boldsymbol{\iota}}\Big) - cU_3\frac{\partial c}{\partial \boldsymbol{\iota}} + \frac{1}{2}\Big(\frac{2}{\iota_1}(c^2 U_3 - r\iota_2 U_2),\, 2rU_2, \\ &\qquad r(\iota_1 U_3 + 2\iota_2 U_4) - 3c^2 U_5 + \chi[c^2 U_4 - r(\iota_1 U_2 + \iota_2 U_3)],\, \mathbf{0}_5\Big),\end{aligned}$$

$$\frac{\partial u_5}{\partial \boldsymbol{\iota}} = \frac{1}{c\iota_1}\Big(-\frac{\iota_2}{\iota_1}U_1,\, U_1,\, \frac{1}{2}[\iota_2 U_3 - \chi(\iota_1 U_1 + \iota_2 U_2)],\, \mathbf{0}_5\Big) + u_5 c\frac{\partial c}{\partial \boldsymbol{\iota}},$$

where $\mathbf{0}_5 \in \mathbb{R}^5$ is a row vector of null entries. Assuming that $\mathscr{U}$ depends only on $\mathbf{r}$, t (see the remark in Section 2.6), we have

$$\frac{\partial \mathscr{U}}{\partial \boldsymbol{\iota}} = \frac{\partial \mathscr{U}}{\partial \mathbf{r}}\frac{\partial \mathbf{r}}{\partial \boldsymbol{\iota}} + \frac{\partial \mathscr{U}}{\partial t}\frac{\partial t}{\partial \boldsymbol{\iota}}. \tag{108}$$

Let us denote by $\mathbf{y}$ either $\mathbf{F}$ or $\mathbf{P}$, and with y_ℓ the component of $\mathbf{y}(\mathbf{r}, \dot{\mathbf{r}}, t)$ along one of the directions associated to $\mathbf{e}_r$, $\mathbf{e}_\nu$, $\mathbf{e}_z$. Then, we can write

$$\frac{\partial y_\ell}{\partial \boldsymbol{\iota}} = \mathbf{e}_\ell^T \frac{\partial \mathbf{y}}{\partial \boldsymbol{\iota}} + \mathbf{y}^T \frac{\partial \mathbf{e}_\ell}{\partial \boldsymbol{\iota}}, \tag{109}$$

where

$$\frac{\partial \mathbf{y}}{\partial \boldsymbol{\iota}} = \frac{\partial \mathbf{y}}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\iota}} + \frac{\partial \mathbf{y}}{\partial \dot{\mathbf{r}}} \frac{\partial \dot{\mathbf{r}}}{\partial \boldsymbol{\iota}} + \frac{\partial \mathbf{y}}{\partial t} \frac{\partial t}{\partial \boldsymbol{\iota}}. \tag{110}$$

The matrices $\partial \mathbf{r}/\partial \boldsymbol{\iota}$, $\partial \dot{\mathbf{r}}/\partial \boldsymbol{\iota}$ are provided in Section 3.1, together with $\partial \mathbf{e}_r/\partial \boldsymbol{\iota}$, $\partial \mathbf{e}_\nu/\partial \boldsymbol{\iota}$, while $\partial \mathbf{e}_z/\partial \boldsymbol{\iota}$ can be easily obtained from the expression

$$\mathbf{e}_z = (2\iota_6\iota_8 + 2\iota_5\iota_7,\, 2\iota_7\iota_8 - 2\iota_5\iota_6,\, \iota_5^2 - \iota_6^2 - \iota_7^2 + \iota_8^2)^T. \tag{111}$$

Also note that

$$\frac{\partial \mathbf{F}}{\partial \mathbf{r}} = \frac{\partial \mathbf{P}}{\partial \mathbf{r}} - \frac{\partial(\nabla \mathscr{U})}{\partial \mathbf{r}}, \qquad \frac{\partial \mathbf{F}}{\partial t} = \frac{\partial \mathbf{P}}{\partial t} - \frac{\partial(\nabla \mathscr{U})}{\partial t}. \tag{112}$$

Finally, we have

$$\frac{\partial t}{\partial \boldsymbol{\iota}} = \Big(U_1,\, U_2,\, \frac{1}{2}[\iota_1 U_3 + 2\iota_2 U_4 + 3\mu U_5 - \chi(\iota_1 U_2 + \iota_2 U_3 + \mu U_4)],\, 1,\, 0,\, 0,\, 0,\, 0\Big). \tag{113}$$

D Identities for the universal functions

We collect the identities for the universal functions introduced in Eq. (11) that we used to derive some equations of this paper (see Battin, 1999, sects. 4.5, 4.6). For simplicity, we omit the argument α in the universal functions. These formulae are:

$$\begin{gathered}
U_n(\chi) + \alpha U_{n+2}(\chi) = \frac{\chi^n}{n!}, \;\; n \in \mathbb{N}, \\
U_0(\chi)^2 + \alpha U_1(\chi)^2 = 1, \\
U_1(\chi)^2 - U_0(\chi)U_2(\chi) = U_2(\chi), \\
U_0(\chi)U_3(\chi) - U_1(\chi)U_2(\chi) = U_3(\chi) - \chi U_2(\chi), \\
U_1(\chi)U_3(\chi) - U_2(\chi)^2 = 2U_4(\chi) - \chi U_3(\chi),
\end{gathered}$$

the double argument identities:

$$\begin{aligned}
U_0(2\chi) &= U_0(\chi)^2 - \alpha U_1(\chi)^2, \\
U_1(2\chi) &= 2U_0(\chi)U_1(\chi), \\
U_2(2\chi) &= 2U_1(\chi)^2, \\
U_3(2\chi) &= 2U_3(\chi) + 2U_1(\chi)U_2(\chi), \\
U_5(2\chi) &= 2U_1(\chi)U_4(\chi) + \chi^2 U_3(\chi) + 2U_5(\chi),
\end{aligned}$$

and the differential relations:

$$\frac{\partial U_0}{\partial \chi} = -\alpha U_1, \qquad \frac{\partial U_m}{\partial \chi} = U_{m-1}, \quad m \in \mathbb{N}^+,$$
$$\frac{\partial U_n}{\partial \alpha} = \frac{1}{2}(nU_{n+2} - \chi U_{n+1}), \quad n \in \mathbb{N}.$$

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