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OVERVIEW – REGULARIZATION AND NUMERICAL METHODS IN CELESTIAL MECHANICS AND DYNAMICAL ASTRONOMY

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Abstract. The relevant study of the n-body problem (predicting individual motions of a group of celestial objects interacting with each other gravitational) is substantial in space dynamics. Further, the various perturbations effects, the collisions or the close encounters between celestial bodies are trajectory modifiers. In the digital age, the behaviour of non-integrable systems is usually and primarily studied with restricted models or coupled with the help of numerical integrators. Over time, these numerical integrators progressed, and the numerical challenge led to the introduction of many new techniques. The question is, which numerical algorithm to choose for the correct research? Is what we get through numerical integration close to the proper orbit? In other words, how can one be sure that the obtained trajectories reflect reality and that their prediction can be taken into account for a long time? This paper presents some analytical and numerical methods with highly accurate computations, such as regularization methods and symplectic integrators, which can be useful in obtaining the corresponding more accurate results.

Key words: celestial mechanics, dynamical astronomy, numerical methods, symplectic integrator, regularization.

1. INTRODUCTION

Poincaré (1890) proved that unlike the two-body problem that is integrable and thus its solutions are completely understood, the three-body problem is not integrable. In most cases, trajectories of the three-body system are chaotic (i.e. non-periodic). In some special cases, there indeed exist periodic orbits. Poincaré indicates that we must use numerical algorithms to solve this problem.

As discovered by Poincaré (1890), computer-generated trajectories of chaotic systems are sensitive to initial conditions (butterfly effect). Namely, a tiny difference in initial conditions might lead to a huge deviation in computer-generated simulation after a long time. Further, Lorenz (2006) found that computer-generated trajectories of chaotic systems are also sensitive to algorithms: different numerical algorithms might give distinctly different computer-generated trajectories of chaotic systems after a long time. The numerical challenge has led to the introduction of many new techniques.

The numerical difficulties associated with integrations of close two-body encounters can be avoided by introducing regularizing transformations which remove the singularity. In 1765, Euler proposed regularizing transformations when studying the motion of three bodies. Regularization is defined as the elimination of singularities occurring in the equations of motion by properly selected variables.

Regularization is essential in space dynamics and stellar dynamics. At the collision, the equations of motion show singularities. When the distance between the bodies approaches zero (close encounters), then the forces acting between particles approach infinity, and this event produces sharp bends of the orbit. The numerical precision after the collision will be worse because of the round-off and truncation errors.

For example, at close encounters, where not actually singularities occur, we can use time-step control decreasing the size of the time-steps. As we all know, the highest accuracy is required at close encounters. The numerous small-time steps of numerical integrations will introduce numerical errors during close encounters. In contrast, all solutions can be determined analytically or numerically if the singularities are eliminated. Therefore, the step size control is not a regularization method. Moreover, the removal of the singularity from the Hamiltonian does not necessarily imply the absence of singular terms in the equations of motion.

The continuation of the orbit after close encounters (collision) is not feasible since the solution encounters the singularity present in the problem.

Apart from the standard procedure of introducing new dependent and independent variables (coordinate and time transformations), singularities may also be removed from the original equations of motion just by the time transformation. Applying a suitable time reparametrization (time transformation or time regularization) that allows one to use constant step size without degrading the accuracy of the computed trajectories. In this case, a new fictitious time s and the original time t are usually related through a differential equation $dt/ds = g(u)$, where u is the vector of state variables.

All regularization methods are a result of choosing the right invariant to represent the reduced phase space and a chart of this reduced phase space.

Regularization methods are also indicative of numerical effectiveness. The key to the further progress of numerical integrators lies in the improved treatment of close encounters that control the dynamical evolution.

It is known that the regularizing technique is very useful for n-body simulations to handle close encounters. Regularized equations of motion can improve numerical integration for the propagation of orbits, and simplify the treatment of mission design problems.

Furthermore, long-term integrations of Hamiltonian systems are preferentially performed using symplectic integrators because they conserve all the Poincaré invariants, such as the phase-space density and have a conserved quantity that is considered a slightly perturbed version of the original Hamiltonian. If the objects of interest are on nearly Keplerian orbits, then a mixed-variable symplectic integrator is particularly useful, allowing for high precision at a relatively large time step.

Symplectic integrators are widely used to study problems in celestial mechanics. These integrators have two advantages over most other algorithms. First, they exhibit no long-term build-up in energy error. Second, the motion of each object about the central body can be built in, so that the choice of step size is determined by the perturbations between bodies, whose magnitude is smaller than the forces due to the central body (Wisdom and Holman, 1991; Wisdom *et al.*, 1997).

In recent years, stellar dynamics have led to an advance in a variety of fields, such as studies of star clusters (i.e. individual, system) formation (Vesperini *et al.*, 2003; Hurley *et al.*, 2005; Adamo *et al.*, 2020), the formation and evolution of higher-order hierarchical systems (i.e. triples, quadruples and higher) (Van den Berk *et al.*, 2007), the Galactic centre and runaway stars (Löckmann and Baumgardt, 2008). I would like to mention that the standard n-body integrators are sensitive to the simulation of the motion of tight binaries or close hyperbolic encounters between stars. Aarseth (2003) summarizes the various regularized schemes that have incorporated into n-body codes to treat strong gravitational interactions with high accuracy and without loss of performance.

Another collision study field can be found between minor and major bodies (i.e. planets, asteroids, comets, satellites, etc.). As an example, one can notice that any minor body that encounters our planet after reaching perihelion inside the orbit of the Earth will approach undetected, hidden in the daytime sky. If the minimum approach distance from Earth is less than 0.001 AU (a configuration called the Red Baron dynamic scenario) and the approaching object cannot be seen due to reflections from the Sun, then this could lead to a possible very close encounter or impact. The most remarkable example of such an occurrence was the Chelyabinsk event on February 15, 2013. Unfortunately, the calculations vary so much that there is no accurate orbital solution that could be used to investigate the origin of the impactor (de la Fuente *et al.*, 2015; Borovička *et al.*, 2013).

This article presents standard techniques and past-recent research in the area, explicitly describes some regularization and symplectic methods, and their application to computer simulations. These methods efficiently treat the close encounters problems.

Moreover, I supply the manuscript with a brief overview of the recent studies in the era of high-performance computers and artificial intelligence.

2. REGULARIZATION METHODS

The numerical integration of the motion of few bodies under a Newtonian gravitational force was difficult in the past, due to the singularities (Levi-Civita, 1920; Kustaanheimo and Stiefel, 1965; Diacu, 1992; Mioc and Csillik, 2002; Anisiu and Szücs-Csillik, 2016). The numerical difficulties associated with direct integrations of close two-body encounters can be avoided by introducing regularizing transformations which remove the disruptive singularity.

In 1893, the mathematician Meissel from Kiel proposed an example of the problem of three bodies which has come to be known as the Pythagorean problem. In 1913, Burrau, hoping to find a periodic solution experimented a numerical integration, with variable step size over a limited period of motion (Burrau, 1913). Later the complete calculation was done by Szebehely and Peters (1967) who succeeded by using KS regularization (Kustaanheimo and Stiefel, 1965) of the relative motion of close pairs and for this the LC regularization (Levi-Civita, 1920).

The KS regularization uses both coordinate transformation and time transformation. The KS regularization leads to regular differential equations, which then can be solved using conventional numerical integrators. Both LC and KS methods are local transformations because applying them allows regularizing collisions with only one of the two primaries (Szebehely, 1967; Stiefel and Scheifele, 1971; Aarseth, 2003; Csillik, 2003; Celletti, 2006; Roa, 2017). Let's mention here, that there are transformations, which can remove both singularities simultaneously for example in the restricted three-body problem. These are called global regularizations. These transformations can be most conveniently given in a coordinate system, where the primaries are located symmetrically with respect to the origin (Érdi, 2004).

The LC and KS regularizations were generalized also Roman and Szücs-Csillik (2014a); Szücs-Csillik and Roman (2014); Szücs-Csillik (2017b, 2021). Techniques to apply KS regularization in multi-particle systems were developed by many authors (Aarseth and Zare, 1974; Aarseth and Heggie, 1976; Mikkola, 1984, 1983; Mikkola and Aarseth, 1996).

Algorithmic regularization uses a transformation of the equations of motion such that the leapfrog algorithm produces exact trajectories for two-body motion as well as regular results in numerical integration of the motion of strongly interacting few-body systems (Mikkola and Tanikawa, 1999; Harfst *et al.*, 2008; Mikkola, 2020). Symplectic integration (like leapfrog) has some important merits over other methods (New *et al.*, 1998), but it also has the shortcoming of requiring the use of a constant integration step, which can be a severe restriction in few-body orbit computations. For example, the basic leapfrog algorithm is time-symmetric, which is not directly possible in the case of velocity-dependent forces, but is usually obtained with the help of the implicit mid-point method.

The treatment of multiple encounters for n-body ($n > 3$) is simplified by the concept of chain regularization introduced by Mikkola and Aarseth (1996). It connects the dominant two-body interactions by a chain of KS-type variables which is updated when the non-chained terms become large. Strong interactions between binaries and single stars or other binaries are treated by chain regularization. This method is particularly useful where the exact orbital phase of binaries is unimportant. The attractive feature of the so-called slow-down method is that it can be applied to binaries of arbitrary size and in the chain formulation. Moreover, several such binaries can be treated simultaneously (Mikkola and Aarseth, 1996).

Let us present some simple and useful regularization methods, which anybody can use to study the dynamics of n-body problem ($n \geq 2$) when close encounters come into account (Roman and Szücs-Csillik, 2011, 2012; Szücs-Csillik and Roman, 2012). Levi-Civita (1920) published the Levi-Civita regularization in plane (see also Szücs-Csillik and Roman (2014); Szücs-Csillik (2017a)). In the following, I will briefly present the KS regularization (in space), which is widely used to remove the singularity in the equations of motion, making it possible to integrate orbits having very high eccentricity (Kustaanheimo and Stiefel, 1965).

As we know, the differential equations of motion of relative two-body problem $\ddot{\mathbf{r}} = -\frac{\mu \mathbf{r}}{r^3}$ are singular at $r = 0$, because in this point the gravitational attraction between bodies is infinite. Here r is the distance between the two bodies, and μ is the gravitational constant. Certainly the Hamiltonian can be directly obtained from the Lagrangian by a transformation known as a Legendre transform (Szebehely, 1967). Therefore, in a fixed reference frame, in space, with relative Cartesian coordinates $\mathbf{q} = (q_1, q_2, q_3)$, the two-body problem is described by the Hamiltonian as

$$H(q_i, p_i) = \frac{\sum_{i=1}^{3} p_i^2}{2} - \frac{\mu}{\sqrt{\sum_{i=1}^{3} q_i^2}}, \tag{1}$$

with the corresponding canonical equations:

$$\begin{aligned} \dot{q}_i &= p_i, \\ \dot{p}_i &= -\frac{\mu q_i}{(q_1^2 + q_2^2 + q_3^2)^{3/2}} = -\frac{\mu q_i}{r^3}, \end{aligned} \tag{2}$$

where q_i and p_i, $i = \overline{1,3}$ are the canonical coordinates in physical space.

In order to achieve the regularization in space, we introduce the $L(\mathbf{Q})$ - KS-matrix, which is orthogonal $L^T(\mathbf{Q})L(\mathbf{Q}) = rE$, where E is the identity matrix, and L^T is the transpose of L matrix, $\mathbf{Q}$ is the new coordinates in parametric space (Csillik, 2003):

$$L(\mathbf{Q}) = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix} \tag{3}$$

As a first step, we introduce the KS transformation, which transforms the $(q_1,q_2,q_3,p_1,p_2,p_3)$ coordinates and momenta in 3-dimensional physical space into the $(Q_1,Q_2,Q_3,Q_4,P_1, P_2,P_3,P_4)$ new coordinates and momenta in 4-dimensional parametric space:

$$\mathbf{q} = \mathbf{L}(\mathbf{Q}) \cdot \mathbf{Q}, \tag{4}$$

where $q_4 = 0 = Q_4Q_1 - Q_3Q_2 - Q_2Q_3 + Q_1Q_4$ is the bilinear relation.

It should be mentioned that for the 2-dimensional physical plane investigations one can use the well-known, simplest Levi-Civita coordinate transformations:

$$\begin{aligned} q_1 &= Q_1^2 - Q_2^2, \\ q_2 &= 2Q_1Q_2. \end{aligned} \tag{5}$$

The new Hamiltonian derived from the KS transformations is:

$$\overline{H}_{KS} = \frac{1}{8} \cdot \frac{\sum_{i=1}^{4} P_i^2}{r} - \frac{\mu}{r}, \qquad r = \sum_{i=1}^{4} Q_i^2. \tag{6}$$

In the second step, we adopt the new fictitious time s as a time transformation:

$$\frac{dt}{ds} = r. \tag{7}$$

Consequently, the new canonical, regular equations become:

$$\begin{aligned} \frac{dQ_i}{ds} &= P_i/4\,, \\ \frac{dP_i}{ds} &= 2\overline{H}_{KS_2}Q_i, \quad i = \overline{1,4}\,, \end{aligned} \tag{8}$$

where the energy $\overline{H}_{KS}$ is constant. Let's mention, that increasing the order of the new canonical equations of motion (8) is not a disadvantage from the numerical point of view, because the regularized equation are more efficient. The KS transformation regularizes the corresponding equations of motion allowing us to understand the near-collision dynamics.

The KS transformation blows up the motion's area near the singularity, and slows down the motion in the parametric plane, using the fictitious time. Besides, the KS regularization is a simple regularization model for the study of motion in physical space. It can be used as a first approximation in regularizing studies. Moreover, using the generalization of the KS-coordinate transformations one can study the orbit's shape of a given celestial object even with small eccentricity around the singularities (Szücs-Csillik and Roman, 2014; Szücs-Csillik, 2017b, 2021).

Funato *et al.* (1997) shown that the time symmetrization scheme, introduced by Hut *et al.* (1992) can be successfully generalized to include KS regularization (Hut and Makino, 2003).

Furthermore, Aarseth and Zare (1974) published a three-particle regularization method. The two shortest distances are regularised with the KS method. Heggie (1974) presented a global n-body regularization using KS-transformations. In this method, each inter-particle vector is an independent variable. Mikkola (1985) wrote a concise algorithm for n-body integration using Heggie's global method (Mikkola, 2008).

Mikkola and Aarseth (1993) elaborated the chain regularization method. Let's briefly present this useful method. Suppose a chain of vectors connecting n bodies. After re-labelling the bodies such that they are along the 1, 2, ..., n chain, the generating function takes the form

$$S = \sum_{i=1}^{n-1} W_k \cdot (q_{k+1} - q_k), \tag{9}$$

where the old momenta $p_k = \partial S / \partial q_k = W_{k-1} - W_k$ is in terms of the new ones W_k for $k = \overline{2, n-1}$, where $p_1 = -W_1$, $p_n = W_{n-1}$. By definition the corresponding chain vectors are given by $R_k = q_{k+1} - q_k$.

The new Hamiltonian becomes

$$\overline{H} = \sum_{k=1}^{n-1} \frac{(m_{k+1} + m_k) \cdot W_k^2}{2 m_k m_{k+1}} - \sum_{k=2}^{n} \frac{W_{k-1} \cdot W_k}{m_k} - \sum_{k=1}^{n-1} \frac{m_k \cdot m_{k+1}}{R_k} - \sum_{1 \le i \le j-2} \frac{m_i \cdot m_j}{R_{ij}},$$

where $R_{ij} = |q_j - q_i|$.

Further, substituting the KS-transformations gives the Hamiltonian in terms of the regularising variables Q_k, P_k. With the time transformation $\frac{dt}{ds} = 1/(T + U)$, where T is the kinetic energy and U is the potential energy, one can obtain the Γ regularized Hamiltonian in the new $(\mathbf{P}, \mathbf{Q}, s)$-system. Consequently, the new canonical equations of motions become

$$\begin{aligned} \frac{d\mathbf{P}_k}{ds} &= -\frac{\partial \Gamma}{\partial \mathbf{Q}_k}, \\ \frac{d\mathbf{Q}_k}{ds} &= \frac{\partial \Gamma}{\partial \mathbf{P}_k}. \end{aligned} \tag{10}$$

In addition, Mikkola and Aarseth (1993) forms a chain of particles such that the shortest relative vectors are in the chain (algorithmic regularization chain).

Experiments made with a *KS-CHAIN* and an *AR-CHAIN* codes have shown that the algorithmic regularized chain method is often efficient even when the mass ratios are large (Mikkola, 2008).

As an example, one can apply the regularization methods to the dynamics of near Earth objects (NEOs) for a long period. As can be observed, the two-body regularization is an efficient tool to integrate perturbed two-body problems numerically (Fukushima, 2007).

A recent new investigation into the existence of ejection–collision orbits in the planar circular restricted three-body problem use for example the simplest planar Levi-Civita regularization (Seara *et al.*, 2022). They use along the paper the local Levi-Civita regularization because it is conceptually simple, suitable for their theoretical purposes and efficient for numerical simulations. Kindly note that not only a complicated regularization can be useful, but sometimes the simplest one will do the same impact.

3. NUMERICAL METHODS

As Poincaré (1890) proved, for three bodies or more there are no general solutions. The trajectories of the bodies depend on their masses, coordinates and velocities at the beginning. In reality, the motion can look very different if the initial conditions are modified, even by minor changes. The three-body problem is a special case of the n-body problem. Unlike two-body problems, no general closed-form solution exists. The resulting dynamical system is chaotic for most initial conditions, and numerical methods are generally required (Hairer and Wanner, 1996; Hairer *et al.*, 2006).

Consequently, we look to perform numerical simulations to describe the motion. This is made by numerical integrations in which the accuracy of the computer and the calculations are essential. The goal is to utilize an adequate method for obtaining precise solutions over a long time.

Note that the chaotic nature of the three-body problem is due to the close encounters which produce large deviations. Thereby errors on small scales are magnified to larger errors in subsequent encounters and the final orbit can be completely different.

For long-term integrations, the most commonly used are symplectic integrators. Symplectic schemes incorporate the symmetries of Hamiltonian systems, and as a result, usually conserve the energy and angular momentum better than non-symplectic integrators. In particular, the angular momentum is usually conserved up to a roundoff error in symplectic integrators.

The literature on the symplectic integration of Hamiltonian problems has rapid growth in the last thirty years. Differential equations used in celestial mechanics are Hamiltonian systems, whose solutions can be obtained by a symplectic (canonical) transformation. Methods of symplectic integration have been constructed for the study of the long-term behaviour of dynamical systems. Early references on symplectic integration are Ruth (1983), Neri (1987), Channell and Scovel (1990), Yoshida (1990), Wisdom and Holman (1991), Kinoshita *et al.* (1991), Saha and Tremaine (1992), Suzuki (1992), Sanz-Serna and Calvo (1994). Yoshida (1993) has discussed the construction of high-order symplectic integrators, while Mikkola and Wiegert (2002) suggested the use of time transformation (Zare and Szebehely, 1975; Zare, 1977).

A common property for all symplectic integrators beyond the second-order derived by using the method of Yoshida (1990) is the unavoidable occurrence of negative integration sub-steps. While negative time steps are not a problem for Newtonian gravitational dynamics due to its time-reversibility, they cause problems for important time-irreversible dynamical processes such as gravitational wave emission and tidal dissipation.

The other approach is to consider higher-order schemes, which permit a very good control of the numerical error by taking advantage of the hierarchical structure of the problem. This has been used with success for long-term integrations of the solar system Farrés *et al.* (2013). The principal limitation of symplectic integrators is that they require a fixed time-step (Gladman *et al.*, 1991).

If the time step is modified between each step, the integrator remains symplectic because each step is symplectic. However, the change in time-step introduces a possible secular energy drift that may reduce the interest in the method. As a consequence, classical symplectic integrators are not very adapted to treat the case of systems that experience occasional close encounters where very small time steps are needed.

To resolve close encounters, Duncan *et al.* (1998) and Chambers (1999) provided solutions in the form of hybrid symplectic integrators. They developed multiple time step symplectic integrators, where the smallest time steps are only used when a close encounter occurs.

Another way to build a symplectic integrator that correctly regularizes close encounters is using time transformation (regularization). Up to an extension of the phase space and a modification of the Hamiltonian, it is indeed always possible to modify the time that appears in the equations of motion. As a result, real time becomes a variable to integrate. It is possible to integrate the motion with a fixed fictitious time-step using an arbitrary splitting scheme (Mikkola, 2008, 2020).

In the following, I review the simplest leapfrog integration and the Neri fourth-order symplectic integrator (Neri, 1987) applied for the relative two-body problem

(Szücs-Csillik, 2010a,b).

The leapfrog method is numerically integrating differential equations as the form of canonical equations of the two-body problem, namely

$$\begin{aligned} \dot{q}_i &= p_i, \\ \dot{p}_i &= -\frac{\mu q_i}{(q_1^2+q_2^2+q_3^2)^{\frac{3}{2}}}, \end{aligned} \tag{11}$$

where q_i and p_i, $i=\overline{1,3}$ are the canonical coordinates in physical space. The leapfrog integrator is also known as the Verlet method (Hairer and Wanner, 2015).

The leapfrog integrator has some advantages. First, it solves the second-order ordinary differential equations directly. Second, it is reversible. Third, it approximately conserves energy.

The leapfrog schema for two-body problem explicitly with h step size can be written as:

$$\begin{aligned} q_i^j &= q_i^{j-1} + hp_i^{j-1} - \frac{1}{2}h^2 \frac{q_i^{j-1}}{((q_1^{j-1})^2+(q_2^{j-1})^2+(q_3^{j-1})^2)^{\frac{3}{2}}}, \quad j=0:h:t_n \\ p_i^j &= p_i^{j-1} - \frac{1}{2}h\left(\frac{q_i^{j-1}}{((q_1^{j-1})^2+(q_2^{j-1})^2+(q_3^{j-1})^2)^{\frac{3}{2}}} + \frac{q_i^j}{((q_1^j)^2+(q_2^j)^2+(q_3^j)^2)^{\frac{3}{3}}}\right), \end{aligned} \tag{12}$$

where $i=\overline{1,3}$, j is the time with t_n - final time.

The Neri fourth-order symplectic integrator schema explicitly is given by:

$$\begin{aligned} q_i^k &= q_i^{k-1} + hc_k p_i^{k-1}, \\ p_i^k &= p_i^{k-1} - hd_k \frac{q_i^k}{((q_1^k)^2+(q_2^k)^2+(q_3^k)^2)^{\frac{3}{2}}}, \quad i=\overline{1,3}, \quad k=\overline{1,4}, \end{aligned} \tag{13}$$

where the value of the coefficient c_k, d_k, $k=\overline{1,4}$ are

$$\begin{aligned} c_1 &= c_4 = \frac{1}{2(2-2^{1/3})}, \qquad c_2 = c_3 = \frac{1-2^{1/3}}{2(2-2^{1/3})}, \\ d_1 &= d_3 = \frac{1}{2-2^{1/3}}, \qquad d_2 = \frac{-2^{1/3}}{2-2^{1/3}}, \qquad d_4 = 0. \end{aligned} \tag{14}$$

Note that the Neri symplectic integrator is suitable for an autonomous Hamiltonian system which can be split into two integrable parts of kinetic and potential energies (Breiter, 1999; Csillik, 2004).

As an application, let's test the simplest leapfrog integrator for simulating the motion of three free bodies in gravitational interaction, which is one of the simplest examples of chaotic behaviour in nature. For this simple application, I wrote the code in MATLAB programming and numeric computing environment*.

As in almost all three-body problems, one of the bodies gets eventually kicked out of the system, while the other two remain stuck together forever (Figs. 1, 2).

Note this problem is more interesting for celestial objects at smaller distances, such as satellites, meteoroids, asteroids, moons, etc., because the changes are faster (Szücs-Csillik, 2017a; Anghel *et al.*, 2021; De Cicco and Szücs-Csillik, 2022).

On the contrary, in triple-star systems at great distances, these changes take a very long time. These generalized results can be useful in the investigation of observed systems, providing a fast method of determining their stability bounds within the large parameter space that results from observational uncertainties (Szenkovits *et al.*, 2002, 2004; Makó *et al.*, 2005; Belbruno *et al.*, 2010).

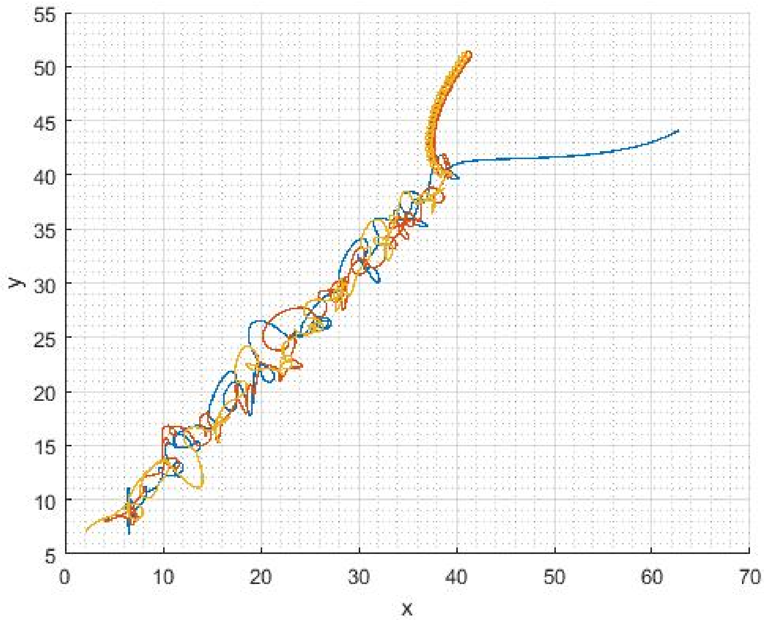

Fig. 1 – Three-body problem simulation using leapfrog symplectic integrator for 10000 seconds

The relationships expressed in the regression models can also be used to guide searches for planets in triple systems and to select candidates for surveys of triple systems. The geometry of the stable zone indicates not only where to look for exoplanets but also the most appropriate technique to search for them (Aarseth, 2004;

*Chosen initial positions and velocities for the three bodies are: $x_1(0) = 6.5$, $y_1(0) = 6.8$, $x_2(0) = 6.4$, $y_2(0) = 9.5$, $x_3(0) = 2.1$, $y_3(0) = 7.1$, $vx_1(0) = 0.002$, $vy_1(0) = 0.001$, $vx_2(0) = 0.006$, $vy_2(0) = 0.004$, $vx_3(0) = 0.004$, $vy_3(0) = 0.006$, $\mu = 0.001$, $dt = 0.1$

Busetti *et al.*, 2018; Asghari *et al.*, 2004; de la Fuente and de la Fuente, 2021).

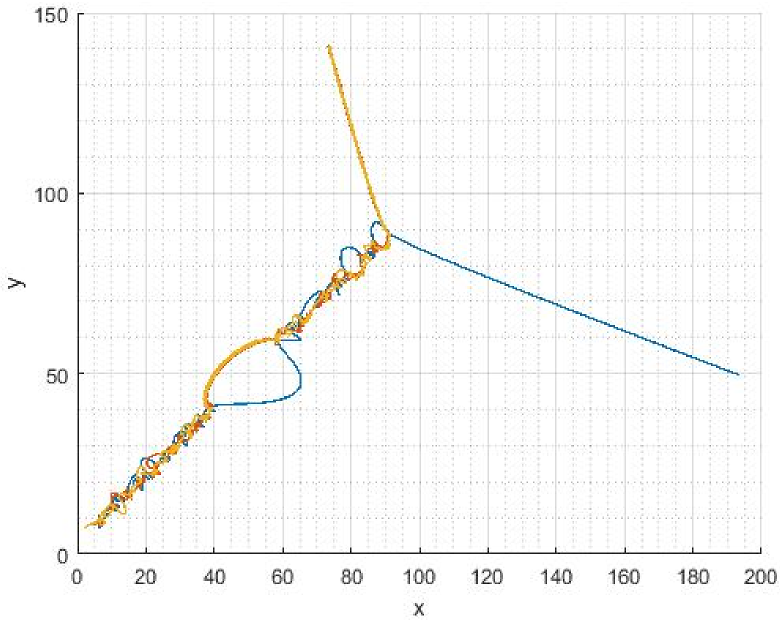

Fig. 2 – Three-body problem simulation using leapfrog symplectic integrator for 25000 seconds.

4. RECENT STUDIES

The work of Poincaré (1890) made a historical turning point: it indicates that we mostly had to use numerical algorithms to solve the n-body ($n \geq 3$) problem.

Nowadays, there is an increasing need for a precise long-term integration. The first long-term direct numerical integration (without averaging) of a realistic model of the Solar System, together with the precession and obliquity equations, was performed by Quinn *et al.* (1991) over 3 Myr. The orbital motion of the full Solar System was computed over 100 Myr using a symplectic integrator with mixed variables (Wisdom and Holman, 1991).

Following the improvement of computer technology, long-term integrations of realistic models of the Solar System have been improved (Ito and Tanikawa, 2002). Now it is possible to integrate the motion of the Solar System over time periods of more than 5 Gyr, which is comparable to its age or expected lifetime (Laskar and Gastineau, 2009; Laskar and Robutel, 2001; Mikkola and Lehto, 2022).

In this paper I wish to indicate how these presented ideas offer a new technique for the numerical solution of initial value problems for ordinary and partial differential equations with particular relevance to certain difficult questions arising from long-term integration.

It must be emphasized that high-performance computers and artificial intelligence (including machine learning) play significant roles in performing the investigation of the n-body problem.

In the following, I will present briefly some integrators, codes, software packages that analysing also close encounter problems:

- *DROMO* allows a new approach to the dynamics of NEOs in the long term, especially appropriated to consider the influence of the anisotropic thermal emission (Yarkovsky and YORP effects) on the dynamics (Peláez *et al.*, 2007; Bau *et al.*, 2011).

- *FCIRK16* is a 16th-order implicit symplectic integrator for long-term high precision Solar System simulations. It takes advantage of the near-Keplerian motion of the planets around the Sun by alternating Keplerian motions with corrections accounting for the planetary interactions. In order to deal with eventual close encounters, *FCIRK16* monitor and accurately resolve eventual close encounters (Antoñana *et al.*, 2022).

- *NBODYx* is a open-source n-body code for high-accuracy simulations of dense stellar systems (Aarseth, 2003). For example, *NBODY4* was successfully tested yielding an unprecedented low-cost tool for astrophysical research in 2014.

- *MSTAR* is an algorithmically regularized integrator for high-accuracy integrations of n-body systems using minimum spanning tree coordinates. It is for large particle numbers and is faster in comparison with the algorithmic regularized chain (AR-CHAIN) method. It is enabled for simulating the dynamics of a galactic scale or supermassive black holes in gas-rich galaxies (Rantala *et al.*, 2020).

- *FROST* is a hierarchical generalization of a fourth-order forward symplectic integrator. The integrator is very suitable for problems with an extremely large dynamical range due to the use of hierarchical Hamiltonian splitting which essentially decouples the evolution of the rapidly evolving parts of the system from the slowly evolving regions. The integrator uses strictly positive (i.e. forward) time steps unlike other high-order symplectic integrators (Yoshida, 1990). There is no secular energy error growth in long-term simulations because the integrator is symplectic (Rantala *et al.*, 2021). *BIFROST* is an extended version of the GPU-accelerated hierarchical fourth-order forward symplectic integrator code *FROST* (Rantala *et al.*, 2022).

- *Swifter* is an improved solar system integration software package. *Swifter* can integrate a set of mutually gravitationally interacting bodies together with a group of massless test particles that feel the gravitational influence of the massive bodies but do not affect each other or the massive bodies. In addition, the *SyMBA* integrator supports the second class of massive bodies whose masses are less than some user-specified value. These bodies gravitationally interact with the more massive bodies but do not interact with each other. Seven integration techniques are included in the current beta release of Swifter: Wisdom-Holman mapping (WHM) (Wisdom and Holman, 1991); Regularized Mixed Variable Symplectic (RMVS) method (Levison and Duncan, 1994); Democratic Heliocentric (DH or HELIO) method (Duncan *et al.*, 1998); Symplectic Massive Body Algorithm (SyMBA) (Levison and Duncan, 2000; Roisin *et al.*, 2022); A fourth-order T+U Symplectic (TU4) method (Gladman *et al.*, 1991); A nonsymplectic fifteenth-order integrator that uses Gauss-Radau spacings (RADAU15) (Everhart, 1985); Bulirsch-Stoer (BS) method (Teukolsky *et al.*, 1992).

- *STARLAB* is a software package for simulating the evolution of dense stellar systems and analyzing the resultant data (see Fig. 3). It is an n-body integrator incorporating both second-order leapfrog and fourth-order Hermite integration algorithms. It includes *Kira* - the general n-body integrator incorporating recursive coordinate transformations, allowing uniform treatment of hierarchical systems of arbitrary complexity within a general n-body framework, and *SeBa* - the stellar and binary evolution package, allowing to follow in time the evolution of any star or binary from arbitrary start conditions. In addition, let's mention some connected integrator-packages *MODEST* (MOdeling DEnse STellar systems), a collaboration between groups working in stellar dynamics, stellar evolution, and stellar hydrodynamics, and the *MANYBODY* collaboration for stellar dynamics software, hardware, and visualization. *GRAPE* (GRAvitational PipelinE) project, creating special-purpose hardware for stellar dynamics. *NEMO* is a software environment for stellar dynamics (Anders *et al.*, 2009).

- *REBOUND* is an n-body integrator, in other words, a software package that can integrate the motion of particles under the influence of gravity. The particles can represent stars, planets, moons, ring or dust particles. It efficiently solves many problems in astrophysics. It includes symplectic integrators as *WHFast, SEI, LEAPFROG, EOS*, high order symplectic integrators for integrating planetary systems as *SABA*, hybrid symplectic integrators for planetary dynamics with close encounters as *MERCURIUS*, high accuracy non-symplectic integrator with adaptive time-stepping like *IAS15* (Rein and Tamayo, 2015; Rein and Spiegel, 2015).

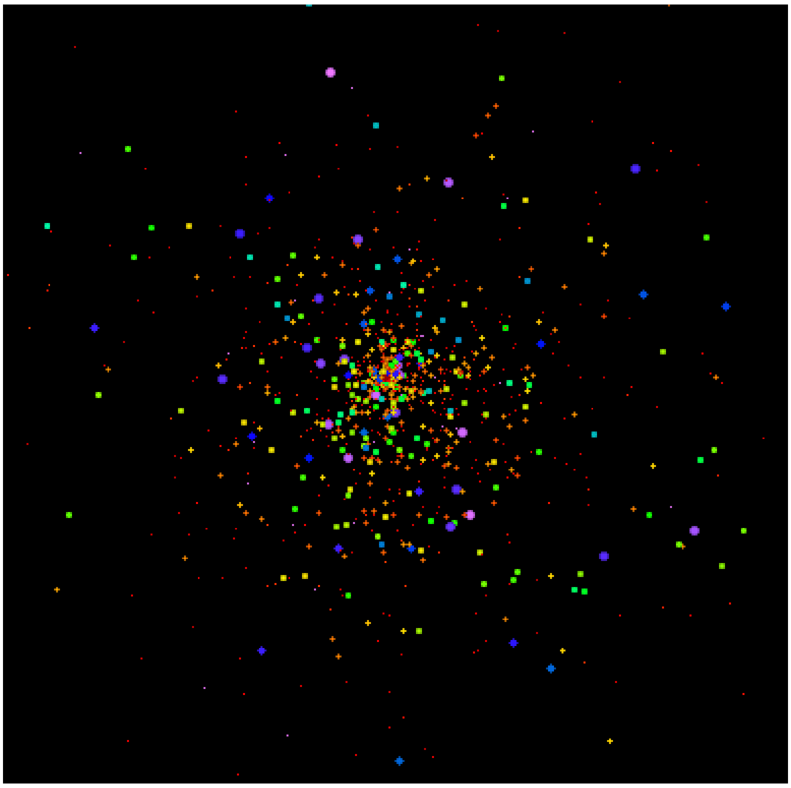

Fig. 3 – Sample animation created with the *STARLAB* toolset (1024 bodies).

- *Changa* (Charm n-body GrAvity solver) is a code to perform collisionless n-body simulations. It employs a tree algorithm to represent the simulation space. An important feature of it is the use of a multi-step integration scheme, which on the smallest (most frequent) timestep updates only those particles with the highest speeds (Menon *et al.*, 2015).

- *OrbFit* software version 5.0 including a new astrometric error model and various other improvements, the capability to determine the semiempirical parameters appearing in the non-gravitational perturbations on asteroids, such as the direct radiation pressure, the Yarkovsky effect, and cometary outgassing. It contains the executable programs *fitobs, catpro, orbfit*. This part provides the main algorithms for orbit propagation, ephemerides computation, orbit determination, close approach analysis, and impact monitoring. *ORBIT9* provides long term orbit propagation for asteroids and other solar system bodies, computation of Lyapunov exponents, computation of proper elements, both analytic and synthetic, and a Graphics Interactive Fourier Filtering program for displaying the results (Gronchi *et al.*, 2010).

- *celmech* an open-source Python package designed to facilitate a wide variety of celestial mechanics calculations. The code can be applied, for example, to isolate the contribution of particular resonances to a system's dynamical evolution and develop simple analytical models with the minimum number of terms required to capture a particular dynamical phenomenon (Hadden and Tamayo, 2022). The *celmech* package is designed to interface with *REBOUND*.

- *Exo-striker* is a transit and radial velocity interactive fitting tool for orbital analysis and n-body simulations. It analyzes exoplanet orbitals, performs n-body simulations, and models the RV stellar reflex motion caused by dynamically interacting planets in multi-planetary systems. It offers a broad range of tools for detailed analysis of transit and Doppler data, including power spectrum analysis for Doppler and transit data. Moreover, it provides Keplerian and dynamical modelling of multi-planet systems, a long-term stability check of multi-planet systems (Trifonov *et al.*, 2019).

These presented n-body integrators suggest that high-performance computer and artificial intelligence (including machine learning) should be the key to future researches. For example, recently thousands of families of periodic orbits of triple systems with three or two equal masses have been found (Liao *et al.*, 2022).

5. CONCLUSION

Regularization is essential in space dynamics. At the collision, the equations of motion show singularities. When the distance between the bodies approaches zero (close encounters), then the forces acting between particles approach infinity, and this event produces sharp bends of the orbit. The numerical precision after the collision will be worse because of the round-off and truncation errors.

The continuation of the orbit after the collision is not feasible since the solution encounters the singularity present in the problem.

Moreover, during a numerical integration, to overcome this difficulty is to use a small step length and many steps of integration surrounding the close approach. In the first instance, the removal of the singularity from the Hamiltonian does not necessarily imply the absence of singular terms in the equations of motion.

Apart from the standard procedure of introducing new dependent and independent variables, singularities may also be removed from the original equations of motion by the time transformation.

Regularization methods are indicative of numerical effectiveness. The key to the further progress of numerical integrators lies in the improved treatment of close encounters that control the dynamical evolution.

Comparing some software packages (i.e. REBOUND, STARLAB, etc.) that can integrate the motion of n particles under the influence of gravity using symplectic, hybrid symplectic, and non-symplectic integrators seems that simultaneous close encounters slow down the integrators.

These integrators must be attentively adapted and well know their properties to avoid unrealistic results.

Retrospectively, high-performance computer and artificial intelligence (machine learning) should be the key to future research.

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