Generalisation of the Levi-Civita/Kustaanheimo-Stiefel regularisation: Scaling invariance

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Abstract.

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1. Introduction

The Levi-Civita (LC) regularisation of the equations for the planar motion (Levi-Civita, 1920), or its extension to the spatial case given by Kustaanheimo and Stiefel (KS) (Kustaanheimo and Stiefel, 1965; Stiefel and Scheifel, 1971) is a standard technique for the numerical integration of eccentric orbits in the Kepler problem. It combines a time-regularisation with a canonical transformation. The time-regularisation removes the singularity, but it makes the system (or Hamiltonian) more complicate. Using a proper canonical transformation the system turns into a harmonic oscillator, making its numerical integration very efficient. This technique has been used as a tool for treating two-body close encounters because it especially reduces the accumulation of numerical error in highly eccentric orbits. Its long-term behavior of the integration errors of the orbital motions has been studied in (Arakida and Fukushima, 2000), showing to be also superior even far from close encounters.

On the other hand, it has been proved that for systems with singularities scaling invariance is a very important property to take into account (Barenblat, 1996; Blanes and Budd, 2002; Budd et al., 2001; Budd and Piggott, 2002; Budd et al., 1997). Numerical integrators preserving (or nearly preserving) this property have proved to be superior to other regularisations for a number of problems. In spite that the Kepler problem is scaling invariant, the LC/KS transformation does not preserve this scaling invariance. Then, its performance can considerably decrease under certain conditions, as shown in (Blanes and Budd, 2002) for a particular example. For this reason, it is important to study under which conditions the LC/KS transformation looses its efficiency, and to analyse if a generalisation of this regularisation (preserving the scaling invariance) works more efficiently.

In this paper we generalise this technique for the two- and three-dimensional problem. It contains the LC/KS regularisation as a particular case as well as a different regularisation which removes the singularity of the Kepler problem, preserving at the same time its scaling invariance. The resulting system will be suitable for being numerically integrated with a symplectic Rung–Kutta–Nyström integrator (see the Appendix). Using this regularisation it is possible to use an explicit adaptive symplectic (EASY) method (Blanes and Budd, 2002) which preserves the scaling invariance of the Kepler problems.

We study the conditions which make the scaling invariant transformation superior. In particular, we consider the collision problem and several perturbations to the Kepler problem: the perturbation due to an oblate planet, the Hill's Lunar problem and an electromagnetic perturbation (the Stark problem can be considered as a particular case). We find that for the pure Kepler problem (with no collision) and for polynomial perturbations to it, the LC/KS regularisation is the most efficient method. However, for the collision problem and for perturbations with higher singularities, the scaling invariant transformation is the most efficient technique. Since the LC/KS regularisation has been widely used for the numerical integration of the N-body problem both with gravitational and Coulombic interactions (Leimkuhler, 1999; Mikkola, 1997b; Waldvogel, 1972), we expect the new regularisation can be very useful for these problems.

The plan of the paper is as follows. In Section 2 the Levi-Civita regularisation is presented as well as its generalisation to the three-dimensional problem. This transformation is generalised in Section 3 to allow to use different regularisation functions. In Section 4 we relate the regularisation function with scaling invariance. Numerical examples are presented in Section 5, and Section 6 gives some conclusions.

2. Levi-Civita and Kustaanheimo-Stiefel regularisations

Let us denote by $\mathbf{q} = (q_1, \ldots, q_k)^T$, $\mathbf{p} = (p_1, \ldots, p_k)^T$, $k = 2, 3$ the coordinates and associated momenta of a system in a $2k$-dimensional phase space with Hamiltonian

$$H = T(\mathbf{p}) + V(\mathbf{q}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}). \tag{1}$$

If the potential has singularities, its numerical integration can produce large errors when the particle approaches the singularity. A standard technique is to regularise the equations in order to remove or reduce the strength of the singularity. This can be achieved if a fictive time is introduced through the ordinary differential equation, $dt/d\tau = g(\mathbf{q}, \mathbf{p})$, defining a *Sundman transformation* Here g is a positive scalar function which is taken to be small if the solution is evolving rapidly. To recover a Hamiltonian structure we introduce two new conjugate coordinates[1]

$$q^t = H(\mathbf{q}_0, \mathbf{p}_0) \quad \text{and} \quad p^t = t.$$

As the Hamiltonian H of the original system is constant we have that $H(\mathbf{p}, \mathbf{q}) - q^t \equiv 0$. To preserve the Hamiltonian structure we can introduce the Poincaré transformation (Waldvogel, 1972). With this transformation the whole system $(\mathbf{q}, q^t, \mathbf{p}, p^t)$ is Hamiltonian and evolves in the fictive time, τ, with Hamiltonian

$$K = g(\mathbf{q}, \mathbf{p})(H(\mathbf{q}, \mathbf{p}) - q^t). \tag{2}$$

Observe that with this choice of q^t and p^t the evolution of the system of ordinary differential equation corresponding to the Hamiltonian (1) is equivalent to the evolution of the extended system with Hamiltonian (2), where the effect of the time transformation is already included.

With this transformation it is possible to remove the singularity of a problem with a proper choice of $g(\mathbf{q})$ but, usually it turns into a more complicate system to be solved numerically. This problem can be simplified if a canonical transformation is found such that the Hamiltonian, in the new coordinates, recovers a simple structure. For the Kepler problem, this can be achieved using the LC or KS regularisation.

[1] In the literature it is usual to take $q^t = t$ and $p^t = -H(\mathbf{q}_0, \mathbf{p}_0)$, but to get a more natural splitting of the extended Hamiltonian, in this paper we consider p^t as the time.

2.1. The Levi-Civita regularisation

Given the Hamiltonian (1) with $k = 2$, the Levi-Civita regularisation takes the Poincaré transformation (2) with $g(q_1, q_2) = r = \sqrt{q_1^2 + q_2^2}$. This leads the following Hamiltonian

$$K(\mathbf{q}, \mathbf{p}) = \frac{1}{2} r \mathbf{p}^T \mathbf{p} + r \left(V(\mathbf{q}) - q^t \right). \tag{3}$$

This transformation is specially suitable for the analysis of eccentric orbits in the Kepler problem, where $V = c/r$, with c a constant, because the singularity in the potential is removed. As mentioned, the original Hamiltonian H is separable, but the transformed Hamiltonian K contains the term $\frac{1}{2} r \mathbf{p}^T \mathbf{p}$. This term is exactly solvable, but it is computationally expensive, and the benefits of using, for example, an explicit symplectic integrator (see the Appendix) breaks down.

Fortunately, there is a simple solution. It is possible to find a canonical transformation (CT) which allows to rewrite K as a simple and separable Hamiltonian in the new coordinates. This CT can be written using complex notation (Waldvogel, 1972) in the form

$$\begin{cases} q_1 + i q_2 = (Q_1 + i Q_2)^2 \\ p_1 + i p_2 = \dfrac{P_1 + i P_2}{2(Q_1 - i Q_2)}, \end{cases} \tag{4}$$

and $(Q^t, P^t) = (q^t, p^t)$, or using real matrix expressions

$$\begin{cases} \mathbf{q} = \hat{Q} \mathbf{Q}, \\ \mathbf{p} = \dfrac{1}{2R^2} \hat{Q} \mathbf{P}, \end{cases} \qquad \text{with} \qquad \hat{Q} = \begin{pmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{pmatrix} \tag{5}$$

and $\mathbf{Q} = (Q_1, Q_2)^T$, $\mathbf{P} = (P_1, P_2)^T$, $R = \sqrt{Q_1^2 + Q_2^2}$.

If a transformation $(\mathbf{q}, \mathbf{p}) = \mathcal{C}(\mathbf{Q}, \mathbf{P})$ is canonical, the Hamiltonian which describes the evolution on the new coordinates is $H(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}(\mathbf{Q}, \mathbf{P}), \mathbf{p}(\mathbf{Q}, \mathbf{P}))$. Then, for completeness, before substituting this transformation into the Hamiltonian (3) we prove that (5) is canonical. This can be easily achieved with the help of the following

THEOREM 1. *The transformation*

$$\begin{cases} \mathbf{q} = \Phi(\mathbf{Q}) \\ \Phi'(\mathbf{Q})^T \mathbf{p} = \mathbf{P}, \end{cases} \tag{6}$$

where Φ is a diffeomorphism of $\mathbb{R}^{2k}$, is canonical.

2.1.0.1. *Proof:* A well known technique for building canonical transformations is by using generating functions. Let us consider the following generating function depending on the new coordinates and old momenta

$$F(\mathbf{Q},\mathbf{p}) = -\Phi(\mathbf{Q})^T\mathbf{p} \tag{7}$$

then, the following equations define a canonical transformation (Goldstein, 1980; **?**)

$$\mathbf{q} = -\frac{\partial F}{\partial \mathbf{p}} = \Phi(\mathbf{Q}), \qquad \mathbf{P} = -\frac{\partial F}{\partial \mathbf{Q}} = \Phi'(\mathbf{Q})^T\mathbf{p} \tag{8}$$

which correspond just to (6). □

As a consequence we have

COROLLARY 1. *The transformation (5) is canonical.*

2.1.0.2. *Proof:* Let us consider $\Phi(\mathbf{Q}) = \hat{Q}\mathbf{Q}$ then, it is immediate to check that

$$\Phi'(\mathbf{Q}) = 2\hat{Q}. \tag{9}$$

Substituting Φ and Φ' in (6) and considering that

$$\hat{Q}^T\hat{Q} = \hat{Q}\hat{Q}^T = R^2 I, \tag{10}$$

where I is the identity matrix, we get (5) so, it is canonical. □

If we consider that

$$r = \sqrt{\mathbf{q}^T\mathbf{q}} = \sqrt{\mathbf{Q}^T\hat{Q}^T\hat{Q}\mathbf{Q}} = R^2, \qquad \frac{1}{2}r\mathbf{p}^T\mathbf{p} = \frac{1}{8R^2}\mathbf{P}^T\hat{Q}^T\hat{Q}\mathbf{P} = \frac{1}{8}\mathbf{P}^T\mathbf{P} \tag{11}$$

the Hamiltonian K in the new coordinates takes the form

$$K = \frac{1}{8}\mathbf{P}^T\mathbf{P} + R^2V(\mathbf{Q}) - R^2Q^t, \tag{12}$$

which is separable in two trivially solvable parts, $K = \tilde{T}(\mathbf{P}) + \tilde{V}(\mathbf{Q}, Q^t)$ with $\tilde{T}$ again quadratic in momenta. For the Kepler problem ($V = -1/r = -1/R^2$) we have

$$K = \frac{1}{8}\mathbf{P}^T\mathbf{P} - 1 - R^2Q^t. \tag{13}$$

Since Q^t is constant, this corresponds to a harmonic oscillator.

2.2. The Kustaanheimo-Stiefel transformation

The generalisation of the Levi-Civita transformation to three dimensions is called the Kustaanheimo-Stiefel (KS) transformation. It can be written using the 4-dimensional KS-variables $\mathbf{Q} = (Q_1, Q_2, Q_3, Q_4)^T$, $\mathbf{P} = (P_1, P_2, P_3, P_4)^T$, where we now consider the 4-dimensional vectors $\mathbf{q} = (q_1, q_2, q_3, 0)^T$, $\mathbf{p} = (p_1, p_2, p_3, 0)^T$. Let us introduce the KS-matrix

$$\hat{Q} = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix}, \tag{14}$$

which is a generalisation of the 2×2 matrix $\hat{Q}$ previously introduced. Observe that the new matrix $\hat{Q}$ also satisfies a similar property to (10) with $R = \sqrt{Q_1^2 + \ldots + Q_4^2}$. If we consider the transformation (5) in the 4-dimensional space, then Corollary 1 also applies, being a CT. Since (**??**) is also satisfied, the Hamiltonian to be solved is (12) in the 4-dimensional space.

As previously mentioned, the LC/KS regularization has been used both in the gravitational and Coulombic case during the last decades as very efficient technique for numerically solving the Kepler problem (as well as for some perturbations to it). However, we must keep in mind that this CT is only useful for one particular regularisation function ($g = r$) which, as we will see, does not preserve the scaling invariance for the Kepler problem. We must also keep in mind that, for different potentials other regularisation functions can be more interesting. For this reason, and in order to keep the advantages of the LC/KS techniques, it seems interesting to look for different CTs for more appropriate regularisation functions, g, such that, at the same time, the final Hamiltonian is still separable like (12), with the kinetic energy quadratic in momenta.

3. Generalisation of the LS/KS transformation

In (Blanes and Budd, 2002) the Lennard-Jones potential is considered and a CT is presented for $g(\mathbf{q}) = r^4$, which makes the system nearly scaling invariant, showing to be clearly superior to the LC/KS regularisation. Thus we are motivated to consider more general CTs which can be applied to a variety of scaling functions $g(\mathbf{q})$.

In this section we apply Theorem 1 to generalise the CT (5) with the goal that for a family of regularisation functions, $g(\mathbf{q})$, the following conditions are satisfied

$$\mathbf{q} = \Phi(\mathbf{Q}), \qquad g(\mathbf{q})\frac{1}{2}\mathbf{p}^T\mathbf{p} = a\mathbf{P}^T\mathbf{P}, \tag{15}$$

with a being a constant and Φ a function depending only on the coordinates. If this CT is found, the Hamiltonian (2), which takes the form

$$K = \frac{1}{2}g(\mathbf{q})\mathbf{p}^T\mathbf{p} + g(\mathbf{q})(V(\mathbf{q}) - q^t) \tag{16}$$

will turn into

$$K = a\mathbf{P}^T\mathbf{P} + \tilde{V}(\mathbf{Q}, Q^t). \tag{17}$$

If g is properly chosen then $a\mathbf{P}^T\mathbf{P}$ and $\tilde{V}(\mathbf{Q}, Q^t)$ will be reasonably small, and symplectic RKN methods with constant time step will work very efficiently, being also computationally more stable.

We present a procedure to find CTs which has the LC/KS transformation as a particular case. Suppose we have found a function $\Phi(\mathbf{Q})$ such that

$$\Phi(\mathbf{Q})^T\Phi(\mathbf{Q}) = R^{2\alpha} \tag{18}$$

and

$$\Phi'(\mathbf{Q})\Phi'(\mathbf{Q})^T = cR^{\beta}I. \tag{19}$$

with c a constant. If this function is used to define the CT (6), conditions (15) are satisfied for $g = r^{\gamma}$, $\gamma = \beta/\alpha$. Observe that for the LC/KS transformation (5) we have $\Phi(\mathbf{Q}) = \hat{Q}\mathbf{Q}$ (and $\alpha = 2$) and $\Phi'(\mathbf{Q}) = \hat{Q}$ (and $\beta = 2$) so, $\gamma = 1$.

We follow this procedure to generalise (5) in order to get different values for γ. Since the performance of a numerical integrator is highly dependent on the choice of γ (Blanes and Budd, 2002), this generalisation will allow to take a more appropriate regularisation function for each particular problem studied.

Let us now consider the following permutations

$$\mathcal{P}^{(1)}\mathbf{Q} = \mathbf{Q}, \qquad \mathcal{P}^{(2)}\mathbf{Q} = (-Q_2, Q_1)^T. \tag{20}$$

With these vectors we form the matrix, $\hat{Q}$, in (5)

$$\hat{Q} = (\mathcal{P}^{(1)}\mathbf{Q}, \mathcal{P}^{(2)}\mathbf{Q}).$$

Next, we define the following sequence of vectors and matrices

$$\begin{aligned} \mathbf{Q}^{(i)} &= \hat{Q}_{i-1}\mathbf{Q} \\ \hat{Q}_i &= \left(\mathcal{P}^{(1)}\mathbf{Q}^{(i)}, \mathcal{P}^{(2)}\mathbf{Q}^{(i)}\right), \qquad i \geq 1 \end{aligned} \tag{21}$$

with $\hat{Q}_0 = I$, which have the following properties.

LEMMA 1. *The matrices $\hat{Q}_i$ defined in (21) with $\mathcal{P}^{(j)}$ given in (20) satisfy*

$$\hat{Q}_i\hat{Q}_i^T = \hat{Q}_i^T\hat{Q}_i = R^{2i}I. \tag{22}$$

3.0.0.3. *Proof:* From (20) we have

$$(\mathcal{P}^{(l)}\mathbf{Q}^{(k)})^T(\mathcal{P}^{(m)}\mathbf{Q}^{(k)}) = \delta_{lm}(\mathbf{Q}^{(k)})^T\mathbf{Q}^{(k)}, \qquad \forall\ \mathbf{Q}^{(k)} \in \mathbb{R}^2$$

so

$$\hat{Q}_i\hat{Q}_i^T = \hat{Q}_i^T\hat{Q}_i = (\mathbf{Q}^{(i)})^T\mathbf{Q}^{(i)}I = \mathbf{Q}^T\left(\hat{Q}_{i-1}^T\hat{Q}_{i-1}\right)\mathbf{Q}\,I, \tag{23}$$

and by simple induction the lemma is proved. $\square$

This is a generalisation of property (10). The relation between vectors and matrices given in (21) is as follows.

LEMMA 2. *Given the vectors $\mathbf{Q}^{(i)}$ and matrices $\hat{Q}_i$ defined according to (21), then*

$$(\mathbf{Q}^{(m+1)})' = (m+1)\hat{Q}_m. \tag{24}$$

3.0.0.4. *Proof:* This is done by induction. From (9) we have

$$(\mathbf{Q}^{(2)})' = 2\hat{Q}_1, \tag{25}$$

and from (21) we have

$$\begin{aligned} (\mathbf{Q}^{(m+1)})'_{ij} &= \frac{\partial \mathbf{Q}_i^{(m+1)}}{\partial \mathbf{Q}_j} = \frac{\partial}{\partial \mathbf{Q}_j}\left(\hat{Q}_m\mathbf{Q}\right)_i = \frac{\partial}{\partial \mathbf{Q}_j}\left(\sum_k \mathbf{Q}_k\mathcal{P}^{(k)}\mathbf{Q}^{(m)}\right)_i \\ &= \left(\mathcal{P}^{(j)}\mathbf{Q}^{(m)}\right)_i + \left(\sum_k \mathbf{Q}_k\mathcal{P}^{(k)}\frac{\partial \mathbf{Q}^{(m)}}{\partial Q_j}\right)_i \end{aligned}$$

$$
\begin{aligned}
&= \left(\mathcal{P}^{(j)}\mathbf{Q}^{(m)}\right)_i + \left(\sum_k \mathbf{Q}_k \mathcal{P}^{(k)} \left(m\mathcal{P}^{(j)}\mathbf{Q}^{(m-1)}\right)\right)_i \\
&= \left(\mathcal{P}^{(j)}\mathbf{Q}^{(m)}\right)_i + \left(m\mathcal{P}^{(j)} \underbrace{\sum_k \mathbf{Q}_k \mathcal{P}^{(k)}\mathbf{Q}^{(m-1)}}_{\mathbf{Q}^{(m)}}\right)_i = (m+1)\left(\mathcal{P}^{(j)}\mathbf{Q}^{(m)}\right)_i \\
&= (m+1)(\hat{Q}_m)_{ij}. \qquad (26)
\end{aligned}
$$

□

Next, we generalise the CT (5) as follows

THEOREM 2. *The following family of transformations*

$$
\begin{cases}
\mathbf{q} = \mathbf{Q}^{(m+1)} \\
\mathbf{p} = \dfrac{1}{(m+1)R^{2m}} \hat{Q}_m \mathbf{P},
\end{cases} \qquad (27)
$$

for $m \in \mathbb{Z}^+$, *is canonical.*

3.0.0.5. *Proof:* From Theorem 1, the following transformation

$$
\begin{cases}
\mathbf{q} &= \mathbf{Q}^{(m+1)} \\
(\mathbf{Q}^{(m+1)})'^T \mathbf{p} &= \mathbf{P},
\end{cases} \qquad (28)
$$

is canonical, and from Lemma 2 it is equivalent to

$$
\begin{cases}
\mathbf{q} &= \mathbf{Q}^{(m+1)} \\
(m+1)\hat{Q}_m^T \mathbf{p} &= \mathbf{P}.
\end{cases} \qquad (29)
$$

Multiplying the second equation by $\hat{Q}_m$ and using Lemma 1, the transformation (27) is obtained and then, it is canonical. □

Notice that the LC/KS transformation corresponds to the particular case $m = 1$. Similarly to (4) and (5), the transformation (27) can also be written using complex notation as

$$
\begin{cases}
q_1 + iq_2 = (Q_1 + iQ_2)^{m+1} \\
p_1 + ip_2 = \dfrac{P_1 + iP_2}{(m+1)(Q_1 - iQ_2)^m}.
\end{cases} \qquad (30)
$$

Observe that if we define $\Phi = \mathbf{Q}^{(m+1)}$ then

$$
\Phi^T \Phi = \mathbf{Q}^T \hat{Q}_m^T \hat{Q}_m \mathbf{Q} = R^{2m} \mathbf{Q}^T I \mathbf{Q} = R^{2(m+1)}
$$

and

$$\Phi'\Phi'^T = (m+1)^2 \hat{Q}_m^T \hat{Q}_m R^{2m} = (m+1)^2 R^{2m}.$$

If we compare with (18) and (19) we have that $\alpha = m+1$ and $\beta = 2m$. This implies that for the family of regularisation functions

$$g(\mathbf{q}) = r^{\gamma}, \qquad \text{with} \qquad \gamma = \frac{2m}{m+1}, \tag{31}$$

condition (15) are satisfied using the previous CT. Substituting in (16) gives

$$K = \frac{1}{2(m+1)^2}\mathbf{P}^T\mathbf{P} + R^{2m}V(\mathbf{Q}) - R^{2m}Q^t. \tag{32}$$

This regularisation removes the singularity for the following family of potentials

$$V(r) = \frac{c}{r^{\frac{2m}{m+1}}}, \tag{33}$$

with c a constant. Although a number of potentials can be considered, it still have the constraint that $0 \leq 2m/(m+1) < 2$. On the other hand, as mentioned previously, a CT for the regularisation function $g = r^4$ (removing the singularity for the potential $V(r) = c/r^4$) is presented in (Blanes and Budd, 2002). For a one-dimensional potential it is possible, in general, to find a regularisation function and CT which removes the singularity (Blanes and Budd, 2002), but this seems not to be the case for higher dimensional problems.

The generalisation to the 4-dimensional case can simply be obtained taking the following set of permutations

$$\begin{array}{ll} \mathcal{P}^{(1)}\mathbf{Q} = \mathbf{Q}, & \mathcal{P}^{(3)}\mathbf{Q} = (-Q_3, -Q_4, Q_1, Q_2)^T, \\ \mathcal{P}^{(2)}\mathbf{Q} = (-Q_2, Q_1, Q_4, -Q_3)^T, & \mathcal{P}^{(4)}\mathbf{Q} = (Q_4, -Q_3, Q_2, -Q_1)^T. \end{array} \tag{34}$$

Using these vectors we rewrite the matrix (14) as follows

$$\hat{Q} = \left(\mathcal{P}^{(1)}\mathbf{Q}, \mathcal{P}^{(2)}\mathbf{Q}, \mathcal{P}^{(3)}\mathbf{Q}, \mathcal{P}^{(4)}\mathbf{Q}\right).$$

Considering that $(\mathcal{P}^{(l)}\mathbf{Q})^T(\mathcal{P}^{(m)}\mathbf{Q}) = \delta_{lm}R^2$, if we define the new vectors, $\mathbf{Q}^{(i)}$, and matrices, $\hat{Q}_i$, similarly to (21), and consider that Lemmas 1 and 2 also apply, the CT we are looking for is just (27) but, in the 4-dimensional space.

The inverse of (27), $(\mathbf{Q}, \mathbf{P}) = \mathcal{C}^{-1}(\mathbf{q}, \mathbf{p})$, can be numerically expensive to compute. But, it has to be evaluated only once for starting the computation. For the output we have to compute the transformation

(27), $(\mathbf{q},\mathbf{p}) = \mathcal{C}(\mathbf{Q},\mathbf{P})$, which requires only few and simple arithmetic operations and it is, in general, not necessary at each step.

This new technique can also be useful for potentials with no singularities. For example, suppose we find a function, g, and a CT such that the new potential $\tilde{V}(\mathbf{Q}, Q^t)$ and the transformation $(\mathbf{q},\mathbf{p}) = \mathcal{C}(\mathbf{Q},\mathbf{P})$ are easy and cheap to compute. In other words, the complexity of the original potential, $V(\mathbf{q})$, moves to the CT, $(\mathbf{Q},\mathbf{P}) = \mathcal{C}^{-1}(\mathbf{q},\mathbf{p})$, which, as previously mentioned, is only required once for starting the computation, and has not to be computed at each step. Then, the new algorithm for the integration will be faster and can be more efficient even for smooth trajectories, where the variable time-step technique seems not appropriate.

4. Scaling Invariance

TO COMPLETE THIS SECTION

-To mention this is a important property.

-Identify the scaling invariance for a problem, and in particular for the Kepler problem.

-To indicate that for $m = 3$ we obtain, for the Kepler problem, a separable Hamiltonian with no singularities and preserving the scaling invariance.

Given the potential $V = c/r^{\alpha}$ and the regularisation function $g = r^{\gamma}$, it is well known that the choice of γ which makes the Hamilton equations scaling invariant is

$$\gamma = \gamma_s = 1 + \alpha/2.$$

If we choose $\gamma_s = 2m/(m+1)$ we have:

1. The singularity is removed for $\alpha < 2$ because $\gamma > \alpha$.

2. The family of potentials such that the singularity is removed, preserve scaling invariance and a CT is known is

$$V(r) = \frac{c}{r^{\frac{2(m-1)}{m+1}}}, \tag{35}$$

   which contains (33) as particular cases (when m in (35) is odd).

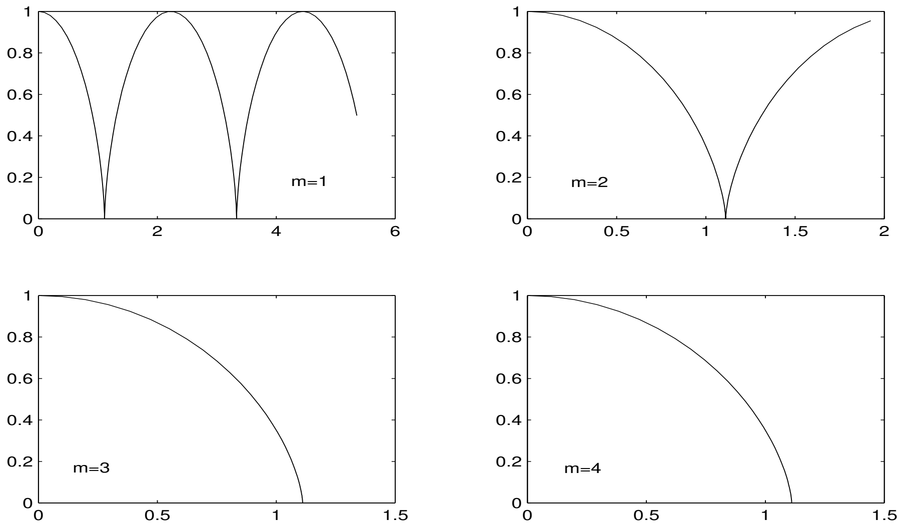

Figure 1. Trajectories obtained for the collapsing problem taking different values of m in the generalisation of the LC/KS regularisation. The case $m = 1$ corresponds to LC/KS, showing a wrong qualitative result.

5. Numerical Examples

5.1. The collision problem

As a first test, we consider a collision in the Kepler problem. This can be described by the one-dimensional Hamiltonian

$$H = \frac{1}{2}p^2 - \frac{1}{q}. \tag{36}$$

We take as initial conditions $(q(0), p(0)) = (1, 0)$, which has a solution which collapses at the finite time $p^t = T = \frac{\pi}{2\sqrt{2}} = 1.11072\ldots$. (Such a solution is asymptotically self-similar.) We consider the fictive time step $\Delta\tau = 0.1$ and integrate until $\tau = 10$, using as the numerical integrator the 6 stages fourth-order symplectic RKN methods given in (Blanes and Moan, 2002). In Fig. 1 we show the curves obtained for $m = 1, 2, 3, 4$, where only for $m \geq 3$ the collapsing point is reached asymptotically. Observe that using the LC regularisation the Hamiltonian (36) is equivalent to

$$K = \frac{1}{8}P^2 + Q^2 \tag{37}$$

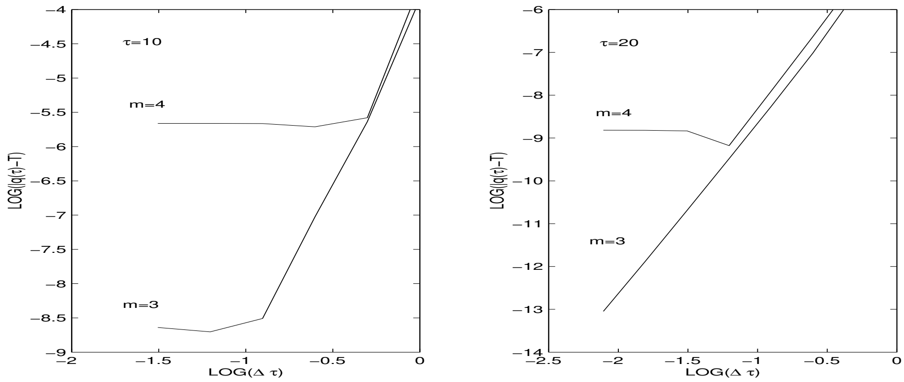

Figure 2. Error in the collision time, T, for different values of the fictive time step, taking as the final fictive time $\tau = 10$ and $\tau = 20$. Only $m = 3, 4$ are considered since they approach to the collision asymptotically.

with initial conditions $(Q(0), P(0)) = (1, 0)$, giving oscillatory solutions, and then crossing the singularity (q takes positive values because $q = Q^2$). If we want to approach the singular point asymptotically, this method is not convenient. However, with the scaling invariant regularisation, the Hamiltonian to be solved is

$$K = \frac{1}{32} P^2 - Q^2 + Q^6, \tag{38}$$

with initial conditions $(Q(0), P(0)) = (1, 0)$, which approaches to the origin asymptotically, as the exact solution. In order to know how accurately the methods approach this collapsing time, in Fig. 2 we present $|q^t(\tau) - T|$ for $m \geq 3$ and different values of $\Delta\tau$ and τ (same cost). It seems clear that for this particular problem the choice $m = 3$, preserving scaling invariance, is optimal, consistent with the previous theory.

5.2. Perturbed Kepler problem

Let us now consider the following Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} + \frac{\varepsilon}{2r^3}\left(1 - \alpha \frac{3q_1^2}{r^2}\right), \qquad r = (q_1^2 + q_2^2)^{1/2}. \tag{39}$$

This Hamiltonian describes in first approximation the dynamics of a satellite moving into the gravitational field produced by a slightly oblate spherical planet. The motion takes place in a plane containing the symmetry axis of the planet when $\alpha = 1$, whereas $\alpha = 0$ corresponds to a plane perpendicular to that axis.

Taking the general regularisation function $g = r^{\frac{2m}{m+1}}$ and the generalised transformation (27), the Hamiltonian (39) turns into

$$\begin{aligned} K &= \tilde{T}(\mathbf{P}) + \tilde{V}(\mathbf{Q}, Q^t) \qquad (40) \\ &= \frac{1}{2(m+1)^2}(P_1^2 + P_2^2) - R^{m-1} + \frac{\varepsilon}{2R^{m+3}}\left(1 - \alpha\frac{q_1^2(\mathbf{Q})}{R^{2(m+1)}}\right) - Q^t R^{2m} \end{aligned}$$

where the function $q_1(\mathbf{Q})$ can be obtained from (30)

$$q_1(\mathbf{Q}) = Re\,(Q_1 + iQ_2)^{m+1} = \sum_{i=0}^{\lfloor \frac{m+1}{2} \rfloor} (-1)^i \binom{m+1}{m+1-2i} Q_1^{m+1-2i} Q_2^{2i}, \qquad (41)$$

where $\left\lfloor \frac{m+1}{2} \right\rfloor$ represents the integer part of $\frac{m+1}{2}$.

We study the performance of the methods taking $\alpha = 1$ and different values of m. This problem is neither integrable nor scaling invariant, although it does have an approximate scaling symmetry if ε/r^3 is small. We take as initial conditions

$$q_1 = 1 - e, \quad q_2 = 0, \quad p_1 = 0, \quad p_2 = \sqrt{(1+e)/(1-e)}, \qquad (42)$$

which, for the unperturbed problem, would correspond to a periodic orbit with eccentricity e and energy $-1/2$. We integrated until $t_f = 20\pi$ for different values of $e \in (0, e^*)$, where e^* is the largest value for e which gives bounded trajectories, and measured the average relative error in energy. The fictive time step is adjusted such that t_f is reached with approximately 200 steps. The numerical integration is carried out with the 11 stages sixth-order symplectic RKN integrator given in (Blanes and Moan, 2002). We considered three cases: (i) $m = 0$ (non regularisation); (ii) $m = 1$ (the standard Levi-Civita regularisation), and (iii) $m = 3$ (the scaling invariant regularisation for the unperturbed Kepler problem). We started the experiments with $\varepsilon = 0$ (unperturbed problem) and results are shown in Fig. 3. Three important facts can be deduced:

1. For the regularised schemes ($m = 1, 3$), the error is nearly independent on the eccentricity. The error increases when e is very close to 1 because a large fictive time step is necessary to reach the final

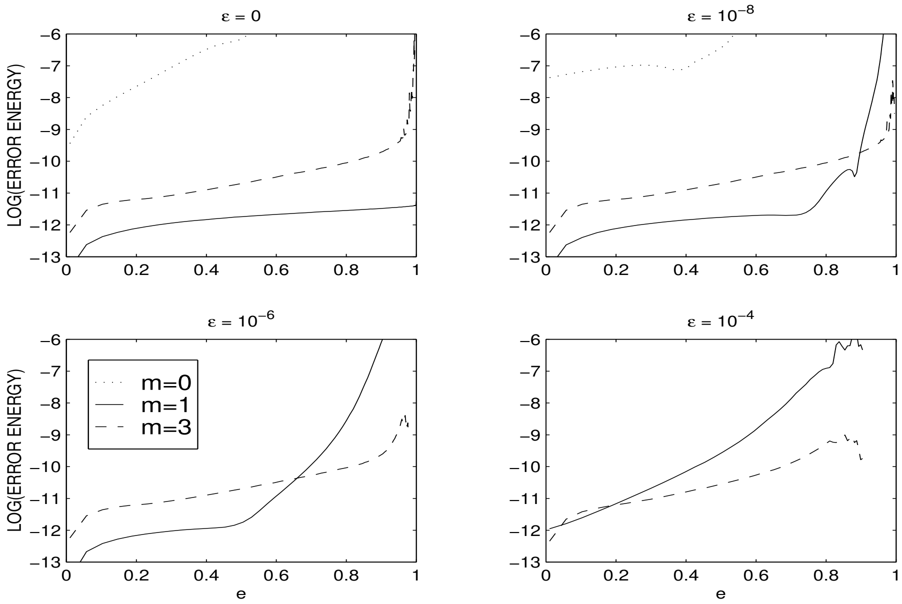

Figure 3. Average relative error in energy as a function of the eccentricity for $m = 0, 1, 3$ using the same fictive time-step, and for different values of ε. Only values of e giving bounded trajectories are considered.

computational time t_f with the fixed number of steps, and the numerical integrator is unstable for these steps.

2. The performance of the regularised schemes is considerably superior to those with constant step size, even for small eccentricities, as already observed in (Arakida and Fukushima, 2000).

3. The Levi-Civita is more accurate than the optimal scaling invariant scheme.

Next, we take $\varepsilon = 10^{-8}$ corresponding to a very small perturbation (see Fig. 3). For $m = 3$ this small perturbation only change slightly the performance of the method. However, the performance of LC is severely deteriorated for high eccentricities (as observed in (Blanes and Budd, 2002)) and it is out performed by the scaling invariant regularisation. This is because the system is now no longer integrable. We also show the results for $\varepsilon = 10^{-6}$ and $\varepsilon = 10^{-4}$ where this effect is magnified.

The reason for the good performance of the Levi-Civita regularisation on the unperturbed problem comes because, when taking $\varepsilon = 0$

and $m = 1$ in (40), the Hamiltonian to be solved is (13) which is exactly solvable. This is possible because the original system is also integrable. The symplectic integrators used solve exactly a perturbed harmonic oscillator or, equivalently, they solve exactly a Kepler problem, with slightly different parameters, giving also a closed trajectory (this is a surprising fact since it is well known that most symplectic integrators, when applied to the Kepler problem give trajectories with a precession of the orbit). However, this only happens when solving the Kepler problem in Cartesian coordinates, but not in polar coordinates as observed in (Blanes and Budd, 2002). Since the fictive time in the new Hamiltonian is not scaling invariant, its performance is drastically deteriorated for high eccentricities when the perturbation is introduced. The choice $m = 3$ (or $g = r^{3/2}$) resulting a nearly scaling invariant scheme, gives the best results for high eccentricities for this perturbed Kepler problem.

To better illustrate the performance of the methods at high eccentricities, we consider the following cases: (i) $\varepsilon = 0$ and $e = 0.999$; (ii) $\varepsilon = 10^{-8}$ and $e = 0.98$. As the numerical integrators we consider the following symplectic RKN integrators: the second order (47), the 6 stages fourth-order and the 11 stages sixth-order given in (Blanes and Moan, 2002). We compare the LC regularisation (LCn, $n = 2, 4, 6$) versus the nearly scaling invariant ($m = 3$) regularisation (En, $n = 2, 4, 6$). We measure the average relative error in energy versus the number of potential evaluations. Fig.**??** show the results obtained. For the pure Kepler problem, the LC regularisation is always more efficient. However the performances completely change when the small perturbation in introduced. Observe that the difference between En and LCn increase with n in agreement with the general results obtained for the one-dimensional problem studied in (Blanes and Budd, 2002).

5.3. The Hill's Lunar problem

It describes the motion of the moon under the influence of the earth and an infinitely remote sun on a circular orbit. Hill's lunar problem can be represented by the two-dimensional Hamiltonian (Waldvogel, 1996)

$$H = \frac{1}{2}\mathbf{p}^T\mathbf{p} + \mathbf{p}^T M\mathbf{q} + \mathbf{q}^T S\mathbf{q} - \frac{1}{r}, \qquad \text{with} \qquad M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad S = \begin{pmatrix} -1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{43}$$

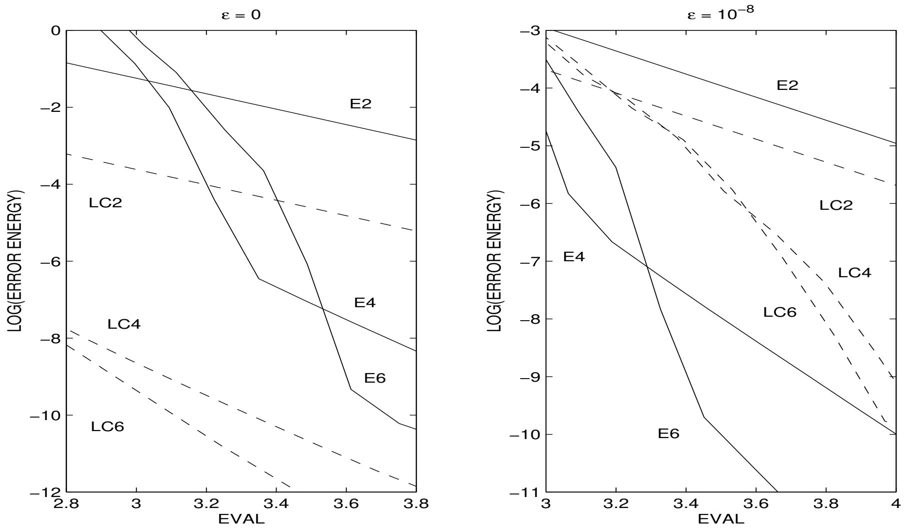

Figure 4. Average relative error in energy versus the number of potential evaluations for the LC regularisation (LCn, $n = 2, 4, 6$) and the nearly scaling invariant ($m = 3$) regularisation (En, $n = 2, 4, 6$).

Let us consider $g = r^{\frac{2m}{m+1}}$ with the CT (27) and

$$r = R^{m+1}, \qquad \mathbf{p}^T\mathbf{p} = \frac{1}{(m+1)^2R^{2m}}\mathbf{P}^T\mathbf{P}, \qquad g = R^{2m},$$

$$\mathbf{p}^T M\mathbf{q} = \frac{1}{(m+1)R^{2m}}\mathbf{P}^T\hat{Q}_m^T M\hat{Q}_m\mathbf{Q} = \frac{1}{m+1}\mathbf{P}^T M\mathbf{Q},$$

where $\hat{Q}_m^T M\hat{Q}_m = R^{2m}M$, then, the Hamiltonian to be solved is

$$K = \frac{1}{2(m+1)^2}\mathbf{P}^T\mathbf{P} + \frac{R^{2m}}{m+1}\mathbf{P}^T M\mathbf{Q} + R^{2m}\mathbf{Q}^T\hat{Q}_m^T S\hat{Q}_m\mathbf{Q} - R^{m-1} + R^{2m}Q^t, \tag{44}$$

which has no singularities for $m > 0$. If m is even, a square root is necessary in the computation of R^{m-1}, but this is not the case if m is odd. This Hamiltonian is separable in three solvable parts $K = K_1(\mathbf{P}) + K_2(\mathbf{Q}, \mathbf{P}) + K_3(\mathbf{Q})$. Here, K_1 and K_3 are trivially solvable since they only depend on the coordinates and momenta, respectively. The evolution due to K_2 is also trivial if we take into account that for this Hamiltonian both R as well as $\mathbf{P}^T M\mathbf{Q}$ are constants of the motion. This involve the computation of the exponential of M, but this has to be done only once (and to store it) because the integration is done with a fixed time-step in the fictive time. An efficient splitting method for this problem is, for example, to consider first the splitting $K = A + B$ with $A = K_1 + K_2$ and $B = K_3$. Observe that $\{B, \{B, \{B, A\}\}\} = 0$ and a Nyström method can be used. Next, to solve the evolution of A we can use a second splitting method. In this case, as the only nested commutators which are different from 0 are $\{K_2, \{K_2, \ldots \{K_2, K_1\} \ldots\}\}$ we can use the methods for the near integrable problem $(s, 2)$ presented in (McLachlan, 1995b) to have a method of order s. Here, K_1 plays the role of the small term.

Several numerical experiments indicate that the LC/KS regularisation works more efficiently than the scaling invariant regularisation method even when nearly collisions happens. The reason comes from the fact that the Hamiltonian (43) corresponds to the Kepler problem with a perturbation which can be neglected when the body is close to a collision. This means that during a near-collision the system can be considered as purely Keplerian and, as observed in the previous example, in this case the LC regularisation works more efficiently.

Similar results are obtained, for example, with a system in a constant electrical and magnetic field with Hamiltonian

$$H = \frac{1}{2}\left(\mathbf{p} - \frac{1}{2}\hat{B}\mathbf{q}\right)^T \left(\mathbf{p} - \frac{1}{2}\hat{B}\mathbf{q}\right) - \frac{1}{r} + E\mathbf{q} \tag{45}$$

with $E \in \mathbb{R}^3$ the electric field and $\hat{B} \in \mathbb{R}^{3\times 3}$ the matrix associated to the magnetic field. The particular case $\hat{B} = 0$ corresponds also to the Stark problem in celestial mechanics. However, if a perturbation with a singularity which can not be removed with the LC/KS regularisation is introduced to those problems, the performance of LC/KS will deteriorate as the previous example.

6. Conclusions

From the theoretical analysis and the numerical experiments carried out in this paper for several perturbations to the Kepler problem it seems clear that for the numerical integration of the pure Kepler problem or some polynomial perturbations to it, the LC/KS regularisation, in general, gives the most efficient techniques . However, for collision problems as well as if the perturbation contains a higher order singularity, the scaling invariant regularisation is more efficient for eccentric orbits. At this moment, the performance of this new scaling invariant regularisation on the N-body problem in under investigation.

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Appendix

A. Symplectic Integrators

Given the Hamiltonian (1) with initial conditions $\mathbf{q}_0$, $\mathbf{p}_0$ and $H_0 = H(\mathbf{q}_0, \mathbf{p}_0)$, the evolution of this system can formally be written as

$$(\mathbf{q}, \mathbf{p}) = e^{-t\hat{H}}(\mathbf{q}_0, \mathbf{p}_0), \tag{46}$$

where $\hat{H}$ is the Lie operator associated to the Hamiltonian[2], and t is the time. The Lie transformation, $e^{-t\hat{H}}$, acts on each component and (46) defines a canonical or symplectic transformation. If $H = T(\mathbf{p} + V(\mathbf{q})$ then T and V are exactly solvable and the second order symmetric and symplectic Störmer/leapfrog/Verlet method, for one time step h, is

$$S_2(h) = e^{-\frac{h}{2}\hat{V}}\, e^{-h\hat{T}}\, e^{-\frac{h}{2}\hat{V}} = e^{-h\hat{H}} + O(h^3) \tag{47}$$

so that the algorithm for one step is given by

$$\begin{aligned} \mathbf{p}_{n+1/2} &= \mathbf{p}_n - \tfrac{h}{2}\nabla_{\mathbf{q}} V(\mathbf{q}_n) \\ \mathbf{q}_{n+1} &= \mathbf{q}_n + h\mathbf{p}_{n+1/2} \\ \mathbf{p}_{n+1} &= \mathbf{p}_{n+1/2} - \tfrac{h}{2}\nabla_{\mathbf{q}} V(\mathbf{q}_{n+1}), \end{aligned} \tag{48}$$

where $(\mathbf{q}_n, \mathbf{p}_n) \simeq (\mathbf{q}(t_n), \mathbf{p}(t_n))$ with $t_n = t_0 + nh$. For N steps, the last computation of $\nabla_{\mathbf{q}} V(\mathbf{q}_{n+1})$ at each step can be reused in the next step, and only one evaluation of $\nabla_{\mathbf{q}} V$ per step is required.

Higher order symplectic methods can be obtained by composition of this method (Suzuki, 1990; Yoshida, 1990). For example, a well known symmetric fourth order method is given by

$$\begin{aligned} S_4(h) &= S_2(x_1 h) S_2(x_0 h) S_2(x_1 h) \qquad (49) \\ &= e^{-h\frac{x_1}{2}\hat{V}}\, e^{-hx_1\hat{T}}\, e^{-\frac{x_1+x_0}{2}\hat{V}}\, e^{-hx_0\hat{T}}\, e^{-\frac{x_1+x_0}{2}\hat{V}}\, e^{-hx_1\hat{T}}\, e^{-h\frac{x_1}{2}\hat{V}} \end{aligned}$$

with $x_1 = 1/(2 - 2^{1/3})$, $x_0 = 1 - 2x_1$. Higher order methods are also presented in (Yoshida, 1990). These methods have become very well

[2] It is defined by its action on a differentiable function, $f(\mathbf{q}, \mathbf{p})$ as $\hat{H}f = \{H, f\}$, being $\{\cdot, \cdot\}$ the usual Poisson bracket

known due to their good behaviour for long time integration (Yoshida, 1993; Sanz-Serna and Calvo, 1994; Hairer et al., 2002) but, they are not very accurate. Recently, a number of new splitting methods have appeared which are more efficient. For Hamiltonians like (1), which are quadratic in momenta, more efficient symplectic RKN methods can be used. A symmetric k stages integrator can be written as

$$\Phi_h = \prod_{i=0}^{k} e^{-a_i h \hat{T}} \, e^{-b_i h \hat{V}} \tag{50}$$

with $a_0 = 0, a_{k-i} = a_{i+1}, b_{k-i} = b_i$ or $b_k = 0, b_{k-i-1} = b_i, a_{k-i} = a_i, \ i = 0, \ldots, k$. For example, the following 6 stages fourth order symmetric method presented in (Blanes and Moan, 2002) has been shown to be highly efficient

$$\begin{array}{ll} b_6 = b_0 = 0.0829844064174052 & a_0 = 0 \\ b_5 = b_1 = 0.396309801498368 & a_6 = a_1 = 0.245298957184271 \\ b_4 = b_2 = -0.0390563049223486 & a_5 = a_2 = 0.604872665711080 \\ b_3 = 1 - 2(b_0 + b_1 + b_2) & a_4 = a_3 = 1/2 - (a_1 + a_2). \end{array} \tag{51}$$

This integrator requires twice the number of evaluations than S_4, but it is several orders of magnitude more accurate, and this compensates the extra cost. Sixth order RKN methods are also presented in (Blanes and Moan, 2002), and methods up to order eight, using the processing technique, are presented in (Blanes et al., 2001).

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