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Conservative discretizations of the Kepler motion

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Abstract

Modified vector fields are used to construct high-order conservative discretizations of the three-dimensional Kepler motion. The numerical integrators preserve the Hamiltonian function, the angular momentum and Runge–Lenz vector. In particular, the exact integrator of the Kepler motion is found. The proposed numerical schemes permit explicit implementation.

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1. Introduction

Kepler problem is a well-known completely integrable system. The equations of motion preserve the Hamiltonian function, the angular momentum and Runge–Lenz vector. There is a sufficient number of independent first integrals for integrability of the differential equations (in contrast, the N-body problem is in general non-integrable for $N \geqslant 3$). Furthermore, Kepler problem is super-integrable, i.e. any bounded orbit is closed and periodic. Therefore, it is beneficial to preserve this property under discretization.

Conservative discretization methods for the two- and three-dimensional Kepler problems were recently presented in [10, 11]. These discretization methods are based on Levi-Civita [16] and Kustaanheimo and Stiefel [7] transformations, which link the two- and three-dimensional Kepler problems to the two- and four-dimensional harmonic oscillators, respectively. The discretizations conserve all first integrals of motion, namely, the energy, the angular momentum and Runge–Lenz vector.

The only drawback of these schemes is the second order of approximation. In the present paper we show how to construct high-order methods. Using the modified vector field framework developed in [2, 3], we obtain numerical integrators of orders 4 and 6. Moreover, the exact integrator of Kepler motion is found. Such numerical realization of the exact solution is new and can be useful for splitting methods which include two-body problems as components.

The paper is organized as follows: in section 2 we present a regularization of the three-dimensional Kepler problem, which links it to the four-dimensional harmonic oscillator. In

section 3, we consider transformation of the first integrals. Section 4 describes a discrete Kepler motion through a discretization of the harmonic oscillator. The discrete motion has the same first integrals as the continuous Kepler motion. In section 5, we present numerical experiments. The final section 6 contains concluding remarks.

2. Kepler motion and Kustaanheimo–Stiefel transformation

The three-dimensional Kepler motion is described by the equations

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{p}, \qquad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{K^2}{r^3}\mathbf{q}, \qquad r = |\mathbf{q}| \qquad \mathbf{q}, \mathbf{p} \in \mathbb{R}^3 \tag{2.1}$$

with the initial data

$$\mathbf{q}(0) = \mathbf{q}_0, \qquad \mathbf{p}(0) = \mathbf{p}_0. \tag{2.2}$$

This system is defined by the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}|\mathbf{p}|^2 - \frac{K^2}{r}. \tag{2.3}$$

The equations of the three-dimensional Kepler motion can be transformed to the equations of the four-dimensional harmonic oscillator. First, we perform a time transformation

$$\frac{\mathrm{d}t}{\mathrm{d}s} = r. \tag{2.4}$$

The transformation preserves the canonical form of the differential equations provided that a new Hamiltonian

$$\hat{H}(\mathbf{q}, \mathbf{p}) = r(H(\mathbf{q}, \mathbf{p}) + A), \qquad A = -H(\mathbf{q}_0, \mathbf{p}_0)$$

is used. This transformation is called Poincaré transform [9]. For Kepler motion we get the new Hamiltonian

$$\hat{H}(\mathbf{q}, \mathbf{p}) = \tfrac{1}{2}r|\mathbf{p}|^2 + Ar - K^2.$$

It removes the singularity of the potential, but leads to a more complicated system.

It is well known that the orbits of the Keplerian motion are classified according to the values of A:

(1) if $A > 0$, the orbit is an ellipse;
(2) if $A = 0$, the orbit is a parabola;
(3) if $A < 0$, the orbit is a hyperbola.

Secondly, we use a canonical transformation

$$\mathbf{q} = \Lambda(\mathbf{Q})\mathbf{Q}, \qquad \mathbf{p} = \frac{1}{2|\mathbf{Q}|^2}\Lambda(\mathbf{Q})\mathbf{P}, \qquad \mathbf{Q}, \mathbf{P} \in \mathbb{R}^4, \tag{2.5}$$

$$\Lambda(\mathbf{Q}) = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \end{pmatrix}, \tag{2.6}$$

which recovers a simple structure of the differential equations.

It transforms $\hat{H}(\mathbf{q}, \mathbf{p})$ to a simple and separable Hamiltonian in the new coordinates

$$H_{\mathrm{osc}}(\mathbf{Q}, \mathbf{P}) = \tfrac{1}{8}|\mathbf{P}|^2 + A|\mathbf{Q}|^2 - K^2, \tag{2.7}$$

which describes a four-dimensional harmonic oscillator

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}s} = \frac{1}{4}\mathbf{P}, \qquad \frac{\mathrm{d}\mathbf{P}}{\mathrm{d}s} = -2A\mathbf{Q}. \tag{2.8}$$

In the parametric variables, the time transformation (2.4) takes the form

$$\frac{\mathrm{d}t}{\mathrm{d}s} = |\mathbf{Q}|^2. \tag{2.9}$$

The transformation (2.5) combined with the time transformation (2.9) generates a transformation that maps the three-dimensional Kepler motion to the system of four-dimensional harmonic oscillator. Let us note that the regularization of the three-dimensional Kepler problem cannot be achieved without this increase of the degrees of freedom [16].

It was proved in [16] that the transformation (2.5) is canonical if the bi-linear relation

$$l(\mathbf{Q})\mathbf{P} = 0, \qquad l(\mathbf{Q}) = (Q_4 \quad -Q_3 \quad Q_2 \quad -Q_1) \tag{2.10}$$

holds. Since this bi-linear relation is a first integral of equations (2.8) it is necessary to choose the initial values $\mathbf{Q}_0$ and $\mathbf{P}_0$, so that

$$l(\mathbf{Q}_0)\mathbf{P}_0 = 0$$

is satisfied. We can use the formulae

$$\mathbf{q}_0 = L_1(\mathbf{Q}_0)\mathbf{Q}_0, \qquad \mathbf{P}_0 = 2L_1^T(\mathbf{Q}_0)\mathbf{p}_0. \tag{2.11}$$

From the former equation one finds some vector $\mathbf{Q}_0$. The solution $\mathbf{Q}_0$ is not unique because Kustaanheimo–Stiefel transformation is not one-to-one. Then, from the latter equation $\mathbf{P}_0$ is uniquely determined. A particular suggestion for the choice of the initial values $(\mathbf{Q}_0, \mathbf{P}_0)$ of the parametric coordinates can be found in [16].

3. Conservation properties

The equations of the three-dimensional Kepler motion (2.1) have the following first integrals:

(1) Hamiltonian function $H(\mathbf{q}, \mathbf{p})$ given in (2.3).

(2) Angular momentum

$$\mathbf{L}(\mathbf{q}, \mathbf{p}) = \mathbf{q} \times \mathbf{p}. \tag{3.1}$$

(3) Runge–Lenz vector

$$\mathbf{A}(\mathbf{q}, \mathbf{p}) = \mathbf{p} \times \mathbf{L} - \frac{K^2}{r}\mathbf{q} = \mathbf{q}\left(H(\mathbf{q}, \mathbf{p}) + \frac{1}{2}|\mathbf{p}|^2\right) - \mathbf{p}(\mathbf{q}, \mathbf{p}). \tag{3.2}$$

Not all first integrals are independent. There are two relations between them given by the equations

$$|\mathbf{A}|^2 - 2H|\mathbf{L}|^2 = K^4 \qquad \text{and} \qquad (\mathbf{A}, \mathbf{L}) = 0.$$

Kustaanheimo–Stiefel transformation (2.5) transforms first integrals of three-dimensional Kepler motion to the following first integrals of the four-dimensional harmonic oscillator [11]:

(1) Hamiltonian function $H_{\mathrm{osc}}(\mathbf{Q}, \mathbf{P})$ given in (2.7).

(2) Angular momentum

$$\mathbf{L}(\mathbf{Q}, \mathbf{P}) = \frac{1}{2}\begin{pmatrix} (Q_1P_4 - Q_4P_1) + (Q_2P_3 - Q_3P_2) \\ -(Q_1P_3 - Q_3P_1) + (Q_2P_4 - Q_4P_2) \\ (Q_1P_2 - Q_2P_1) + (Q_3P_4 - Q_4P_3) \end{pmatrix}. \tag{3.3}$$

(3) Runge–Lenz vector

$$\mathbf{A}(\mathbf{Q}, \mathbf{P}) = \begin{pmatrix} H_{\mathrm{osc}}\left(Q_1^2 - Q_2^2 - Q_3^2 + Q_4^2\right) - \frac{1}{8}\left(P_1^2 - P_2^2 - P_3^2 + P_4^2\right) \\ 2H_{\mathrm{osc}}(Q_1Q_2 - Q_3Q_4) - \frac{1}{4}(P_1P_2 - P_3P_4) \\ 2H_{\mathrm{osc}}(Q_1Q_3 + Q_2Q_4) - \frac{1}{4}(P_1P_3 + P_2P_4) \end{pmatrix}. \tag{3.4}$$

4. Discrete Kepler motion

To find a numerical solution of the Kepler motion one can perform computations in the parametric coordinates $(\mathbf{Q}, \mathbf{P})$ and fictitious time s and transfer the solution back to the physical coordinates $(\mathbf{q}, \mathbf{p})$. Computations in fictitious (or computational) time became popular for adaptive numerical schemes [1]. Kustaanheimo–Stiefel regularization leads to the linear equations of motion and any solution of these equations is stable in contrast to the solutions of the Newtonian classical equations of the two-body problem [16]. As a consequence, it is preferable to perform numerical integration in the parametric coordinates. The equation for computation of the physical time t is added to the system. The equations can be combined as

$$\frac{\mathrm{d}}{\mathrm{d}s}\begin{pmatrix}\mathbf{Q}\\ \mathbf{P}\\ t\end{pmatrix} = \begin{pmatrix}\frac{1}{4}\mathbf{P}\\ -2A\mathbf{Q}\\ |\mathbf{Q}|^2\end{pmatrix}. \tag{4.1}$$

Here $A = -H(\mathbf{q}_0, \mathbf{p}_0)$ and the initial values $(\mathbf{Q}_0, \mathbf{P}_0)$ are found from the initial values for $(\mathbf{q}_0, \mathbf{p}_0)$ by (2.11).

4.1. The basic numerical integrator

Conservation of the Hamiltonian $H_{\mathrm{osc}}(\mathbf{Q}, \mathbf{P})$, angular momentum $\mathbf{L}(\mathbf{Q}, \mathbf{P})$ and Runge–Lenz vector $\mathbf{A}(\mathbf{Q}, \mathbf{P})$ can be achieved if we employ a numerical method which preserves quadratic first integrals [4]. The Hamiltonian function and the angular momentum are quadratic. Runge–Lenz vector $\mathbf{A}(\mathbf{Q}, \mathbf{P})$ is a polynomial of the fourth order. However, it is quadratic if we consider $H_{\mathrm{osc}}(\mathbf{Q}, \mathbf{P})$, a quadratic first integral on its own, as a constant.

For example, we can choose midpoint rule

$$y_{n+1} = y_n + hf\left(\frac{y_n + y_{n+1}}{2}\right). \tag{4.2}$$

It is the simplest scheme that conserves quadratic first integrals. The scheme has a second-order approximation of the differential equations.

Applied to the system (4.1), the midpoint rule gives the numerical scheme

$$\frac{\mathbf{Q}^{j+1} - \mathbf{Q}^j}{h} = \frac{1}{4}\frac{\mathbf{P}^j + \mathbf{P}^{j+1}}{2}, \tag{4.3}$$

$$\frac{\mathbf{P}^{j+1} - \mathbf{P}^j}{h} = -2A\frac{\mathbf{Q}^j + \mathbf{Q}^{j+1}}{2}, \tag{4.4}$$

$$\frac{t^{j+1} - t^j}{h} = \left|\frac{\mathbf{Q}^j + \mathbf{Q}^{j+1}}{2}\right|^2, \tag{4.5}$$

which permits an explicit implementation. First, equations (4.3) and (4.4) can be solved for $(\mathbf{Q}^{j+1}, \mathbf{P}^{j+1})$. After that, the new physical time can be calculated. To find physical variables $(\mathbf{q}, \mathbf{p})$ we use the transformation (2.5).

The proposed discretization has all first integrals of Kepler motion. However, it has only second order of approximation. In the next section, we will consider how one can improve the order of the midpoint rule scheme using the modified differential equations.

4.2. Modified differential equations

An approach for the construction of high-order numerical integrators which preserve structural properties of the differential equations was recently developed in [2, 3]. Let us briefly present this framework.

We consider an initial value problem

$$\dot{y} = f(y), \qquad y(0) = y_0 \tag{4.6}$$

and a numerical one-step integrator $y_{n+1} = \Phi_{f,h}(y_n)$. We search for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + \cdots, \qquad z(0) = y_0 \tag{4.7}$$

such that the numerical solution $\{z_n\}$ of the method applied with step size h to (4.7) yields formally the exact solution of the original differential equation (4.6), i.e. $z_n = y(nh)$ for $n = 0, 1, 2, \ldots$. The coefficient functions $f_j(z)$ can be computed recursively.

Having found first functions $f_j(z)$, one can use the truncation

$$\dot{z} = f_h^{[r]}(z) = f(z) + hf_2(z) + \cdots + h^{r-1} f_r(z) \tag{4.8}$$

of the modified differential equation corresponding to $\Phi_{f,h}(y)$. A numerical method $z_{n+1} = \Phi_{f_h^{[r]},h}(z_n)$ approximates the solution of (4.6) with order r. It was called a *modifying integrator* because it applies to the modified vector field $f_h^{[r]}$ instead of $f(y)$.

Truncation $f_h^{[5]}$ of the modifying vector field corresponding to the implicit midpoint rule (4.2) was found in [2, 5]:

$$\begin{aligned} f_h^{[5]} = f &+ \frac{h^2}{12}\left(-f'f'f + \frac{1}{2}f''(f,f)\right) + \frac{h^4}{120}\left(f'f'f'f'f - f''(f,f'f'f) + \frac{1}{2}f''(f'f,f'f)\right) \\ &+ \frac{h^4}{120}\left(-\frac{1}{2}f'f'f''(f,f) + f'f''(f,f'f) + \frac{1}{2}f''(f,f''(f,f))\right. \\ &\left. - \frac{1}{2}f^{(3)}(f,f,f'f)\right) + \frac{h^4}{80}\left(-\frac{1}{6}f'f^{(3)}(f,f,f) + \frac{1}{24}f^{(4)}(f,f,f,f)\right). \end{aligned}$$

The midpoint rule (4.2) applied to $\dot{z} = f_h^{[5]}(z)$ yields a numerical approximation of order 6.

Let us note that if we drop the terms with h^4, we will obtain a modified vector field

$$f_h^{[3]} = f + \frac{h^2}{12}\left(-f'f'f + \frac{1}{2}f''(f,f)\right),$$

which provides us with a numerical method of order 4.

For the equations of the harmonic oscillator (4.1) we obtain the following modified vector fields:

$$f_h^{[3]} = \begin{pmatrix} \frac{1}{4}\left(1 + \frac{h^2}{24}A\right)\mathbf{P} \\ -2A\left(1 + \frac{h^2}{24}A\right)\mathbf{Q} \\ \left(1 + \frac{h^2}{12}A\right)|\mathbf{Q}|^2 + \frac{h^2}{192}|\mathbf{P}|^2 \end{pmatrix} \tag{4.9}$$

and

$$f_h^{[5]} = \begin{pmatrix} \frac{1}{4}\left(1 + \frac{h^2}{24}A + \frac{h^4}{480}A^2\right)\mathbf{P} \\ -2A\left(1 + \frac{h^2}{24}A + \frac{h^4}{480}A^2\right)\mathbf{Q} \\ \left(1 + \frac{h^2}{12}A + \frac{h^4}{160}A^2\right)|\mathbf{Q}|^2 + \left(\frac{h^2}{192} + \frac{h^4}{1920}A\right)|\mathbf{P}|^2 \end{pmatrix}. \tag{4.10}$$

Applying the midpoint rule to the modified vector fields $f_h^{[3]}$ and $f_h^{[5]}$, we obtain numerical schemes of orders 4 and 6. These schemes can be presented in the form

$$\begin{aligned}
&\frac{\mathbf{Q}^{j+1}-\mathbf{Q}^j}{h} = \frac{1}{4}a(h)\frac{\mathbf{P}^{j+1}+\mathbf{P}^j}{2},\\
&\frac{\mathbf{P}^{j+1}-\mathbf{P}^j}{h} = -2Ab(h)\frac{\mathbf{Q}^{j+1}+\mathbf{Q}^j}{2},\\
&\frac{t^{j+1}-t^j}{h} = \alpha(h)\left|\frac{\mathbf{Q}^j+\mathbf{Q}^{j+1}}{2}\right|^2 + \beta(h)\left|\frac{\mathbf{P}^j+\mathbf{P}^{j+1}}{2}\right|^2.
\end{aligned} \tag{4.11}$$

Here

$$a(h) = b(h) = \left(1+\frac{h^2}{24}A\right), \qquad \alpha(h) = \left(1+\frac{h^2}{12}A\right), \qquad \beta(h) = \frac{h^2}{192}$$

provide the fourth-order method and

$$\begin{aligned}
&a(h) = b(h) = \left(1+\frac{h^2}{24}A+\frac{h^4}{480}A^2\right),\\
&\alpha(h) = \left(1+\frac{h^2}{12}A+\frac{h^4}{160}A^2\right), \qquad \beta(h) = \left(\frac{h^2}{192}+\frac{h^4}{1920}A\right)
\end{aligned}$$

give the sixth-order method. Both methods conserve all first integrals of the Kepler motion (2.7), (3.3) and (3.4).

4.3. The exact integrator

The form of the modified vector fields (4.9) and (4.10) suggests to look for higher order modified vector fields of the form

$$f_h = \begin{pmatrix} \frac{1}{4}a(h)\mathbf{P} \\ -2Ab(h)\mathbf{Q} \\ \alpha(h)|\mathbf{Q}|^2+\beta(h)|\mathbf{P}|^2 \end{pmatrix}, \tag{4.12}$$

where $a(0)=1, b(0)=1, \alpha(0)=1$ and $\beta(0)=0$. The modification of the vector field is different from a time rescaling since the new term $\beta(h)|\mathbf{P}|^2$ appears in the last equation of the system.

Application of the midpoint rule to the modified equations gives us the numerical scheme (4.11). Using Taylor series expansions for function values present in the scheme equations, we can find closed form solutions for the modifying coefficients

$$\begin{aligned}
&a(h) = b(h) = \frac{c_1\left(\frac{Ah^2}{8}\right)}{c_0\left(\frac{Ah^2}{8}\right)}, \qquad \alpha(h) = \frac{1+c_1\left(\frac{Ah^2}{2}\right)}{2c_0^2\left(\frac{Ah^2}{8}\right)},\\
&\beta(h) = \frac{1-c_1\left(\frac{Ah^2}{2}\right)}{16Ac_0^2\left(\frac{Ah^2}{8}\right)} \quad \text{for} \quad A\neq 0, \qquad \beta(h) = \frac{h^2}{192} \quad \text{for} \quad A=0,
\end{aligned}$$

where $c_0(z)$ and $c_1(z)$ are Stumpff functions defined as

$$c_n(z) = \sum_{k=0}^{\infty}(-1)^k\frac{z^k}{(2k+n)!}, \quad n=0,1,2,\ldots. \tag{4.13}$$

These functions were introduced by Stumpff [16] for uniform treatment of the Kepler motion. Let us remark that functions $\alpha(h)$ and $\beta(h)$ are related as

$$\alpha(h) + 8A\beta(h) = \frac{1}{c_0^2\left(\frac{Ah^2}{8}\right)}.$$

Stumpff functions $c_n(z)$ can be related to trigonometric or hyperbolic functions depending on the values of z. In particular,

$$c_0(x^2) = \cos x, \qquad c_0(-x^2) = \cosh x,$$
$$c_1(x^2) = \frac{\sin x}{x}, \qquad c_1(-x^2) = \frac{\sinh(x)}{x}.$$

Therefore, we can consider the following cases corresponding to the different types of motion:

(1) Elliptic Kepler motion, $A = 2\omega^2 > 0$:

$$a(h) = b(h) = \frac{\tan\left(\frac{\omega h}{2}\right)}{\frac{\omega h}{2}}, \tag{4.14}$$

$$\alpha(h) = \frac{1 + \frac{\sin(\omega h)}{\omega h}}{1 + \cos(\omega h)}, \qquad \beta(h) = \frac{1}{8A}\frac{1 - \frac{\sin(\omega h)}{\omega h}}{1 + \cos(\omega h)}. \tag{4.15}$$

(2) Hyperbolic motion, $A = -2\omega^2 < 0$:

$$a(h) = b(h) = \frac{\tanh\left(\frac{\omega h}{2}\right)}{\frac{\omega h}{2}}, \tag{4.16}$$

$$\alpha(h) = \frac{1 + \frac{\sinh(\omega h)}{\omega h}}{1 + \cosh(\omega h)}, \qquad \beta(h) = \frac{1}{8A}\frac{1 - \frac{\sinh(\omega h)}{\omega h}}{1 + \cosh(\omega h)}. \tag{4.17}$$

(3) Parabolic motion, $A = 0$:

$$a(h) = b(h) = \alpha(h) = 1, \qquad \beta(h) = \frac{h^2}{192}. \tag{4.18}$$

These coefficients can be obtained from the coefficients of the two other cases in the limit $A \to 0$.

The proposed formulae give the exact solution of the Kepler motion. First terms of the Taylor series of the coefficients $a(h)$, $b(h)$, $\alpha(h)$ and $\beta(h)$ match the modifying factors of the vector fields (4.9) and (4.10).

It is interesting to note that there is a restriction on the time step in the case of elliptic motion

$$\omega h < \pi. \tag{4.19}$$

The time step cannot exceed half of the period. Otherwise, the scheme (4.11) might be undefined ($a(h) = b(h) = \infty$) and the time transformation equation gives the wrong value of t^{j+1}.

5. Numerical test

For a numerical experiment we consider the elliptic Kepler motion with initial conditions $\mathbf{q}_0 = (0.8, 0.6, 0)^T$ and $\mathbf{p}_0 = (0, 1, 0.5)^T$ on the time interval $[0, 100]$. First, we use the

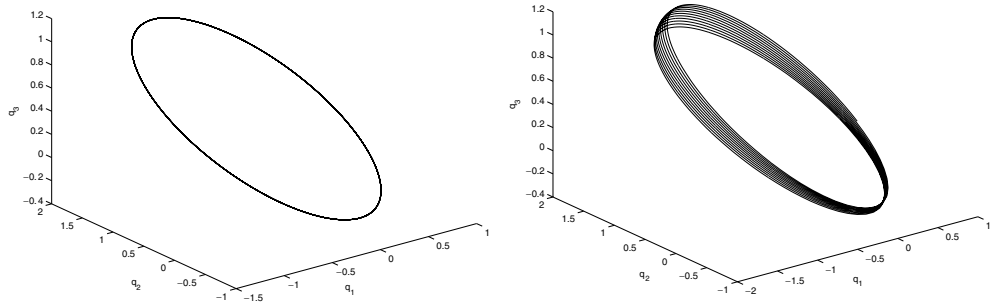

Figure 1. Numerical solution of the Kepler problem by the exact integrator (left plot) and the midpoint rule (right plot).

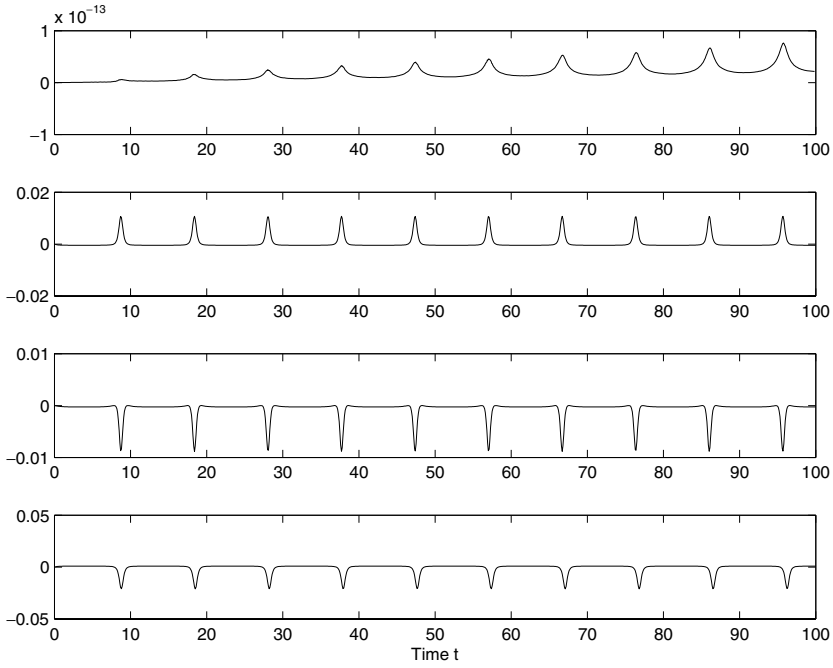

Figure 2. The errors in the Hamiltonian $|H(\mathbf{q},\mathbf{p}) - H(\mathbf{q}_0,\mathbf{p}_0)|$ for the exact integrator, the midpoint rule, the Störmer–Verlet method and the trapezoidal rule (from top to bottom).

exact integrator—the numerical scheme (4.11) with modifying coefficients given by (4.14) and (4.15). The computation with fictitious time step $\Delta s = h = 0.1$ shows that the numerical method does not distort the elliptical orbit (figure 1, left plot). The method used 746 steps to go through the physical time interval [0, 100].

For comparison we choose the midpoint rule (4.2), the Störmer–Verlet method

$$\mathbf{p}_{n+1/2} = \mathbf{p}_n - \frac{h}{2}\frac{K^2}{|\mathbf{q}_n|^3}\mathbf{q}_n$$
$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\mathbf{p}_{n+1/2}$$
$$\mathbf{p}_{n+1} = \mathbf{p}_{n+1/2} - \frac{h}{2}\frac{K^2}{|\mathbf{q}_{n+1}|^3}\mathbf{q}_{n+1}$$

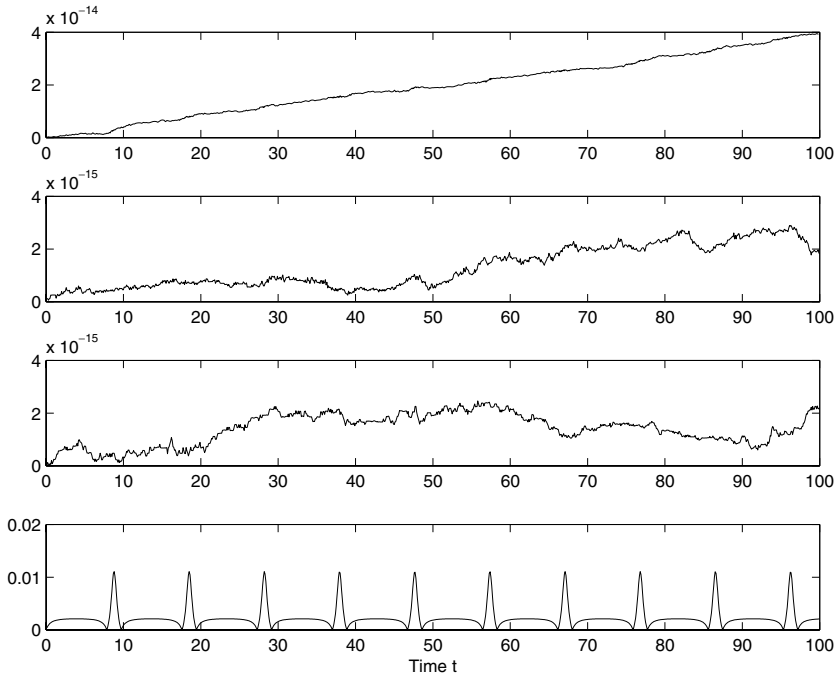

Figure 3. The errors in the angular momentum $|\mathbf{L}(\mathbf{q}, \mathbf{p}) - \mathbf{L}(\mathbf{q}_0, \mathbf{p}_0)|$ for the exact integrator, the midpoint rule, the Störmer–Verlet method and the trapezoidal rule (from top to bottom).

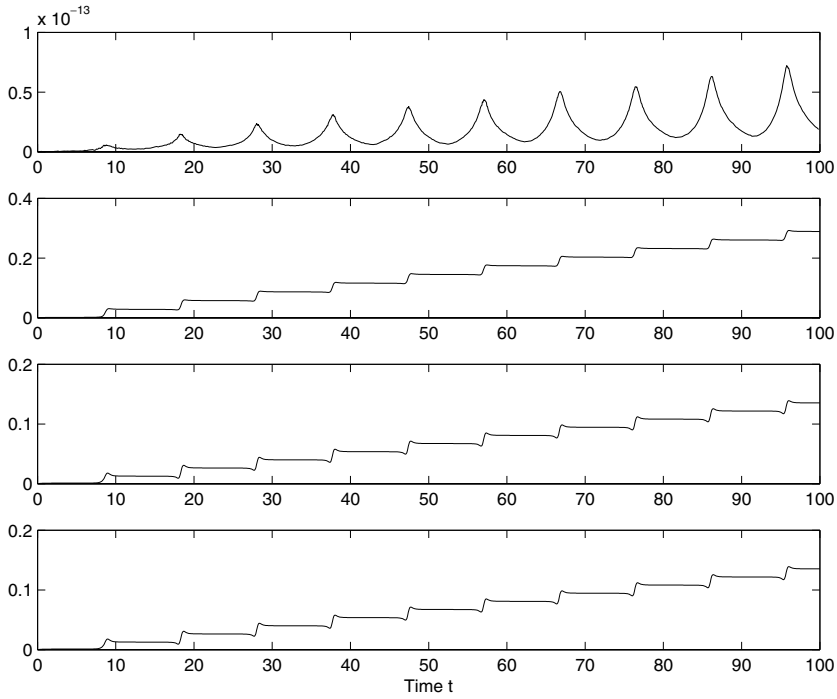

Figure 4. The errors in Runge–Lenz vector $|\mathbf{A}(\mathbf{q}, \mathbf{p}) - \mathbf{A}(\mathbf{q}_0, \mathbf{p}_0)|$ for the exact integrator, the midpoint rule, the Störmer–Verlet method and the trapezoidal rule (from top to bottom).

and the trapezoidal rule

$$y_{n+1} = y_n + \frac{h}{2}(f(y_n) + f(y_{n+1}))$$

applied to the Kepler motion (2.1) with time step $\Delta t = 0.1$ (1000 steps to cover the interval [0, 100]). The midpoint rule and the Störmer–Verlet method are symplectic [4]. All the three methods are of second order. We will not consider higher order methods because we are interested in qualitative properties of numerical integrators.

Conservation of the Hamiltonian, the angular momentum and Runge–Lenz vector is presented in figures 2–4, respectively. The exact integrator preserves all first integrals up to round-off errors. For the other methods we observe the following: the angular momentum is preserved by the midpoint rule and the Störmer–Verlet method, but not by the trapezoidal rule. The Hamiltonian is not conserved (the midpoint rule and the Störmer–Verlet method conserve approximate Hamiltonian functions because they are symplectic [4]). More importantly, Runge–Lenz vector is not preserved in the numerical integration. Runge–Lenz vector points along the major axis of the conic section determined by the elliptical orbit, its magnitude determining the eccentricity [17]. Non-conservation of Runge–Lenz vector causes the precession effect clearly seen in the right plot of figure 1 on the example of the midpoint rule.

6. Conclusion

A discretization of the three-dimensional Kepler motion based on the midpoint rule applied to the regularized equations, i.e. the equations of the four-dimensional oscillator, was proposed in [11]. In the present paper we improved this discretization scheme using modified vector fields. It allows us to find discretizations of orders 4 and 6 as well as to find the exact integrator of the Kepler motion. It is interesting to note that higher order is obtained more or less for free, by introducing scalar factors.

The numerical integrator of the harmonic oscillator supplemented by the time transformation equation (4.1) can be used for a harmonic oscillator of any dimension. We considered the three-dimensional Kepler problem, which is related to the four-dimensional harmonic oscillator by Kustaanheimo–Stiefel transformation. However, the three-dimensional Kepler problem can be linked to the four-dimensional harmonic oscillator by a much wider family of L-transformations [15]. The two-dimensional Kepler problem is related to the two-dimensional harmonic oscillator by Levi-Civita transformation [16]. The five-dimensional Kepler is linked to the eight-dimensional oscillator [12–14]. In [6, 8] it was proved that the Kepler problem in dimension $q + 1$ can be converted into a harmonic oscillator system in dimension N via a generalization of the Kustaanheimo–Stiefel transformation if and only if $N = 2q$ and $q = 2^h$, $h = 0, 1, 2, \ldots$. For all these cases a higher order or exact integrator of the harmonic oscillator presented here can be used to solve the corresponding Kepler problem.

The proposed numerical integrators can also be used in splitting methods which include two-body problems as components. For example, for three-body and many-body problems one can use the exact integrator to construct numerical schemes which have only errors introduced by the splitting.

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