Geometric Numerical Propagation of Redundant Orbital Problems

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Abstract. In order to increase the efficiency in the numerical integration of orbital problems it is need, firstly, the formulation of the problem in the adequate set of variables. It has been revealed that the formulation in regularized projective variables referred to the ideal frame is very adequate. The difficulty of this formulation is based on the existence of constrains, which, traditionally, have been used as control for the progress of the numerical calculations. In the other side, and, particularly, when a long time propagation is need, it must be exigible the use of numerical methods that supply the solution showing a qualitative behaviour as close as possible to the exact solution; this behaviour can be realized by means of backward error analysis. It is checked that the partitioned symplectic integrators, particularly, the Lobatto IIIA-IIIB, are well adapted to the propagation of differential problems with constrains, because they preserve some integrals of motion as well as the constrains. The use of the propagators and the formulation just mentioned allows us to advance one more step in the long time propagation orbits.

Keywords: orbital problem, ideal frames, redundant variables, partitioned Runge-Kutta methods

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§1. Introduction

Years ago we started our work on orbital problems with the aim of obtaining a good numerical propagation of such problems. This goes through the formulation of the problems in an adequate set of variables that allows us not only its analytical study, but a good numerical propagation. We found [10], for instance, that the formulation in projective regularized variables referred to the ideal frame of Hansen come to an improvement of the solution in at least two digits when a numerical propagation is performed, whatever be the numerical procedure used. Some difficulty appears when this formulation is used, because the ideal frame is defined from initial system of reference by means of quaternions and for the transformation from cartesian coordinates to another with quaternions be univocally defined, it is need that the quaternions verify some constraints. Usually, this type of restrictions have been used to control the progress in the numerical propagation of the solutions to the problem.

In the other side, this projective variables with quaternions do not form a canonical systems of variables. The advantage of the use of canonical systems is well-known; from a numerical point of view, it rest on the fact that with them one can use the so called geometric numerical

propagators, which exhibit in their behaviour some characteristics of the differential system, as, for instance, the preservation of some invariants or integrals of the motion.

Currently, to propagate Hamiltonian problems, in particular, to long time periods, geometric methods are considered, it is to say, methods symmetric and symplectic. The construction of such methods as collocation methods is very interesting and their use shows advantages when two methods of this type are used together to form a partitioned one; for instance, the partitioned methods formed by a Lobatto IIIA and a Lobatto IIIB methods based on the same nodes. It has been proved [6] the symplecticity of this methods. This type of partitioned methods is specially adequate to be used with Hamitonian systems, because one can integrate the momenta with an element of the pair and coordinates with the other element. They are also interesting to propagate the solutions of problems with constraints [8].

The aim of this paper is to construct, following the technique proposed by Cid [3] and others, an extended system of five canonical variables including as coordinates the components of the quaternion defining the instantaneous rotation and the corresponding conjugate momenta. Next, we include the partitioned Runge-Kutta methods (PRK in short) and their use to propagate canonical problems with constraints; finally, we show some numerical results.

§2. A canonical system

An election of coordinates [10] very adequate to describe the orbital problems is one that considers the coordinates (q_1, q_2, q_3, q_4, r), where the first four are the components of a quaternion $\mathbf{q} = (q_1, q_2, q_3, q_4)$ and the last one is the radial distance. The quaternion $\mathbf{q}$ allows to define the instantaneous rotation of the initial coordinates system to the Hansen ideal frame, which main plane of reference coincides with the instantaneous orbital plane. As the position of a point in the orbit is defined in this way by the radial distance and a rotation, i. e., an angle, we can call them projective coordinates. A later regularization and the consideration of the reciprocal of the distance as new variable, $\rho = 1/r$, allows us to write the equations of motion as the ones of a perturbed harmonic oscillator.

Nevertheless, the mentioned variables do not permit to describe the motion in a canonical form. With the purpose of be able of applying geometric numerical integrators to propagate the orbits, we construct a canonical extension of that set of variables. Transformations of variables of this type, that enlarge in one or two the number of canonical variables, have been frequently considered by several authors (Broucke [1], Cid and SanSaturio [3], Ferrándiz and SanSaturio [4], Ferrer [5], among others).

The process of construction of the new transformation can be planning in the following way. Let (x_1, x_2, x_3) be the cartesian coordinates in an initial system of reference. We consider a new system of variables $\mathbf{Q} = (q_1, q_2, q_3, q_4, r)$, composed by the four coordinates of the quaternion that allows to define the instantaneous rotation of the initial reference system to the new one (for instance, the ideal frame of Hansen) and the radial distance. This transformation can be defined [1] by means of the following equations:

$$
\begin{aligned}
x_1 &= r\,(q_1^2 - q_2^2 - q_3^2 + q_4^2) \\
x_2 &= 2\,r\,(-q_1\,q_2 + q_3\,q_4) \\
x_3 &= 2\,r\,(q_1\,q_3 + q_2\,q_4).
\end{aligned}
\tag{1}
$$

Nevertheless, this transformation is univocally defined only in the case that the coordinates q_j fulfill the following constraints:

$$
\begin{aligned}
x_4 &= q_1^2 + q_2^2 + q_3^2 + q_4^2, \\
x_5 &= \frac{q_1\,q_3 - q_2\,q_4}{q_1\,q_4 + q_2\,q_3},
\end{aligned}
\tag{2}
$$

where x_4 and x_5 must be constants, in particular, $x_4 = 1$.

Now, one canonical extension of the transformation of variables $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$ to the variables $\mathbf{Q}$ can be performed, defining the new momenta $\mathbf{P} = (P_1, P_2, P_3, P_4, P_5)$ by means of the following matricial equation

$$
\mathbf{X} = M\,\mathbf{P}, \qquad M = (A^T)^{-1}, \quad A = \frac{\partial \mathbf{x}}{\partial \mathbf{Q}},
\tag{3}
$$

proposed by Ferrándiz and Sansaturio [4] and already used by Ferrer [5], where $\mathbf{X} = (X_1, X_2, X_3, X_4, X_5)$ are the old momenta.

Nevertheless, some of the expressions obtained for the momenta are no very simple, due to the complicated expression of the elements of the matrix M, for what we have performed the mentioned transformation using the steps proposed by Cid [3].

The equations of the transformation proposed by Cid [3], equivalent to the (3), are

$$
\mathbf{P} = J\,\mathbf{X}, \qquad J = \left(\frac{\partial \mathbf{x}}{\partial \mathbf{Q}}\right)^T,
\tag{4}
$$

where only the first three components of vectors $\mathbf{x}, \mathbf{X}$ are considered. These equations define a invertible system, if some restrictions are accomplished, which solution we have obtained after a long process of Gaussian elimination with the help of a symbolic manipulator, resulting

$$
\begin{aligned}
X_1 &= \frac{(-q_1\,q_3 + q_2\,q_4)\,P_3 - (q_1\,q_2 + q_3\,q_4)\,P_2 + (q_1^2 + q_4^2)\,P_1}{2\,r\,q_1}, \\
X_2 &= \frac{(q_2\,q_3 + q_1\,q_4)\,P_3 + (-q_1\,q_2 + q_3\,q_4)\,P_2 - (q_1^2 + q_3^2)\,P_1}{2\,r\,q_1}, \\
X_3 &= \frac{(-q_2\,q_3 + q_1\,q_4)\,P_3 + (q_1\,q_3 + q_2\,q_4)\,P_2 + (q_1^2 + q_2^2)\,P_1}{2\,r\,q_1},
\end{aligned}
\tag{5}
$$

being the constraints the following

$$
\begin{aligned}
X_4 &= P_4\,q_1 - P_3\,q_2 + P_2\,q_3 - P_1\,q_4 = 0 \\
X_5 &= P_1\,q_1 + P_2\,q_2 + P_3\,q_3 + P_4\,q_4 - 2\,P_5\,r = 0
\end{aligned}
\tag{6}
$$

Note that the above expressions (5) of the old momenta as function of the new coordinates and new momenta result relatively simple and, besides, the constraints (6) coincide with that obtained by Ferrer [5].

The new Hamiltonian for the non perturbed Keplerian problem is obtained by substituting the expressions of the old coordinates and momenta in the following expression

$$
H = \frac{1}{2}\left(X_1^2 + X_2^2 + X_3^2\right) + \frac{\mu}{r},
$$

resulting

$$H = H(\mathbf{P},\ \mathbf{Q}) = \frac{1}{8} \frac{\left(P_1^2 + P_2^2 + P_3^2\right) q_1^2 + \left(P_3\, q_2 - P_2\, q_3 + P_1\, q_4\right)^2}{8\, q_1^2\, \left(q_1^2 + q_2^2 + q_3^2 + q_4^2\right) r^2} + \frac{\mu}{r}$$

The equations of motion for the Keplerian problem will not be the classical

$$\dot{\mathbf{P}} = -H_{\mathbf{Q}}, \qquad \dot{\mathbf{Q}} = H_{\mathbf{P}},$$

where $H_{\mathbf{Q}}$ and $H_{\mathbf{P}}$ denote the column vectors of partial derivatives, because of the existence of the constraints, but they must be formulated in the following form:

$$\dot{\mathbf{P}} = -H_{\mathbf{Q}} - \mathbf{g}_{\mathbf{Q}}(\mathbf{Q})\, \lambda,$$
$$\dot{\mathbf{Q}} = H_{\mathbf{P}}, \tag{7}$$
$$\mathbf{g}(\mathbf{Q}) = 0,$$

where the function $\mathbf{g}(\mathbf{Q})$ has as components the constraints among the coordinates $\mathbf{Q}$. In our case, there are two of them and vector λ belong to $\mathbb{R}^2$; it can be obtained differentiating twice the constraint in (7) with respect to time

$$\mathbf{g}'(\mathbf{Q})\, H_{\mathbf{P}} = 0,$$
$$\frac{\partial}{\partial q}(\mathbf{g}'(\mathbf{Q})\, H_{\mathbf{P}})\, H_{\mathbf{P}} - \mathbf{g}'(\mathbf{Q})\, H_{\mathbf{PP}}\, (H_{\mathbf{Q}} + \mathbf{g}'(\mathbf{Q})^T\, \lambda) = 0 \tag{8}$$

Hence, if the matrix

$$\mathbf{g}'(\mathbf{Q})\, H_{\mathbf{PP}}\, \mathbf{g}'(\mathbf{Q})^T$$

is regular, vector λ can be obtained from equation (8) as a function $\lambda = \lambda\,(\mathbf{P},\ \mathbf{Q})$.

Inserting this result into (7) gives a differential equation for $(\mathbf{P},\ \mathbf{Q})$ on the manifold

$$\mathcal{M} = \{(\mathbf{P},\ \mathbf{Q})\,|\, \mathbf{g}(\mathbf{Q}) = 0, \quad \mathbf{g}'(\mathbf{Q})\, H_{\mathbf{P}} = 0\}, \tag{9}$$

which is reversible if $H(-\mathbf{P},\ \mathbf{Q}) = H(\mathbf{P},\ \mathbf{Q})$, what is verified in our case.

It can be proved [6] that the flow of the system (7) is a symplectic transformation on $\mathcal{M}$.

§3. Lobatto IIIA-IIIB for constrained canonical systems

Classical techniques to solve numerically the above algebraic-differential equations, as the index reduction, are not very adequate, because index reduction is not compatible with symplectic integration. Different extensions of symplectic method to Hamiltonian system with constraints have been proposed; basically, they integrate momenta and coordinates and then make an adequate projection on the manifold $\mathcal{M}$. High order symplectic integrator can be obtained, in another way, by the use of partitioned Runge-Kutta methods as suggested by Jay [8], which proposes the use of a pair of Lobatto IIIA-IIIB method to integrate these problems.

Lobatto IIIA-IIIB methods, as partitioned Runge-Kutta, can be formulated as

$$q_1 = q_0 + h \sum_{i=1}^{s} b_i \, k_i, \quad p_1 = p_0 + h \sum_{i=1}^{s} \hat{b}_i \, l_i$$

where

$$k_i = H_{\mathbf{P}}(P_i, \, Q_i), \quad l_i = -H_{\mathbf{Q}} - \mathbf{g_Q}(\mathbf{Q}) \, \lambda,$$

and the internal stages are given by

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} \, k_j, \quad P_i = p_0 + h \sum_{j=1}^{s} \hat{a}_{ij} \, l_j$$

These methods are symplectic, because they satisfy the following conditions of symplecticity

$$b_i = \hat{b}_i, \quad \text{for } i = 1, ..., 2, \text{ and}$$

$$b_i \, \hat{a}_{ij} + \hat{b}_j \, a_{ji} - b_i \, \hat{b}_j = 0, \text{for } i, j = 1, ..., s.$$

The Lobatto IIIA methods of s stages are collocation methods with nodes $c_i, i = 1, ..., s$, equal to the zeros of polynomial

$$\frac{d^{s-2}}{dx^{s-2}} \left(x^{s-1} \, (x-1)^{s-1} \right),$$

and are equivalent to s-stage Runge-Kutta methods with coefficients determined by the following conditions:

$$C(s) : \sum_{j=1}^{s} a_{ij} \, c_j^{k-1} = \frac{c_i^k}{k}, \quad k = 1, ..., s, \forall i$$

$$B(s) : \sum_{j=1}^{s} b_i \, c_i^{k-1} = \frac{1}{k}, \quad k = 1, ..., s$$

Lobatto IIIB methods are discontinuous collocation methods, based on the same nodes that Lobatto IIIA, and are equivalent to s-stage Runge-Kutta methods with coefficients determined by the following conditions:

$$c_1 = 0, \quad c_s = 1, \quad a_{i1} = b_1, \quad a_{is} = 0, \text{ for } i = 1, ..., s$$
$$C(s-2) \text{ and } B(s-2)$$
$$\text{and} \quad C(s) \text{ and } B(s)$$

In this way, solving the corresponding equations with the help of an algebraic manipulator, we have obtained, among others, the following Lobatto IIIA-IIIB pair with $s = 5$ stages.

0	0	0	0	0	0
$\dfrac{7-\sqrt{21}}{14}$	$\dfrac{119+3\sqrt{21}}{1960}$	$\dfrac{343-9\sqrt{21}}{2520}$	$\dfrac{8(-49+12\sqrt{21})}{2205}$	$\dfrac{343-69\sqrt{21}}{2520}$	$\dfrac{3(-7+\sqrt{21})}{1960}$
$\dfrac{1}{2}$	$\dfrac{13}{320}$	$\dfrac{7(56+15\sqrt{21})}{2880}$	$\dfrac{8}{45}$	$\dfrac{7(-56+15\sqrt{21})}{2880}$	$\dfrac{3}{320}$
$\dfrac{7+\sqrt{21}}{14}$	$\dfrac{119-3\sqrt{21}}{1960}$	$\dfrac{343+69\sqrt{21}}{2520}$	$\dfrac{8(49+12\sqrt{21})}{2205}$	$\dfrac{343+9\sqrt{21}}{2520}$	$-\dfrac{3(7+\sqrt{21})}{1960}$
1	$\dfrac{1}{20}$	$\dfrac{49}{180}$	$\dfrac{16}{45}$	$\dfrac{49}{180}$	$\dfrac{1}{20}$
	$\dfrac{1}{20}$	$\dfrac{49}{180}$	$\dfrac{16}{45}$	$\dfrac{49}{180}$	$\dfrac{1}{20}$

Lobatto IIIA, s = 5

0	$\dfrac{1}{20}$	$\dfrac{-7-\sqrt{21}}{120}$	$\dfrac{1}{15}$	$\dfrac{-7+\sqrt{21}}{120}$	0
$\dfrac{7-\sqrt{21}}{14}$	$\dfrac{1}{20}$	$\dfrac{343+9\sqrt{21}}{2520}$	$\dfrac{56-15\sqrt{21}}{315}$	$\dfrac{343-69\sqrt{21}}{2520}$	0
$\dfrac{1}{2}$	$\dfrac{1}{20}$	$\dfrac{49+12\sqrt{21}}{360}$	$\dfrac{8}{45}$	$\dfrac{49-12\sqrt{21}}{360}$	0
$\dfrac{7+\sqrt{21}}{14}$	$\dfrac{1}{20}$	$\dfrac{343+69\sqrt{21}}{2520}$	$\dfrac{56+15\sqrt{21}}{315}$	$\dfrac{343-9\sqrt{21}}{2520}$	0
1	$\dfrac{1}{20}$	$\dfrac{119-3\sqrt{21}}{360}$	$\dfrac{13}{45}$	$\dfrac{119+3\sqrt{21}}{360}$	0
	$\dfrac{1}{20}$	$\dfrac{49}{180}$	$\dfrac{16}{45}$	$\dfrac{49}{180}$	$\dfrac{1}{20}$

Lobatto IIIB, s = 5

§4. Numerical results

Special attention must be paid to the starting process because the methods we are considering are implicit and at each step a system of implicit equations must be solved. The most simple method used [6] is the functional iteration, but several starting method improving it have been proposed. For instance, Laburta [9, 2] construct much more accurate starting approximation with the aid of a few additional function evaluations for the Gauss method. Very recently Higueras and Roldan [7] have proposed an starting algorithm for the Lobatto IIIA-IIIB methods that we have been no possibility to use.

Remark that the first row of the Butcher's matrix of coefficients of Lobatto IIIA and the last column of the Lobatto IIIB are vectors of zeros. This fact must be taken into account when the methods are implemented in order to reduce the number of evaluations of functions.

We have implemented the Lobatto IIIA-IIIB (LAB in short) method of s stages and order $p = 2s - 2 = 8$ with several values of s, taking into account the previous considerations on the number of function evaluations and considering an adaptation of the starting algorithm of Laburta [9], for the Kepler's problem with eccentricity $e = 0.6$.

We have compared method LAB of $s = 4, 5$ stages with the methods Runge-Kutta-Gauss (Gs in short) of $s = 2, 4, 6$ stages. In table 4, we can see that the number of function evaluations for method LAB of s stages is between the Gauss methods of $s - 1$ and s, respectively, but methods LAB4 and LAB5 are closer to G2 and G4 than to G4 and G6, respectively.

	h	Num. steps	N. eval. func.
G2	0.10	62	627
LAB4	0.10	62	733
G4	0.10	62	883
LAB5	0.10	62	947
G6	0.10	62	1059

Table 1: Number of function evaluations after two revolutions

In figure 4, we can see the error in energy after 200 revolutions for stepsizes $h = 0.5, 0.1, 0.05,$ $0.01, 0.005$ and methods Runge-Kutta-Gauss of $s = 2, 4$ stages and Lobatto IIIA-IIIB of $s = 4$ stages. We can see that error for LAB4 is between that for G2 and G4, which corresponds with the fact that the order of Gauss methods is $p = 2s$ while is $p = 2s - 2$ for LAB. Note that error of LAB4 is closer to G4 when the stepsize decreases.
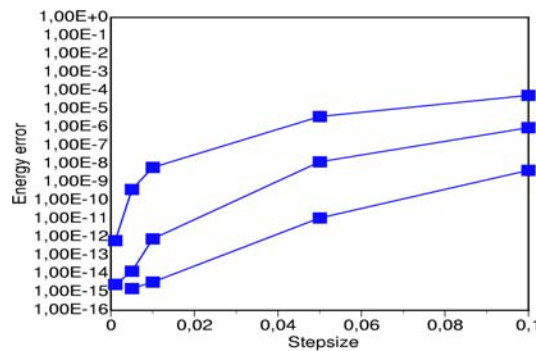

Figure 1: Gauss s=2, LIIIA-IIIB s =4, Gauss s=4 (top to bottom). Energy error after two hundred revolutions

In figure 4, we can see the relative error in radial distance after 200 revolutions for stepsizes $h = 0.5, 0.1, 0.05, 0.01, 0.005$ and methods Runge-Kutta-Gauss of $s = 2, 4$ stages and Lobatto IIIA-IIIB of $s = 4$ stages. We can observe that the behaviour is quite similar to that observed in the energy error, once .

§5. Conclusions

A set of redundant canonical variables including the components of the quaternion defining instantaneous rotations to the ideal frame of reference has been constructed for orbital problems. The equations of motion have been formulated as the canonical equations with constraints. To solve numerically this equations, i. e., for the numerical propagation of the orbits, partitioned Runge-Kutta methods of Lobatto IIIA-IIIB has been considered. Application to the Kepler problem has been performed. First results enlarge the field of methods to attack the problem of propagation of orbits in redundant systems of variables.
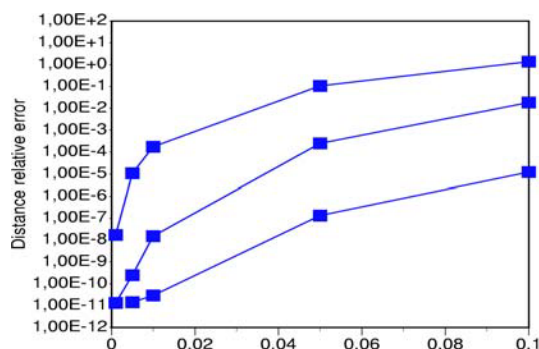
Figure 2: Gauss s=2, LIIIA-IIIB s =4, Gauss s=4 (top to bottom). Distance relative error after two hundred revolutions

Acknowledgements

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