An asynchronous leap-frog method

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A second order explicit one-step numerical method for the initial value problem of the general ordinary differential equation is proposed. It is obtained by natural modifications of the well-known leap-frog method, which is a second order, two-step explicit method. According to the latter method, the input data for an integration step are two system states which refer to different times (we employ the terminology of dynamical systems). The usage of two states instead of a single one can be seen as the reason for the robustness of the method. Since the time step size thus is part of the step input data, it is complicated to change this size during the computation of a discrete trajectory. This is a serious drawback when one needs to implement automatic time step control.

The proposed modification transforms one of the two input states into a velocity and thus gets rid of the time step dependency in the step input data. For these new step input data, the leap-frog method gives a unique prescription how to evolve them stepwise.

The method is exemplified with the equation of motion of a one-dimensional non-linear oscillator describing the radial motion in the Kepler problem. For this equation the modified leap-frog method is shown to be significantly more accurate than the original method.

As a result, we have a second order explicit method that, just as the simple explicit Euler method, needs only one evaluation of the right-hand side of the differential equation per integration step, and allows to change the time step without any additional computational burden after each integration step. Unlike the Euler method and the explicit Runge-Kutta methods it is robust in the sense that it allows us to reliably model the dynamics of a wide variety of physical systems over extended periods of time.

1 Introduction

We consider the initial value problem of the general ordinary differential equation

$$\dot{\psi}(t) = F(t, \psi(t)) \tag{1}$$

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for a time-dependent quantity ψ which takes values in a real finite-dimensional vector space $\mathcal{H}$. Here F is a function $\mathbb{R} \times \mathcal{H} \to \mathcal{H}$ [1] . Equations of this kind arise from ordinary differential equations of finite order and from discrete approximations to partial differential equations like the time-dependent Schrödinger equation or Maxwell's equations. The main example here will be $\mathcal{H} = \mathbb{R}^2$

$$\begin{aligned} F &: \mathbb{R} \times \mathbb{R}^2 \to \mathbb{R}^2 \\ &(t,(x,v)) \mapsto \left(v, \frac{1}{x^2}\left(\frac{1}{x} - 1\right)\right) \end{aligned} \tag{2}$$

which describes the radial motion in the Kepler problem. This is a convenient test problem since its initial value problem can be solved directly without making use of time stepping by solving Kepler's famous transcendental equation. Since it is equivalent to a Hamiltonian problem, there are many integration methods available (e.g. [6]) to compare with. More demanding applications of the method, in which $\mathcal{H}$ is a higher-dimensional space, are considered in [12] and presented in [13].

The *computational initial value problem* associated with this equation (1) asks for an algorithm which determines for each $\mathbb{R}$-valued increasing list $t_0, t_1, \ldots, t_n$ and each value $\psi_0 \in \mathcal{H}$ (the initial value) a $\mathcal{H}$-valued list $\psi_1, \ldots, \psi_n$ such that the $\mathbb{R} \times \mathcal{H}$-valued list $(t_0, \psi_0), (t_1, \psi_1), \ldots, (t_n, \psi_n)$ is a reasonable approximation to a solution curve $t \mapsto \psi(t)$, $\psi(t_0) = \psi_0$, of the differential equation (1) whenever the regularity properties of F suffice for determining such a curve, and the gaps between adjacent $t-$values are small enough. If such an algorithm works only for equidistant time lists (for which $t_i - t_{i-1}$ is independent of i by definition) it is said to be *synchronous* and otherwise it is said to be *asynchronous*. Asynchronous algorithms may be developed into adaptive ones, which adjust their step size $t_{i+1} - t_i$ to the size (according to a suitable notion of size in $\mathcal{H}$) of $F(t_i, \psi_i)$. For a $\mathbb{R}$-valued function F that depends on its second argument trivially, the initial value problem is simply the problem of computing the definite integral. It is straightforward and instructive to specialize the proposed algorithms to this simplified concrete situation.

Starting from the well-known leap-frog algorithm, the present article develops and analyzes an economic and robust asynchronous solution of the computational initial value problem associated with (1). Section 2 recalls the leap-frog method, and Section 3 carries out the general development of the new asynchronous algorithm. Section 4 will apply this integration method and related methods to the differential equation defined by (2).

[1] As is well-known, one may increase formal simplicity by transforming away the explicit t-dependence of the right-hand side of this equation, thus rendering it *autonomous*. However, I refrain from assuming autonomy, since the algorithms to be considered should apply to time-dependent real-world problems directly, without a need to transform them into autonomous ones.

2 The leap-frog method

A marvelously simple synchronous solution algorithm for the computational initial value problem of (1) is the *leap-frog method* or *explicit midpoint rule*, see e.g. [7], eq. (3.3.11). It seems to be the first method that has been successfully applied to the initial value problem of the time-dependent Schrödinger equation (see [2] and the citation of this work in [3]). It is most conveniently considered as the map

$$\begin{aligned} \mathcal{L} : (\mathbb{R}\times\mathcal{H})\times(\mathbb{R}\times\mathcal{H}) &\to (\mathbb{R}\times\mathcal{H})\times(\mathbb{R}\times\mathcal{H}) \\ ((t_0,\psi_0),(t_1,\psi_1)) &\mapsto ((t_1,\psi_1),(t_2,\psi_2)) \,, \end{aligned} \tag{3}$$

where

$$\begin{aligned} t_2 &:= 2t_1 - t_0 \,, \\ \psi_2 &:= \psi_0 + (t_2 - t_0)\, F(t_1,\psi_1) \,. \end{aligned} \tag{4}$$

The equivalent form

$$\begin{aligned} \frac{t_0+t_2}{2} &= t_1 \,, \\ \frac{\psi_2-\psi_0}{t_2-t_0} &= F(t_1,\psi_1) \end{aligned} \tag{5}$$

of these equations, together with equation (1), makes the reasons for choosing them evident:

$$F(t_1,\psi(t_1)) = \dot{\psi}(t_1) = \frac{\psi(t_2)-\psi(t_0)}{t_2-t_0} + O((t_2-t_0)^3) \,. \tag{6}$$

Iterating the map $\mathcal{L}$ determines a *leap-frog trajectory*, $((t_j,\psi_j))_{j\in\mathbb{N}}$ if (t_0,ψ_0) and (t_1,ψ_1) are given:

$$(t_{i+1},\psi_{i+1}) = \pi_2(\mathcal{L}((t_{i-1},\psi_{i-1}),(t_i,\psi_i))) = \pi_2(\mathcal{L}^i((t_0,\psi_0),(t_1,\psi_1))) \,, \tag{7}$$

where π_2 is the canonical projection to the second component of a pair. According to the initial value problem we are given t_0, t_1 (which determines, due to the assumed synchronicity, all further t-values) and ψ_0. For starting iteration (7) we need also ψ_1. This has to be added in a way consistent with (1), e. g. by employing the *explicit Euler rule*

$$\psi_1 := \psi_0 + (t_1 - t_0)\, F(t_0,\psi_0) \tag{8}$$

or a more accurate method (with the same order of error as (6)) such as the implicit trapezoidal rule, which gives the iterative limit definition

$$\psi_1^{(i+1)} := \psi_0 + (t_1 - t_0)\,\frac{F(t_0,\psi_0) + F(t_1,\psi_1^{(i)})}{2} \tag{9}$$

for ψ_1 starting with $\psi_1^{(0)} := \psi_0$, for which (8) is the result of the first iteration step.

We have here an interesting situation: Even for arbitrary ψ_1, the iteration (7) can be used to define a leap-frog trajectory. This then is typically a zig-zag line which tends to wiggle around a trajectory of differential equation (1) and initial data (t_0, ψ_0). The closer ψ_1 is set to this trajectory (e.g. by (8) or, better, (9)) the lower the zig-zag amplitude will be. The map (3), considered as a discrete dynamical system, is thus related to the continuous dynamical system associated with (1) in a more sophisticated manner than usual: The state space of the discrete system is $(\mathbb{R} \times \mathcal{H}) \times (\mathbb{R} \times \mathcal{H})$ since only this set allows the leap-frog method to be defined as a map of states into states. Only a subset of this state space (e. g. the one given by (8)) corresponds to potential initial states of the continuous system (1).

Equation (7) defines ψ_i for arbitrarily large i, whereas equation (1) may drive a trajectory in finite time into infinity. In such cases the size of the numbers involved in applying mapping $\mathcal{L}$ repeatedly will grow above the size which can be handled with realistic computational resources (which include computation time). Such exploding situations also occur if the time step size is too large for the differential equation under consideration.

It might be instructive to discuss the close correspondence of this algorithm to the leap-frog game (Bockspringen in German). In the variant which is of interest here, there are two participants A and B in this nice dynamical sportive exercise. There is an intended direction of motion and the participants line up in this direction, B standing a few meters in front of A. This is the initial condition, which corresponds in the algorithm to the ordered input $((t_0, \psi_0) \cong A, (t_1, \psi_1) \cong B)$. After two or three energetic steps, A jumps over B, supporting himself with both palms on the shoulders of B, thereby receiving from B a smooth kick which makes A fly to a position sufficiently far in front of B that now the action can continue with the roles of A and B reversed, then reversed again, and so forth. The kick which A receives from B corresponds to adding the term $(t_2 - t_0) F(t_1, \psi_1)$ (associated with B) to the term ψ_0, which is associated with A. The result of this addition is ψ_2, which corresponds again to A, but at a new position. By continuation we create terms $\psi_3, \psi_4 \ldots$. All terms with even index correspond to A, and those with odd index to B. The index grows with the progress along the intended direction of motion.

The algorithm can easily be shown to be *reversible*: Let the operator of motion reversal be defined as

$$\begin{aligned} \mathcal{T} \,:\, (\mathbb{R} \times \mathcal{H}) \times (\mathbb{R} \times \mathcal{H}) &\to (\mathbb{R} \times \mathcal{H}) \times (\mathbb{R} \times \mathcal{H}) \\ ((t_0, \psi_0), (t_1, \psi_1)) &\mapsto ((t_1, \psi_1), (t_0, \psi_0)) \end{aligned} \tag{10}$$

then we easily verify

$$\mathcal{L} \circ \mathcal{T} \circ \mathcal{L} = \mathcal{T} \,, \quad \mathcal{T} \circ \mathcal{T} = \mathbf{1} \tag{11}$$

from which one concludes that $\mathcal{L}$ is invertible, with the inverse given by $\mathcal{T} \circ \mathcal{L} \circ \mathcal{T}$. This allows us to reconstruct from the last two data $((t_{n-1}, \psi_{n-1}), (t_n, \psi_n))$ of a leap-frog trajectory all previous components (t_k, ψ_k), $k < n - 1$,

$$(t_k, \psi_k) = \pi_2(\mathcal{T} \mathcal{L}^{n-k} \mathcal{T}((t_{n-1}, \psi_{n-1}), (t_n, \psi_n))) \,. \tag{12}$$

The dynamical system defined by (1) needs not to be reversible. Then, executing (12) may involve numbers which transcend the limitations of real-word computations.

If we would like to change time step size after having arrived at some state $((t_{p-1},\psi_{p-1}),(t_p,\psi_p)$ to value τ, we may start a new synchronous trajectory with the state

$$((t_p,\psi_p),(t_p+\tau,\psi_p+\tau F(t_p,\psi_p)) \tag{13}$$

or a more accurate form which also involves ψ_{p-1} (which equation (13) simply forgets).

3 An asynchronous version of the leap-frog method

What I intend here, is to modify the leap-frog method in a way that no tradeoffs between simplicity and accuracy are involved when we start a trajectory or when we change the time step size. A further aim is to preserve the computational simplicity of the algorithm. In a narrower framework than (1) this modified leap-frog method has been introduced in [12] and applied to time-dependent Hartree equations in [13].

We consider four consecutive components of a leap-frog trajectory of (1)

$$(t_k,\psi_k)\,,\quad (t_{k+1},\psi_{k+1})\,,\quad (t_{k+2},\psi_{k+2})\,,\quad (t_{k+3},\psi_{k+3}) \tag{14}$$

and let τ be the time step. Then we define velocity-like quantities ϕ as follows:

$$\phi_k := \frac{\psi_{k+1}-\psi_k}{\tau}\,,\quad \phi_{k+1} := F(t_{k+1},\psi_{k+1})\,,\quad \phi_{k+2} := \frac{\psi_{k+2}-\psi_{k+1}}{\tau}\,. \tag{15}$$

From this definition and from (5) we obtain

$$\frac{\phi_k+\phi_{k+2}}{2} = \frac{\psi_{k+2}-\psi_k}{2\tau} = F(t_{k+1},\psi_{k+1}) = \phi_{k+1}\,. \tag{16}$$

These equations allow us to compute $(t_{k+2},\psi_{k+2},\phi_{k+2})$ if (t_k,ψ_k,ϕ_k) and τ are given:

$$\begin{aligned} t_{k+1} &= t_k+\tau\,,\quad \psi_{k+1}=\psi_k+\tau\phi_k\,,\quad \phi_{k+1}=F(t_{k+1},\psi_{k+1})\,,\\ t_{k+2} &= t_{k+1}+\tau\,,\\ \psi_{k+2} &= \psi_k+2\tau\phi_{k+1}\,,\\ \phi_{k+2} &= \frac{\psi_{k+2}-\psi_{k+1}}{\tau}\,. \end{aligned} \tag{17}$$

Equation (16) allows us to give the last two equations of (17) a more symmetrical form:

$$\begin{aligned} \phi_{k+2} &= 2\phi_{k+1}-\phi_k\,,\\ \psi_{k+2} &= \psi_{k+1}+\tau\phi_{k+2}\,. \end{aligned} \tag{18}$$

The association $(t_k,\psi_k,\phi_k) \mapsto (t_{k+2},\psi_{k+2},\phi_{k+2})$ can now be considered a mapping $\mathbb{R}\times\mathcal{H}\times\mathcal{H} \to \mathbb{R}\times\mathcal{H}\times\mathcal{H}$ which depends on the total time step 2τ and thus will be denoted $\mathcal{A}_{2\tau}$. The data $(t_{k+1},\psi_{k+1},\phi_{k+1})$ are intermediary (or temporary) with respect to this mapping. This mapping may be iterated: Let us apply $\mathcal{A}_{2\tau}$ to $(t_{k+2},\psi_{k+2},\phi_{k+2})$. The

result may be denoted $(t_{k+4}, \chi_{k+4}, \kappa_{k+4})$ and the intermediary data as $(t_{k+3}, \chi_{k+3}, \kappa_{k+3})$. Although the formulas which define $\mathcal{A}_{2\tau}$ are all consequences of the leap-frog law, the iteration of $\mathcal{A}_{2\tau}$ does not exactly continue the leap-frog trajectory. Actually, we have $\chi_{k+3} = \psi_{k+3}$ only up to terms of order τ^2:

$$\begin{aligned} \psi_{k+3} &= \psi_{k+1} + 2\tau F(t_{k+2}, \psi_{k+2}) \,, \\ \chi_{k+3} &= \psi_{k+2} + \tau\phi_{k+2} = 2\psi_{k+2} - \psi_{k+1} = \psi_{k+1} + 2(\psi_{k+2} - \psi_{k+1}) \end{aligned} \tag{19}$$

and thus

$$(\psi_{k+3} - \chi_{k+3})/2 = \tau F(t_{k+2}, \psi_{k+2}) + \psi_{k+1} - \psi_{k+2} = O(\tau^2) \,. \tag{20}$$

The reason for this behavior lies in the fact that in going from the normal leap-frog algorithm to the asynchronous one we change the notion of system state. The new state notion is more conventional in so far as it refers to a single point in time, whereas the normal leap-frog state consists of data that refer to two points in time. If we are given, according to the initial value problem of (1), the initial values t_0 and ψ_0, the augmentation to a full state according to the new state notion is straightforward and does not depend on the next time value t_1. It is simply given by:

$$\phi_0 := F(t_0, \psi_0) \,. \tag{21}$$

From (t_0, ψ_0, ϕ_0) and a list $(t_1, t_2, \ldots)$ we generate a discrete trajectory

$$((t_0, \psi_0, \phi_0), (t_1, \psi_1, \phi_1), (t_2, \psi_2, \phi_2), \ldots)$$

by the iteration of mappings $\mathcal{A}_{2\tau}$ defined earlier

$$(t_{i+1}, \psi_{i+1}, \phi_{i+1}) := \mathcal{A}_{h_i}(t_i, \psi_i, \phi_i) \,, \quad h_i := t_{i+1} - t_i \,. \tag{22}$$

For convenience, let us rewrite the definition of $\mathcal{A}$ in fully explicit terms: For each $h \in \mathbb{R}$ the mapping

$$\begin{aligned} \mathcal{A}_h \,:\, \mathbb{R} \times \mathcal{H} \times \mathcal{H} &\to \mathbb{R} \times \mathcal{H} \times \mathcal{H} \\ (t, \psi, \phi) &\mapsto (\underline{t}, \underline{\psi}, \underline{\phi}) \end{aligned} \tag{23}$$

can be seen from (17) and (18) to be defined by the following chain of formulas:

$$\begin{aligned} \tau &:= \frac{h}{2} \,, \\ t' &:= t + \tau \,, \\ \psi' &:= \psi + \tau\phi \,, \\ \phi' &:= F(t', \psi') \,, \\ \underline{\phi} &:= 2\phi' - \phi \,, \\ \underline{\psi} &:= \psi' + \tau\underline{\phi} = \psi + 2\tau\phi' \,, \\ \underline{t} &:= t' + \tau \,, \end{aligned} \tag{24}$$

where the leap-frog midpoint state data t', ϕ', ψ' appear only as intermediary quantities that help to give the algorithm an elegant form. This corresponds to equation (8) in [12] but is more general since it does not assume the special form of F that was considered there.

Obviously $\mathcal{A}_0$ is the identity map and $\mathcal{A}$ is *reversible* in the sense that for all $h \in \mathbb{R}$ we have — by a non-trivial cancellation of terms — the equation

$$\mathcal{A}_{-h} \circ \mathcal{A}_h = \mathcal{A}_0 \tag{25}$$

which implies that each of the maps $\mathcal{A}_h$ is invertible, as is the product of arbitrarily many such mappings. As mentioned already for the corresponding situation of the normal leap-frog method, this invertibility of all discrete evolution maps does not imply that the dynamical system defined by (1) has invertible evolution maps. The reversion of discrete trajectories is discussed in [12] subsequent to equation (10). It is to be noted that there is no motion reversion operator comparable to (10). One may be tempted to try $\mathcal{T} : (t, \psi, \phi) \mapsto (-t, \psi, -\phi)$, but this fails to satisfy $\mathcal{A}_h \circ \mathcal{T} \circ \mathcal{A}_h = \mathcal{T}$ which would correspond to (11).

For a given state (t, ψ, ϕ), which determines a discrete trajectory by successive application of $\mathcal{A}_h$, one may also define a normal leap-frog trajectory starting from the leap-frog state $(t - \tau, \psi - \tau\phi), (t, \psi)$, $\tau := \frac{h}{2}$, by successive application of $\mathcal{L}$. Therefore, in a sense, the role of ϕ is to memorize information from the foregoing integration step in addition to state data ψ. Also multi-step methods and predictor-corrector methods improve computational economy by memorizing results from antecedent integration steps. But they do so directly, by memorizing a list of previous states, each associated with the time of its validity. Letting information from antecedent integration steps propagate in the form of derived quantities, such as our ϕ-data, is the clue of the present method.

To consider the usage of such derived quantities is most directly motivated by the desire to obtain an asynchronous method, as the matter is presented here. Actually, my motivation was a different one, namely to extend the well-behaved integrator (32) for differential equations (31) of second order to the more general situation (1). The close relation of the arising method to the leap-frog method became apparent only later.

4 The Kepler oscillator as a test example

Computing the motion of a point mass in the gravitation field of a stationary point mass is what the *Kepler problem* is about. The radial motion in elliptic Kepler orbits (as opposed to parabolic and hyperbolic ones) is oscillatory and can be viewed as the motion of a one-dimensional oscillator which deserves interest as a mechanical example system. Unlike other non-linear example oscillators such as the *Duffing oscillator* and the *Van der Pol oscillator* this system seems to be anonymous. The self-suggesting name *Kepler oscillator* can be found in [11] for this system and will be used in the present article. In the literature this name is, however, more often used for the harmonic oscillator

which is related to the Kepler problem by a regularizing transformation, known as the *KS transformation*.

As is well known (e.g. [1], equation (3-14)) the radial Kepler motion is governed by the differential equation

$$m\ddot{r} = -\frac{\partial}{\partial r}\left(-\frac{GMm}{r} + \frac{L^2}{2mr^2}\right) \tag{26}$$

in which L is the constant angular momentum of mass m relative to the position of the space-fixed mass M. Of course, r is the distance between these two masses and G is the constant of gravity. Restricting ourselves to orbits with non-vanishing L and by selecting suitable units of time, mass, and length, we get for the quantities m, GM, and L the common numerical value 1. Writing x for the numerical value of r and v for the numerical value of $\dot{r}$ we get

$$\dot{x} = v\,, \quad \dot{v} = -\frac{\partial}{\partial x}\left(-\frac{1}{x} + \frac{1}{2x^2}\right) = \frac{1}{x^2}\left(\frac{1}{x} - 1\right) \tag{27}$$

which is the differential equation determined by (2) and also is (since, due to $m = 1$, v is the momentum) the system of canonical equations associated with the Hamiltonian

$$H(v,x) := T(v) + V(x) := \frac{1}{2}v^2 + \frac{1}{x}\left(\frac{1}{2x} - 1\right)\,. \tag{28}$$

This quantity is known to be constant on each orbit. Since, as Figure 1 shows, V attains an absolute minimum at $x = 1$: $V(1) = -\frac{1}{2}$ we have $H(v,x) \geq H(0,1) = -\frac{1}{2}$. We consider only states for which $H(v,x) < 0$ and thus $x > \frac{1}{2}$. These correspond to the elliptical orbits in the Kepler problem; for them the radial motion has an oscillatory character. Kepler's ingenious method for computing the system path for given initial state (not simply the orbit, a subject to which surprisingly many physics texts restrict their interest) can be formulated as a simple algorithm: Given (t_0, x_0, v_0) such that $H_0 := H(v_0, x_0) < 0$ and t_1 we have to go through the following chain of formulas (see also [8], Section 4):

$$\begin{aligned}
a &:= -\frac{1}{2H_0} \text{ (major semi-axis)}\\
\varepsilon &:= \sqrt{1 - \frac{1}{a}} \text{ (numerical eccentricity)}\\
n &:= a^{-\frac{3}{2}} \text{ (mean motion)}\\
z &:= 1 - \frac{x_0}{a} + \mathrm{i}\,\frac{x_0 v_0}{\sqrt{a}}\\
E_0 &:= \arg z \text{ (eccentric anomaly)}\\
M_0 &:= E_0 - \varepsilon \sin E_0 \text{ (mean anomaly)}\\
M_1 &:= M_0 + (t_1 - t_0)n\\
E_1 &:= \text{ solution of } E_1 = M_1 + \varepsilon \sin E_1 \text{ (Kepler's equation)}\\
x_1 &:= a(1 - \varepsilon \cos E_1)\\
v_1 &:= \frac{\varepsilon a^2 n \sin E_1}{x_1}
\end{aligned} \tag{29}$$

to get the exactly evolved state (t_1, x_1, v_1). Here the solution E of $M + \varepsilon \sin E$ is given by the algorithm (C++ syntax, `R` is the type for representing real numbers, i.e. `typedef double R;`)

```
R solKepEqu(R M, R eps, R acc)
// M: mean anomaly, eps: numerical eccentricity, acc: accuracy e.g. 1e-8
{
   R xOld=M+1000, xNew=M;
   while ( abs(xOld-xNew) > acc ){
      xOld=xNew;
      R x1=M+eps*sin(xNew);
      R x2=M+eps*sin(x1);
      xNew=(x1+x2)*0.5;   // My standard provision against oscillations.
         // Works extremely well
   }
   return xNew;
}
```

The computational burden for (29) is independent of the time span $t_1 - t_0$, and it does not matter whether this span is positive (prediction) or negative (retro-diction). Hence, there is no relevant distinction between solution (29) and what normally is referred to as a *closed form solution*. So, in assessing the accuracy of numerical integrators, we have the exact solution always available. In addition to the original leap-frog method and the new asynchronous leap-frog method, we consider two established second order methods for further comparison: The traditional *second order Runge-Kutta method* (e.g. [5], (16.1.2)) and the more modern symplectic *position Verlet integrator*, [4], equation (2.22). For this method there are several names in use, cf. [12], above equation (13), and [10]. The present article refers to it as the *direct midpoint integrator* and recalls its definition for the present simple situation that the forces don't depend on the velocity. Equation (27) can be viewed as a single differential equation of second order

$$\ddot{x} = \frac{1}{x^2}\left(\frac{1}{x} - 1\right) \tag{30}$$

and for convenience of comparison with (24) we write this equation in a form similar to (1) as

$$\ddot{\psi}(t) = F(t, \psi(t)) \,, \quad \dot{\psi}(t) =: \phi(t) \,. \tag{31}$$

Since the differential equation is second order, the initial values for ψ *and* ϕ have to come from the problem and the integrator, just as in (24), has the task to promote them both. This is done by formulas very similar to (24):

$$\begin{aligned} \tau &:= \frac{h}{2} \,, \\ t' &:= t + \tau \,, \\ \psi' &:= \psi + \tau\phi \,, \\ \underline{\phi} &:= \phi + hF(t', \psi') \,, \\ \underline{\psi} &:= \psi' + \tau\underline{\phi} \,, \\ \underline{t} &:= t' + \tau \,. \end{aligned} \tag{32}$$

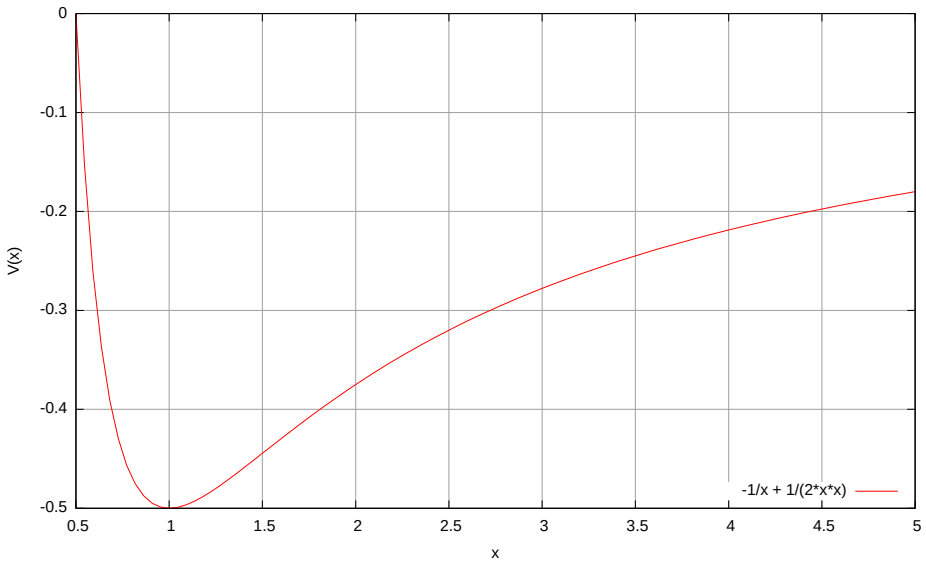

Figure 1: Potential function of the Kepler oscillator

If one accepts to have one equation more than necessary, one may take (24) as it stands, and replace the defining equation for ϕ' by the definition $\phi' := \phi + \tau F(t', \psi')$.

The orbits of the system can be uniquely parametrized by the values $0 \leq \varepsilon < 1$ of the numerical eccentricity, which is related to the total energy H_0 through $\varepsilon^2 = 1 - 2H_0$ (see (29)). The x-values along an orbit range between the solutions $x_{\min}, x_{\max}$ of $V(x) = H_0$ and the v-values range between the solutions $v_{\min}, v_{\max}$ of $T(v) - \frac{1}{2} = H_0$.

Most graphs to be presented here refer to a single path: The one which as an orbit is characterized by $\varepsilon = 0.15$, and the initial state of which is the 'perihelion' i.e. $v_0 = 0$ and that $x_0 = x_{\min}$. The oscillation of this path tuns out to be $t_P = 6.501$. Further we easily find $v_{\max} = -v_{\min} = 0.157$ and $x_{\min} = 0.870$, $x_{\max} = 1.176$ which agrees with the location of the oval shape in Figure 2. As time step for stepwise integration we use $h = t_P/32$ to the effect that 32 computed steps cover the whole period and thus would lead back to the initial position if there would be no integration errors. Each computation yields a discrete trajectory of 512 steps, which corresponds to 16 full 'revolutions'. Figure 2 shows that for these data the Runge-Kutta method does not create a periodic orbit and that the orbit in phase space spirals into the outer space. At this graphical resolution, orbits created by the other methods are hard to distinguish. Figure 2 represents the deviation of the computed position from the exact one for the four methods under consideration. What is displayed here is not simply the difference in phase space location but the phase space position that occurs if the state at time t is back-evolved via the exact dynamics to the initial time $t = 0$. If the stepwise integration would not introduce an error, the point to be displayed would come out as $(0,0)$ in all cases. The errors express themselves as curves (paths) with parameter t and a longer curve indicates a larger total error after the whole integration. Although the dependence on the curve parameter t is not shown

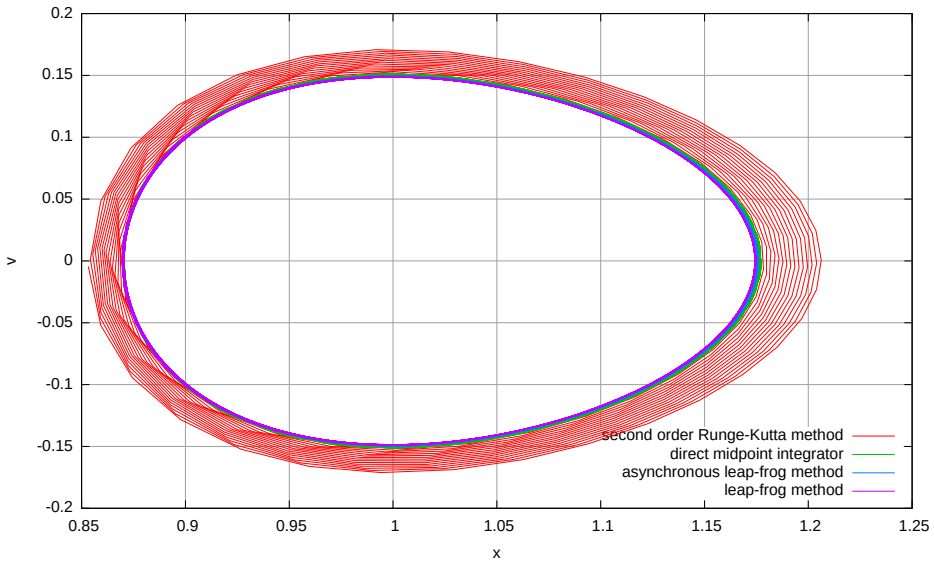

Figure 2: Computed orbits in phase space

in the curves (only the orbit is represented), the 16 approximately repeated substructures in these curves show how the error evolves from revolution to revolution. The coordinates in these diagrams are indexed 'relative' which means that x-differences are divided by $x_{\max} - x_{\min}$ and v-differences are divided by $v_{\max} - v_{\min}$. As already pointed out in [9], near equation (92), these curves can be interpreted as paths in an *interaction picture dynamics*, which again is a dynamical system. This kind of interaction picture (Dirac picture) considers the stepwise integration as the combined action of the exact evolution and a 'discretization interaction' (in analogy to considering a digitized signal as a superposition of the original analog signal and 'digitization noise'). The more accurate the stepwise integration method, the weaker is the interaction and the slower is the motion seen in the interaction picture. As mentioned in [9], this diagnostics based on the interaction picture is not restricted to systems for which the exact solution is directly accessible; an access through stepwise back-evolution methods is sufficient if these are, say, two orders of magnitude more accurate than the method under investigation.

This interaction picture dynamics is related to the usage of evolution operators $\mathrm{e}^{\mathrm{i}Ht}\,\mathrm{e}^{-\mathrm{i}H_0 t}$ in quantum mechanical scattering theory and with backward error analysis in numerical analysis of differential equations, [6], Chapter 10 and [10], Section 4.

Since, as already clear from Figure 2, the error of the Runge-Kutta method is much larger than the error of the other methods, the following Figure 4 gives the corresponding representation for the more accurate methods only. This figure suggests that the direct midpoint integrator is by far more accurate than the two leap-frog integrators. We will see now that this suggestion is misleading. In the application considered in [13] it was found that the asynchronous leap-frog integrator showed similar step size requirements as the direct midpoint integrator when a actual leap-frog step was defined

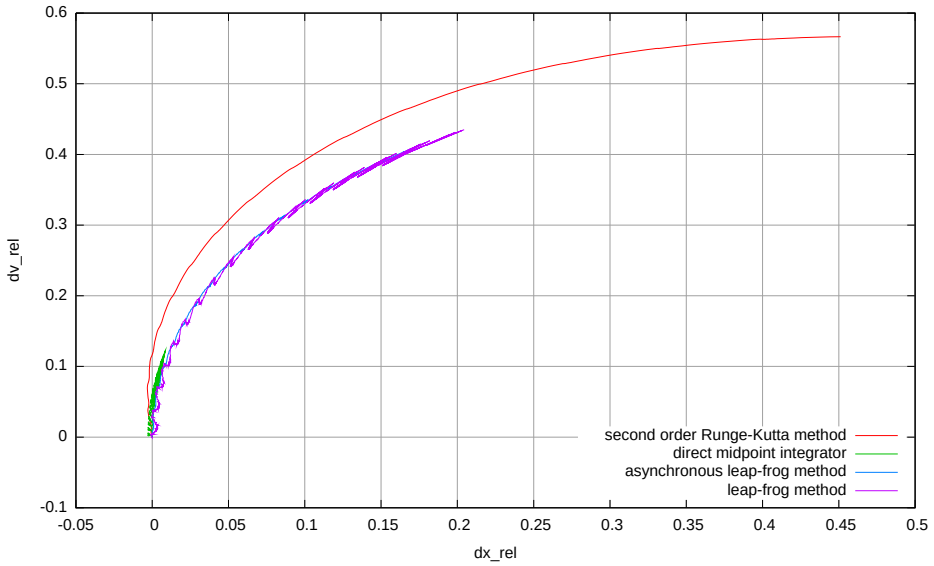

Figure 3: Integration error of four computational methods in the 'interaction picture'

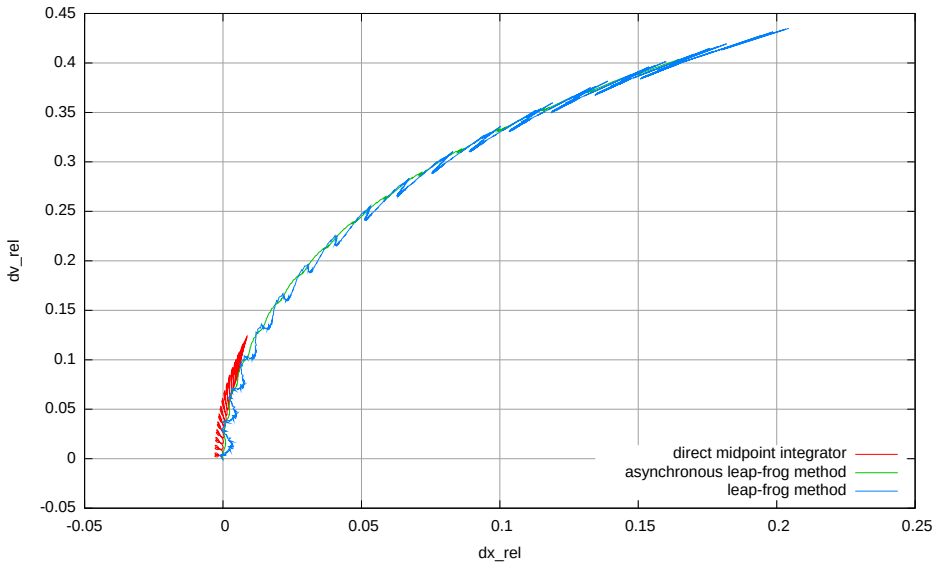

Figure 4: Integration error of the better methods in the 'interaction picture'

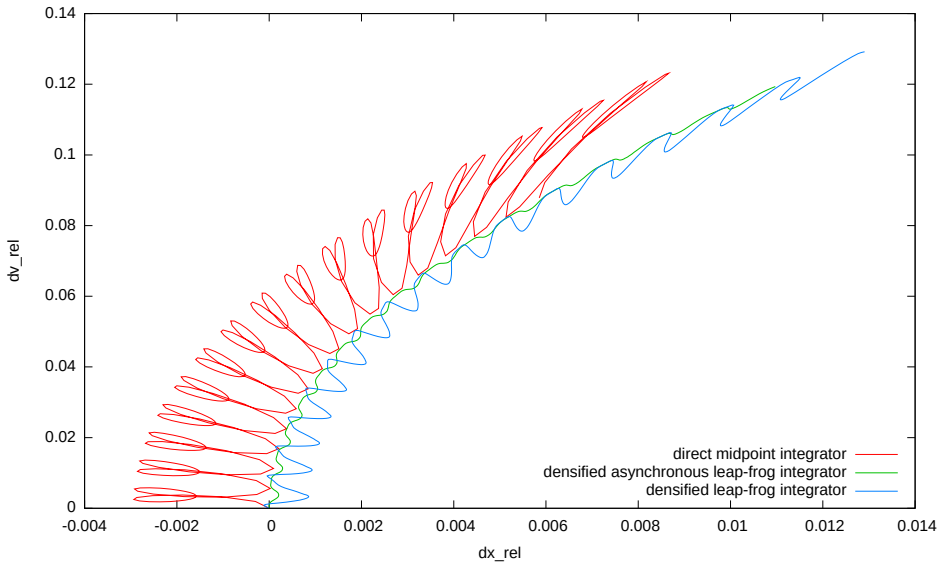

Figure 5: Integration error of the direct midpoint method together with the densified leap-frog methods in the 'interaction picture' for $\varepsilon = 0.15$. Sixteen periods at 32 steps per period.

as consisting of two leap-frog steps of half the step size. Also in the present context it makes sense to consider such a subdivision of a step. We thus define the *densified* leap-frog integrators as

$$\begin{aligned} \tilde{\mathcal{L}} &:= \mathcal{L} \circ \mathcal{L} \\ \tilde{\mathcal{A}}_h &:= \mathcal{A}_{h/2} \circ \mathcal{A}_{h/2} \end{aligned} \tag{33}$$

and display the resulting error orbits in Figure 5. Note that again there are 32 integration steps per orbit, but these are made from substeps so that only every second computed step results in a graphical point. For such a combined step, the computational burden is the same as for one second order Runge-Kutta step, but the accuracy is much better than for Runge-Kutta. It is plausible that only this densified version of the leap-frog methods turns out to come close to the accuracy of the direct midpoint method: The latter has direct access to the second derivative of the solution, whereas the leap-frog methods only accesses the first derivative and thus can be viewed as simulating access to the second derivative by evaluating the first derivative at two different points. One may generate corresponding diagrams for different values of eccentricity and step size and will experience a surprising morphological stability of the curves and their relative length. Figure 6 is an example for this. Here, the number of points per revolution is increased to 64 in response to the increased value of the eccentricity ε.

It is rather evident from all such graphs is that the asynchronous leap-frog method has shorter and more regular error orbits than the standard leap-frog method.

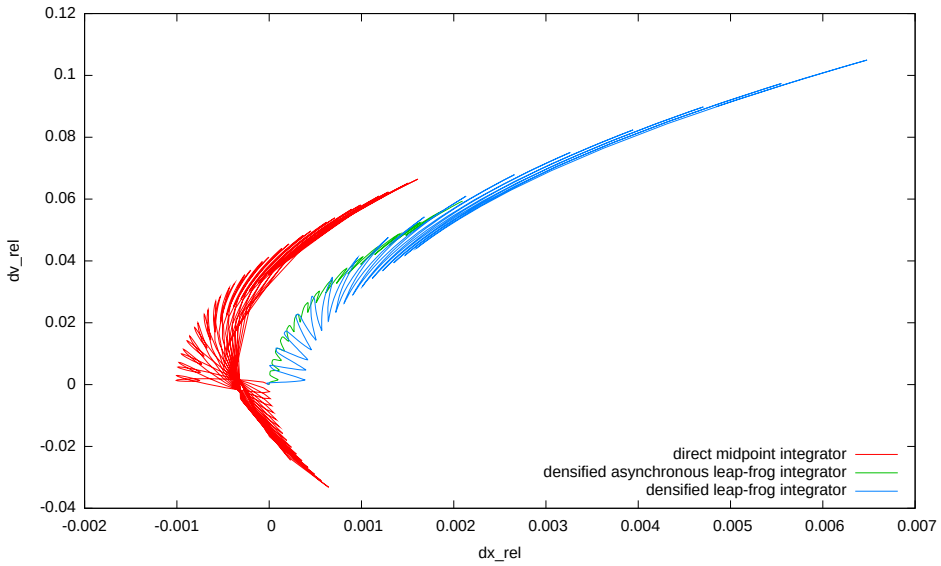

Figure 6: Integration error of the direct midpoint method together with the densified leap-frog methods in the 'interaction picture' for $\varepsilon = 0.30$. Sixteen periods at 64 steps per period.

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