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An efficient computational approach for global regularisation schemes

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Abstract. Due to collisional singularities appearing in gravitational few-body problems, one needs regularisation techniques for their stable approximate solution. We present an efficient computational approach for numerically integrating a symmetrical five body problem called the Caledonian Symmetric Five Body Problem (CS5BP) which is a five-body system with a symmetrically reduced phase space. The proposed global regularisation scheme consists of adapted versions of several known regularisation transformations such as the Levi-Civita-type coordinate transformations together with a time transformation which enables the numerical exploration of the systems as they pass through two-body close encounters. An algebraic optimisation algorithm is adapted for numerically implementing the regularisation scheme which make use of the reverse mode algorithmic differentiation. We show that the proposed regularisation algorithm is numerically and computationally very efficient in handling various two-body close encounters appearing in the CS5BP.
Keywords: Regularisation, singularity, celestial mechanics, few-body problem, optimisation.

1 Introduction

There is a growing interest in studying gravitational few-body problems (with $n > 3$) which makes use of the symmetric boundary conditions to reduce the mathematical complexity of the problem [13],[14], [8], [7].

Several papers in the last decade have studied the the Caledonian Symmetric Four-Body Problem (CSFBP) which is a restricted coplanar four-body system with a symmetrically reduced phase space [5], [12]. The model involves two pairs of non-equal masses moving in coplanar, initially circular orbits, starting in a collinear arrangement [5]. The authors have shown that the global stability of the CSFBP system depends on a parameter called the Szebehely constant C_0. The Szebehely constant $C_0 = -\frac{c^2 E}{G^2 M^5}$ is a dimensionless function of the total energy (E) and the magnitude of the angular momentum of the system

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(c), where G is the gravitational constant, and M is the total mass. A generalization of the CSFBP named the Caledonian Symmetric Five-Body problem (CS5BP) was done by introducing a stationary mass to the centre of mass of the CSFBP with the same analytical stability criteria [8].

Existing numerical integration schemes were inadequate to study orbits with strong close encounters, as the numerical integration fails due to collision singularities [15], [16]. In gravitational few-body problems, singularities normally appear when the distance between objects undergoing orbital motion becomes very small. As a result, the equations describing the dynamics of the system tend towards singular and the numerical integration falls apart [3]. Use of regularisation algorithms to numerically integrate gravitational few-body problems which involve near collisions or close encounters has been widely acknowledged [3], [1]. Recently a global regularisation scheme for the CSFBP is prsented in [11]. In this paper, we extend the regularisation scheme to the Caledonian Symmetric Five-Body problem (CS5BP).

2 Definition of the Caledonian Symmetric Five Body Problem(CS5BP)

Let us consider five bodies P_0,P_1,P_2,P_3,P_4 of masses m_0,m_1, m_2,m_3,m_4 respectively existing in three dimensional Euclidean space [6]. The radius and velocity vectors of the bodies with respect to the centre of mass of the five body system are given by $\mathbf{r}_i$ and $\dot{\mathbf{r}}_i$ respectively, $i = 0, 1, 2, 3, 4$. Let the centre of mass of the system be denoted by O.

The CS5BP involves two types of symmetries; past-future symmetry and dynamical symmetry [8]. Past future symmetry exists in an n-body system when the dynamical evolution of the system after $t = 0$ is a mirror image of the dynamical evolution of the system before $t = 0$. It occurs whenever the system passes through a mirror configuration, *i.e.* a configuration in which the velocity vectors of all the bodies are perpendicular to all the position vectors from the centre of mass of the system [5].

Dynamical symmetry exists when the dynamical evolution of two bodies on one side of the centre of mass of the system is paralleled by the dynamical evolution of the two bodies on the other side of the centre of mass of the system. The resulting configuration is always a parallelogram, but of varying length, width and orientation [8]. See Figure 1 for the configuration of the CS5BP for $t > 0$.

The CS5BP has the following conditions:

1. All five bodies are finite point masses with:

$$m_1 = m_3, \qquad m_2 = m_4 \tag{1}$$

2. P_0 is stationary at origin O, the centre of mass of the system. P_1 and P_3 are moving symmetrically to each other with respect to the centre of mass of the system. Likewise P_2 and P_4 are moving symmetrically to each other. Thus dynamical symmetry is maintained for all time t;

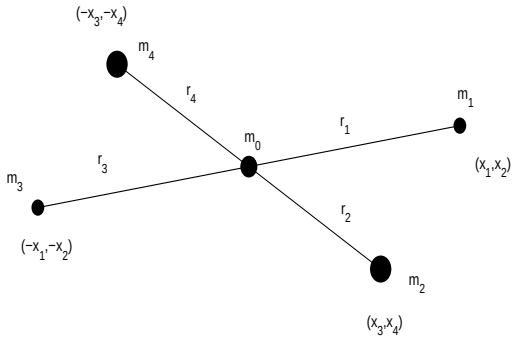

Fig. 1. The configuration of the coplanar CS5BP for $t > 0$

$$\mathbf{r}_1 = -\mathbf{r}_3, \qquad \mathbf{r}_2 = -\mathbf{r}_4, \qquad \mathbf{r}_0 = 0,$$
$$\mathbf{V}_1 = \dot{\mathbf{r}}_1 = -\dot{\mathbf{r}}_3, \qquad \mathbf{V}_2 = \dot{\mathbf{r}}_2 = -\dot{\mathbf{r}}_4, \qquad \mathbf{V}_0 = \dot{\mathbf{r}}_0 = 0. \tag{2}$$

3. At time $t = 0$ the bodies are collinear with their velocity vectors perpendicular to their line of position. This ensures the past-future symmetry and is described by:

$$\mathbf{r}_1 \times \mathbf{r}_2 = 0, \qquad \mathbf{r}_1 \cdot \dot{\mathbf{r}}_1 = 0, \qquad \mathbf{r}_2 \cdot \dot{\mathbf{r}}_2 = 0. \tag{3}$$

We define the masses as ratios to the total mass. Let the total mass M of the system be

$$M = 2\,(m_1 + m_2) + m_0 \tag{4}$$

Let μ_i be the mass ratios defined as $\mu_i = \frac{m_i}{M}$ for $i = 0, 1, 2, 3, 4$ and $\mu = \frac{\mu_1}{\mu_2}$. Equation (4) then becomes

$$2\,(\mu_1 + \mu_2) + \mu_0 = 1, \tag{5}$$

and

$$0 \leq \mu_0 \leq 1, 0 \leq \mu_1 \leq 0.5, 0 \leq \mu_2 \leq 0.5. \tag{6}$$

3 The regularisation scheme

The proposed regularisation scheme consists of a combination of several known regularisation techniques: a Levi-Civita type coordinate transformation, a time transformation function similar to that of [1] and the global formulation of [3]. In general, the proposed scheme follows the transformations described in [4]. We extend the regularisation procedure of the CSFBP [11] into the case of the CS5BP.

Let the position coordinates of the four bodies in cartesian coordinates be $\mathbf{r}_1 = (x_1, x_2)$, $\mathbf{r}_2 = (x_3, x_4)$, $\mathbf{r}_3 = (-x_1, -x_2)$, $\mathbf{r}_4 = (-x_3, -x_4)$, with corresponding momenta $(\omega_1, \omega_2) = \mu_1 M(\dot{x_1}, \dot{x_2})$, $(\omega_3, \omega_4) = \mu_2 M(\dot{x_3}, \dot{x_4})$, $(-\omega_1, -\omega_2)$, $(-\omega_3, -\omega_4)$.

For simplicity, we set the gravitational constant G and total mass M to be equal to unity. According to the symmetrical restrictions, the Hamiltonian function can be written as

$$H = \frac{1}{\mu_1 M}(\omega_1^2 + \omega_2^2) + \frac{1}{\mu_2 M}(\omega_3^2 + \omega_4^2) - 2G\mu_1\mu_2 M^2 \left(\frac{1}{r_{12}} + \frac{1}{r_{14}}\right) - \frac{G\mu_1^2 M^2}{r_{13}} - \frac{G\mu_2^2 M^2}{r_{24}} - 4G\mu_0 M \left(\frac{\mu_1 M}{2r_{13}} + \frac{\mu_2 M}{2r_{24}}\right), \tag{7}$$

where the corresponding inter-body distances are given by

$$\begin{aligned} r_{12} &= \left((x_1 - x_3)^2 + (x_2 - x_4)^2\right)^{1/2} = r_{34}, \\ r_{14} &= \left((x_1 + x_3)^2 + (x_2 + x_4)^2\right)^{1/2} = r_{23}, \\ r_{13} &= \left((2x_1)^2 + (2x_2)^2\right)^{1/2}, \\ r_{24} &= \left((2x_3)^2 + (2x_4)^2\right)^{1/2}. \end{aligned} \tag{8}$$

These four inter-body distances result in collision singularities which is characterised by the following four types of two-body close encounters [10].

1. "12"-type double binary collision: collisions occurring in the binary formed between P_1 and P_2 and the symmetrical binary formed between P_3 and P_4.
2. "14"-type double binary collision: collisions occurring in the binary formed between P_1 and P_4 and the symmetrical binary formed between P_2 and P_3.
3. "13"-type single binary collision: collision occurring in the binary formed between P_1 and P_3.
4. "24"-type single binary collision: collision occurring in the binary formed between P_2 and P_4.

Note that P_0 is stationary at O, the centre of mass of the system and thus P_0 has no influence in deciding the kinetic energy of the system and the collisions.

In order to regularise these singularities first we will map the (x_i, ω_i) physical plane into the (Q_i, P_i) parametric plane using a series of transformation equations so that the new Hamiltonian function will have no singularities as it passes through a two-body close encounter. There are three important steps in the regularisation scheme [9].

Step 1: Coordinate transformation

We first transform the coordinate system to inter-body coordinates.

$$q_1 = x_1 - x_3, \qquad q_2 = x_2 - x_4, \tag{9}$$

$$q_3 = x_3 + x_1, \qquad q_4 = x_4 + x_2, \tag{10}$$

$$q_5 = 2x_1, \qquad q_6 = 2x_2, \tag{11}$$

$$q_7 = 2x_3, \qquad q_8 = 2x_4. \tag{12}$$

This will make sure that all the possible two-body close encounters in the CS5BP system are regularised [11].

We introduce a generating function $F_1(p_k, q_k)$ to obtain conjugate momenta p_k of the corresponding q_k

$$F_1(p_k, q_k) = p_k q_k = (x_1 - x_3)p_1 + (x_2 - x_4)p_2 + (x_3 + x_1)p_3 + (x_4 + x_2)p_4 + 2x_1p_5 + 2x_2p_6 + 2x_3p_7 + 2x_4p_8, \tag{13}$$

which will give

$$\omega_i = \frac{\partial F_1}{\partial x_i}, \tag{14}$$

where i=1 to 4 and k=1 to 8.

Next we find an expression for new momenta, p_k's, in terms of old momenta, ω_i, using an arbitrary relation which is similar to that for the q' s (i.e. $q_5 - q_7 - 2q_1 = 0, q_5 + q_7 - 2q_3 = 0, q_6 + q_8 - 2q_4 = 0, q_6 - q_8 - 2q_2 = 0$), we set

$$\begin{aligned} p_5 - p_7 - 2p_1 &= 0, \\ p_5 + p_7 - 2p_3 &= 0, \\ p_6 + p_8 - 2p_4 &= 0, \\ p_6 - p_8 - 2p_2 &= 0. \end{aligned} \tag{15}$$

Using equation (14) and (15), we can deduce a set of new conjugate momenta p's as

$$\begin{aligned} p_1 &= \frac{1}{6}(\omega_1 - \omega_3), & p_2 &= \frac{1}{6}(\omega_2 - \omega_4), \\ p_3 &= \frac{1}{6}(\omega_1 + \omega_3), & p_4 &= \frac{1}{6}(\omega_2 + \omega_4), \\ p_5 &= \frac{1}{3}\omega_1, & p_6 &= \frac{1}{3}\omega_2, \\ p_7 &= \frac{1}{3}\omega_3, & p_8 &= \frac{1}{3}\omega_4. \end{aligned} \tag{16}$$

Now we perform the Levi-Civita type coordinate transformation on each inter-body coordinate. We introduce the regularising function using the Levi-Civita transformation, in a complex form

$$q_j + iq_{j+1} = (Q_j + iQ_{j+1})^2, \tag{17}$$

where j= 1,3,5,7. Here note that (q_j, q_{j+1}) refers to a physical plane and (Q_j, Q_{j+1}) refers to a parametric plane. Their corresponding conjugate momenta P_k's are given by

$$P_k = \frac{\partial F_2(p_k, Q_k)}{\partial Q_k} \tag{18}$$

where k= 1 to 8 and $F_2(p_k, Q_k)$ is the generating function of the form

$$F_2(p_k, Q_k) = p_j f(Q_j, Q_{j+1}) + p_{j+1} g(Q_j, Q_{j+1})$$

Using these relations, we can write

$$\begin{aligned} P_j &= 2p_jQ_j + 2p_{j+1}Q_{j+1}, \\ P_{j+1} &= -2p_jQ_{j+1} + 2p_{j+1}Q_j, \end{aligned} \tag{19}$$

Step 2: Time transformation

In the next step, we introduce a fictitious time τ, which is a key factor for the regularising effect. The basic principle of regularisation theory is to transform physical coordinates to a parametric plane and physical time to an artificial time by a differential time transformation, which consequently smooths collision effects in the Hamiltonian system. In the literature, we can find a variety of choices for the time transformation function which has a general form

$$dt = gd\tau = R^n d\tau,$$

where R is the separation between the colliding binaries, g is the time re-scaling factor and n has various choices according to the application. We had tried a few arbitrary values for g and we found that, to preserve conservation of energy, it is advantageous to choose a time re-scaling factor of the form

$$\begin{aligned} \frac{dt}{d\tau} = g &= \frac{r_{12}r_{13}r_{14}r_{24}}{(r_{12}+r_{13}+r_{14}+r_{24})^{5/2}} \\ &= \frac{(Q_1^2+Q_2^2)(Q_3^2+Q_4^2)(Q_5^2+Q_6^2)(Q_7^2+Q_8^2)}{(Q_1^2+Q_2^2+Q_3^2+Q_4^2+Q_5^2+Q_6^2+Q_7^2+Q_8^2)^{5/2}}. \end{aligned} \tag{20}$$

Step 3: Fixing the energy

With the introduction of the time rescaling factor, the new Hamiltonian $\tilde{H}(Q_i, P_i)$ takes the following form in the extended phase space

$$\Gamma(Q_i, P_i) = g(\tilde{H} - h_0), \tag{21}$$

where Γ is the transformed Hamiltonian $\tilde{H}(Q_i, P_i)$ in the extended phase space and h_0 is the total energy or the initial value of $\tilde{H}$. For any particular orbit, $\tilde{H}(\tau) = h_0$, a constant and $\Gamma(\tau) = 0$. We have not shown the transformed Hamiltonian $\Gamma(Q_i, P_i)$ in this paper, as the right hand side of the expression is very lengthy due to a large number of multiplicative terms. The numerator terms in the time rescaling factor g cancel out the singular terms in the denominator of the Hamiltonian function and prevent the increase of the velocity to infinity at the collision stages.

We can derive the Hamilton equations of motion with respect to the fictitious time, using this transformed Hamiltonian in the new set of parametric coordinates:

$$\begin{aligned} \frac{dQ_i}{d\tau} &= \frac{\partial \Gamma}{\partial P_i}, \\ \frac{dP_i}{d\tau} &= -\frac{\partial \Gamma}{\partial Q_i}. \end{aligned} \tag{22}$$

Equation (22) is the final regularised equation of motion, which is a set of ordinary differential equations whose solution is a function of the fictitious time τ and these equations are regular, for any $q_i \to 0$.

There can be singularities when all $q_i \to 0$, where i= 1 to 8. This situation is only possible for a CS5BP system with $C_0 = 0$. This corresponds to a singularity at the origin in the physical plane. For $C_0 \neq 0$; regions of forbidden motion appear very close to the origin and a total central collision is not theoretically possible.

4 Optimisation of the regularised Hamiltonian

An optimisation strategy is not generally required for restricted few-body problems for $n < 4$, since the equations of motion derived using standard regularisation schemes usually contain algebraic terms which can be easily handled by most of the standard numerical integrators. However, the transformed Hamiltonian $\Gamma(Q_i, P_i)$ in Equation (21) is determined using a large number of algebraic multiplications. It is evident that the symbolic differentiation to derive the gradient of $\Gamma(Q_i, P_i)$ will produce a large number of additive and multiplicative terms, leading to an inefficient evaluation of the right hand side of the Equation (22). The direct numerical integration of the regularised Equation (22) (i.e. without using any optimisation techniques) required an excessive amount of computational time even for a very small time period of 10 due to the large number function evaluations involved.

We adapt an algebraic optimisation algorithm of [2] to simplify the Equation 22. The first step in the optimisation process is to rewrite the regularised Hamiltonian $\Gamma(Q_i, P_i)$ in terms of the most frequently appearing terms as a MAPLE procedure [9]. Then we split up the product terms in the MAPLE procedure in calculating the regularised Hamiltonian to avoid the generation of common subexpressions while computing its partial derivatives [2].

We also make use of the reverse-mode algorithmic differentiation to reduce the total number of multiplicative operations (multiplication and addition) to derive the partial derivatives of the regularised Hamiltonian $\Gamma(Q_i, P_i)$. The reverse-mode of automatic differentiation allows computation of gradients at a small cost of computing functions by decomposing the function into a sequence of elementary assignments. The forward-mode differentiation of $\Gamma(Q_i, P_i)$ will generate more than 2100 multiplicative terms, whereas the reverse mode algorithmic differentiation leads to a procedure with only about 320 multiplications. Then we convert repeating symbolic expressions into computation sequences needed for the algorithmic differentiation using the built-in MAPLE functions. In general, this algebraic optimisation procedure can be extended to majority of the global regularisation schemes used in gravitational few-body problems (with $n \geq 3$) and fast numerical realization can be achieved.

5 Numerical experiments

We show some preliminary numerical results using the non-regularised and regularised integration schemes for a regular quasi-periodic orbit. The initial conditions for integrating equation (20) and (22) were fixed using the energy and angular momentum equations of the CS5BP. Numerical experiments were

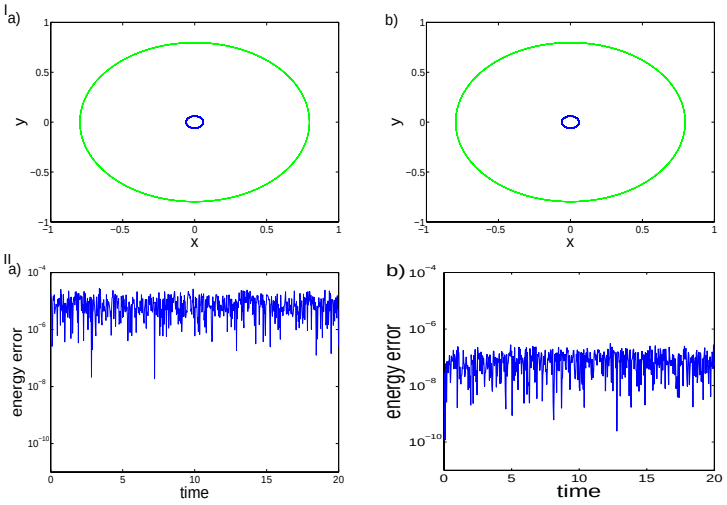

Fig. 2. A quasi-periodic orbit over the time $[0, 20]$ ($\mu = 1$, $\mu_0 = 0$, $E = -7$, $C_0 = 60$ initial $\mathbf{r}_1 = 0.80$ and $\mathbf{r}_2 = 0.06$); with a) non-regularised; b) regularised equations. I. Trajectories of P_1(green) and P_2 (blue) in the xy-plane of motion; II. Energy error over the time period $[0, 20]$

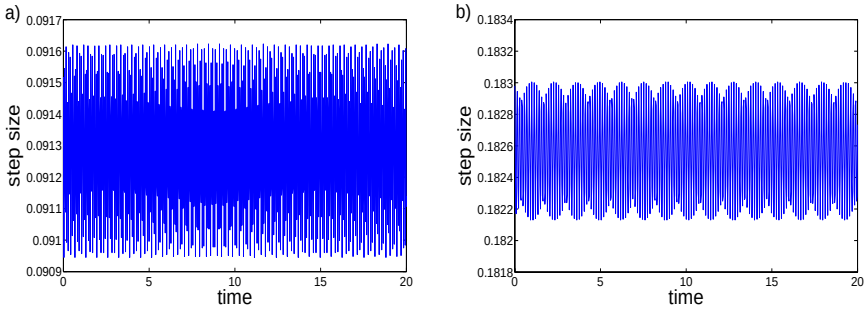

Fig. 3. Time step variations over the time $[0, 20]$ with a) non-regularised; b) regularised equations.

conducted using the standard MATLAB multi-step integrator ode113 which is a variable order Adams-Bashforth-Moulton PECE solver. The orbital trajectories in the xy-plane of motion are shown in Figure 2.1.A central binary is formed (with P_2 and P_4) and the other symmetrical pair P_1 and P_3 orbit around the binary's centre of mass. Only the positions of masses m_1 (x_1, x_2) (green) and m_2 (x_3, x_4)(blue) are shown. The orbits are well separated and remained bounded for some reasonable amount of integration time.

Figure 2.II shows the numerical energy error versus time over a 20 time unit period. Although the orbital trajectories appear to be identical, the regularised integration scheme exhibits a better energy error profile by a factor of 100. Figure 3 shows the corresponding time step variations for the above integrations. The regularised integration scheme has improved the CPU workload

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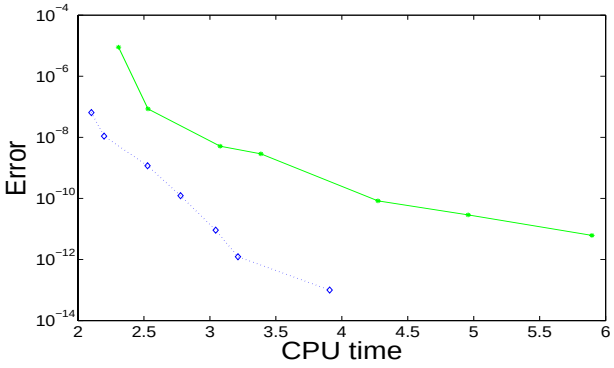

Fig. 4. Comparisons of the errors with variable absolute tolerance error and relative tolerance error; green (non-regularised) and blue (regularised).

by a factor of 1.4 by allowing the integrator to choose bigger step-sizes resulting in decreased number of time steps. Figure 4 shows a comparison between the CPU time and the maximum observed energy error for the given simulation time. It is clear that the regularised scheme allows better accuracy with improved CPU run time. Despite the regularity of the orbit and the absence of extreme close encounters, our numerical tests indicate that the overall CPU workload has been improved. The computational cost involved in each time step differs for both the non-regularised and regularised integrations, since the regularised scheme has twice as many equations in the non-regularised scheme and it involved a large number of algebraic multiplications and additions due to several coordinate transformations forward and backwards. The regularised treatment combined with the algebraic optimisation scheme outperforms the non-regularised approach in terms of computational efficiency and numerical accuracy.

6 Conclusions

We developed a global regularisation scheme that consists of adapted versions of several known regularisation transformations such as the Levi-Civita-type coordinate transformations; that together with a time transformation, removes all the singularities due to colliding pairs of masses in the CS5BP. An algebraic optimisation algorithm is proposed for numerically implementing the regularisation scheme. Regardless of the nature of the orbits, it was found that the regularised integration scheme outperformed the standard non-regularised integration schemes in terms of computational performance and improved numerical accuracy characterized by stable energy profiles.

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