Predicting Classical Motion Directly from the Action Principle

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Abstract

Time-discrete non-relativistic classical dynamics for d degrees of freedom is here formulated in a new way: Discrete approximations to the action (i.e. the time integral of the Lagrangian) determine the new state from a given one, and no differential equations or discretized differential equations are being used. The basis for this dynamical law is a formulation of initial conditions by position and $d+1$ velocities. The mean value of these velocities corresponds to the ordinary initial velocity. The dynamical law works as follows: for an initial configuration we consider $d+1$ rectilinear paths corresponding to the $d+1$ velocities of the initial condition. After a time step τ all paths change their velocity in such a manner, that they re-unite after a second time step τ. The *principle of stationary action* is then applied to these paths to determine the position of the merging point. The $d+1$ new velocities are taken as the velocities associated with the sub-paths of the second time step.

The method is as straightforward and as careless about achieving numerical accuracy as the Euler discretization of differential equations. It turns out, however, that it is closely related—both in explicit representation and in performance—to the more powerful modern *symplectic integration methods* for Hamiltonian systems.

For $d = 1$, the method actually defines a symplectic integrator, which in the limit of vanishing velocity spread is well known. The numerical behavior of the method is studied for the radial part of the Kepler problem, which is an exactly solvable anharmonic oscillator.

For more degrees of freedom the method is formulated in a way that it includes dissipative forces. The numerical behavior is exemplified with an Hamiltonian system only: the solar system 10-body problem. Comparison is made between ephemeris data, the results of the present integration method, and a symplectic Störmer method. As in the case $d = 1$, the behavior with respect to motion reversal is also considered.

1 Introduction

Hamilton's principle of stationary action ('principle of least action' [1], [3]) expresses classical mechanics in a concise and economic manner. With respect to the central problem of dynamics, which is finding the system trajectory from given initial conditions, this principle works rather indirectly: only after having transformed the variation principle into the corresponding Euler-Lagrange differential equations, we are in a position to calculate future system states from a given one.

Feynman's path integral representation of quantum mechanical transition amplitudes [2] shows that the 'selection of the path of least action' can be interpreted in a causal manner: partial waves propagate, interfere, and create the illusion of a trajectory along the space-time points of maximum constructive interference. In Feynman's words [1]: 'So our principle of least action is incompletely stated. It isn't that a particle takes the path of least action but that it smells all the paths in the neighborhood and chooses the one that has the least action by a method analogous to the one by which light chose the shortest time.'

This paper describes what is essentially a mathematical formulation of this concept in the framework of classical mechanics. It will be shown that the infinite manifold of paths to be considered in quantum mechanics can be reduced to a finite number in classical mechanics. This number is $d+1$ for a system of d degrees of freedom. Maximum constructive interference will be described without having to introduce waves as the condition of having equal action along the interfering paths.

These $d+1$ paths will be organized in a way that minimum deviation from the standard notion of a classical trajectory is necessary: Whereas each point of a standard trajectory has a unique velocity vector associated with it, the present formulation associates $d+1$ velocities with a trajectory point. The mean value of these velocities corresponds to the standard velocity, and the spread in velocity allows the particle 'to smell the neighborhood': shortly after the space-time point to which the velocities were attributed, the particle 'occupies' $d+1$ different space points and is influenced by the physical quantities (e.g. potentials) valid at these space points. After the elapse of a time step Δt, the 'non-localized' state has contracted again to a point, again having $d+1$ velocities associated with it. It is only this point in which the system state can be compared with a state of the traditional trajectory according to the rule introduced already: space-time points correspond directly, and the mean value of the $d+1$ velocities corresponds to the traditional velocity.

The essential point is, that this new state is determined from the actions along the $d+1$ paths by the condition of 'maximum constructive interference'. No intermediate differential equation is needed. Since this determines the system state after elapse of a finite time step, this defines the time evolution operator of a time-discrete dynamical system.

Since the traditional trajectory obeys the Euler-Lagrange differential equations, and the present method produces states which approximate such trajectory states on a lattice of time points, the method can also be interpreted as generating an *integrator* of the Euler-Lagrange differential equations. This integrator can directly be compared with known integrators for these differential equations, and this will be done on various levels. A close relation to known symplectic integrators will become apparent.

Looking only at the integrator, one has not to concern oneself with the ingredients of its derivation: a continuum of states, in which only a discrete subset allows an interpretation as a classical particle, and which behaves quantum mechanically in so far, as velocity spread and position spread never vanish at the same time. Also the derivation itself can be given a more conventional interpretation. In essence, it says that the 'least-action path' is determined by an algebraic equation if we restrict the search to a subset of paths which allows a sufficiently simple parametrization and which is sufficient to represent the trajectory over the time step of the integrator. Having looked at the matter from various directions, I hope that the present formulation of the method, which introduces a fixed system of 'smelling'-paths and which considers the descriptors of these paths—the $d+1$ velocities mentioned above—as dynamical variables of the system[1], offers a good starting

[1] this means that initial conditions have to specify values for these quantities

point for further developments of the method.

2 A single particle in one-dimensional space

This section describes the method for a system of one degree of freedom for which the basic equations are very simple, and interesting structural properties, such as symplecticity and motion reversal invariance, can easily be verified.

We assume a Lagrangian

$$L(v,x,t) = T(v) - V(x,t) = \frac{m}{2}v^2 - V(x,t)\ . \tag{1}$$

The intrinsic meaning of this can be seen in associating the action

$$S(x,t;\underline{x},\underline{t}) := (\underline{t}-t)\left(T\left(\frac{\underline{x}-x}{\underline{t}-t}\right) - V\left(\frac{x+\underline{x}}{2},\frac{t+\underline{t}}{2}\right)\right) \tag{2}$$

with a pair $(x,t),(\underline{x},\underline{t})$ of space-time points[2] which are sufficiently close together that all relevant system path connecting them can be considered recti-linear and thus identical. At the next level of detail, we add to the descriptors of a short path an intermediate point (x',t'). Again, the paths between the points can be considered rectilinear. We associate with the corresponding triplet of points (or with the piecewise rectilinear path they are representing) the action

$$\begin{aligned} S(x,t;x',t';\underline{x},\underline{t}) :=& \\ & (t'-t)T\left(\frac{x'-x}{t'-t}\right) + (\underline{t}-t')T\left(\frac{\underline{x}-x'}{\underline{t}-t'}\right) - (\underline{t}-t)V\left(x',t'\right) \\ =& \ (t'-t)L\left(\frac{x'-x}{t'-t},x',t'\right) + (\underline{t}-t')L\left(\frac{\underline{x}-x'}{\underline{t}-t'},x',t'\right)\ , \end{aligned} \tag{3}$$

which enjoys the obvious consistency property

$$S(x,t;\underline{x},\underline{t}) = S(x,t;\tfrac{x+\underline{x}}{2},\tfrac{t+\underline{t}}{2};\underline{x},\underline{t})\ ,$$

which would not hold for the trivial three-point generalization

$$S(x,t;x',t';\underline{x},\underline{t}) := S(x,t;x',t') + S(x',t';\underline{x},\underline{t}).$$

[2]to be called simply *points* in the sequel

At the starting point (x,t) of a trajectory, we are given the velocity v and ask for the system state $(\underline{v},\underline{x})$ at time $\underline{t} = t+\Delta t = t+2\tau$. The function (3) allows to formulate an equation which determines this state if we specify, in addition to v, a velocity spread Δv: This then defines two paths from (x,t) to $(\underline{x},\underline{t})$ for which the condition of constructive interference can be posed in the form

$$S(x,t;x+(v+\Delta v)\tau,t+\tau;\underline{x},\underline{t}) = S(x,t;x+(v-\Delta v)\tau,t+\tau;\underline{x},\underline{t}) \,. \tag{4}$$

If $\underline{x}$ is found from this central equation of this section, the new velocity is given by

$$\underline{v} = \frac{\underline{x}-x}{\tau} - v \,, \tag{5}$$

as will become clear soon. In order to express the solution $\underline{x}$ of (4) compactly, we need some notation:

$$v_1 := v+\Delta v \,, \quad v_2 := v-\Delta v \,, \quad x'_p := x+\tau v_p \,, \quad t' := t+\tau \tag{6}$$

$$S_p := S(x,t;x'_p,t';\underline{x},\underline{t}) \,, \quad p \in \{1,2\} \tag{7}$$

The actions S_p [3], which allow to express (4) simply as

$$S_1 = S_2 \,, \tag{8}$$

are given by (1) and (3) as

$$\begin{aligned} S_p &= T_p - V_p \,, \\ T_p &= \frac{\tau}{2} m v_p^2 + \frac{\tau}{2} m \left| \frac{\underline{x}-x}{\tau} - v_p \right|^2 \\ &= \tau m \left(v_p^2 - 2 v_p \frac{\underline{x}-x}{2\tau} + 2 \left| \frac{\underline{x}-x}{2\tau} \right|^2 \right) \,, \\ V_p &= 2\tau V(x'_p,t') \,. \end{aligned} \tag{9}$$

In the difference of the S_p, the term which contains the square of the unknown $\underline{x}$ cancels out and we simply get

$$S_1 - S_2 = m(v_1 - v_2)\left(x - \underline{x} + 2\tau v + 2\tau^2 a\right) \,, \tag{10}$$

where

$$a = -\frac{V(x'_2,t') - V(x'_1,t')}{m(x'_2 - x'_1)} \,. \tag{11}$$

[3] Throughout this section, the path-index p varies from 1 to 2.

Equations (8)–(11) imply:

$$\underline{x} = x + \Delta t\, v + \tfrac{1}{2}(\Delta t)^2 a\,. \tag{12}$$

The two velocities $\underline{v}_1$, $\underline{v}_2$ in point $(\underline{x}, \underline{t})$ are given by the velocities in the last half of the path:

$$\underline{v}_p := \frac{\underline{x} - x'_p}{\tau}\,. \tag{13}$$

Forming their mean value, we get (5). Equations (6), (11)–(13) allow to to express the state at $(\underline{x}, \underline{t})$ in a compact manner:

$$\begin{aligned}
a &= \frac{V\,(x+\tau(v-\Delta v), t+\tau) - V\,(x+\tau(v+\Delta v), t+\tau)}{2\tau\Delta v m}\,, && (14)\\
\underline{v} &= v + \Delta t\, a\,, && (15)\\
\underline{x} &= x + \Delta t \frac{v+\underline{v}}{2}\,, && (16)\\
\Delta\underline{v} &= -\Delta v\,, && (17)\\
\underline{v}_1 &= \underline{v} + \Delta\underline{v}\,, && (18)\\
\underline{v}_2 &= \underline{v} - \Delta\underline{v}\,. && (19)
\end{aligned}$$

This set of formulae defines a map operating on ordinary[4] system states; to have a name for this map (integrator) we write

$$(\underline{v}, \underline{x}, \underline{t}) = \Phi^1{}_{\Delta t, \Delta v}(v, x, t)\,, \tag{20}$$

where the upper index serves as a distinction from similar maps to be considered later.

If Δv is very small, formula (14) becomes inaccurate numerically and may better be expressed by derivatives:

$$\begin{aligned}
&\frac{V\,(x'_2, t') - V\,(x'_1, t')}{x'_2 - x'_1} = \\
&\qquad V'(x+\tau v, t') + \frac{V'''(x+\tau v, t')}{3!}(2\Delta v \Delta t)^2 + \cdots\,. && (21)
\end{aligned}$$

In the limit $\Delta v \to 0$ we get

$$a = -\frac{V'(x+\tau v, t+\tau)}{m}\,. \tag{22}$$

[4]described by a single velocity instead of two velocities

Then, we don't need the two velocities any longer and have a time-stepping scheme given by (22), (15), (16) which, for future reference, will be denoted

$$(\underline{v},\underline{x},\underline{t}) = \Phi^1{}_{\Delta t}(v,x,t)\ . \tag{23}$$

For a given τ, we could equally well describe the initial configuration by the three positions x, x'_1, x'_2 instead of one position and two velocities. Then, the time step equations (14)–(19) become particularly simple:

$$\underline{x} = x'_1 + x'_2 - x + 2\tau^2 a\ , \quad \underline{x}'_1 = \underline{x} + x'_1 - x\ , \quad \underline{x}'_2 = \underline{x} + x'_2 - x\ . \tag{24}$$

Let us compare (14)–(19) with time-stepping schemes (integrators) for the differential equation of motion

$$\ddot{x} = -\frac{V'(x,t)}{m} =: f(x,t) \tag{25}$$

belonging to the Lagrangian (1). We consider the Euler method [4], equation (16.1.1), the second-order Runge-Kutta (midpoint) method [4], equation (16.1.2), and a second-order Störmer method [5] [4], equation (16.5.2) for $m=1$:

$$\begin{aligned}
a &= f(x,t)\ , \\
\underline{x} &= x + \Delta t\, v + \tfrac{1}{2}(\Delta t)^2 a\ , \\
\underline{v}_{\text{Euler}} &= v + \Delta t\, a\ , && (26) \\
\underline{v}_{\text{Runge-Kutta}} &= v + \Delta t\, f(x+\tau v, t+\tau)\ , && (27) \\
\underline{v}_{\text{Störmer}} &= v + \Delta t\,\frac{a + f(\underline{x}, t+\Delta t)}{2}\ . && (28)
\end{aligned}$$

Also of interest is the implicit second-order Runge-Kutta (implicit midpoint) method, e.g. [5], p. 219, case $m = 1 (q_l = 3)$

$$\begin{aligned}
a &= f(x + \tau v + \tau^2 a, t+\tau)\ , && (29) \\
\underline{v} &= v + \Delta t\, a\ , \\
\underline{x} &= x + \Delta t \frac{v + \underline{v}}{2}\ .
\end{aligned}$$

More sophisticated integrators evaluate the function f at even more positions, but they never change the derivative V' into a finite difference quotient as it appears in (11). Thus, by discretization of the action

[5] also known as the Verlet velocity algorithm

principle we obtain an equation which can't arise from discretizing the corresponding ordinary differential equation. This is also supported by the fact that equations (14)–(19) contain the parameter Δv, which has no analogue in the discretized differential equation.

However, (23) is an ordinary integrator for (25) and can directly be compared with the methods (26)–(29). Although not being a member of this list verbally, it is there as the first iteration step in solving the implicit midpoint method (29): starting with $a = 0$ on the right-hand side, we get to $a = f(x + \tau v, t + \tau)$, i.e. to equation (22).

Recent research on integrators for equations of motion concentrated on methods which define symplectic time evolution operators just as the exact solutions do [7] [8]. The integrators (29), (28), (23) are known to be symplectic i.e. to satisfy

$$\mathrm{d}\underline{v} \wedge \mathrm{d}\underline{x} = \mathrm{d}v \wedge \mathrm{d}x \,. \tag{30}$$

Interestingly, (20) is also symplectic. To show this, and to prepare the argument for a similar integrator to be defined later, we consider integrators of the form

$$\begin{aligned} \underline{v} &= v + 2\tau a \,, \\ \underline{x} &= x + \tau(v + \underline{v}) \,. \end{aligned} \tag{31}$$

Then we have

$$\begin{aligned} \mathrm{d}\underline{v} \wedge \mathrm{d}\underline{x} &= (\mathrm{d}v + 2\tau \mathrm{d}a) \wedge (\mathrm{d}x + \tau \mathrm{d}v + \tau \mathrm{d}\underline{v}) \\ &= (\mathrm{d}v + 2\tau \mathrm{d}a) \wedge (\mathrm{d}x + 2\tau \mathrm{d}v + 2\tau^2 \mathrm{d}a) \\ &= \mathrm{d}v \wedge \mathrm{d}x + \mathrm{d}a \wedge (\mathrm{d}x + \tau \mathrm{d}v) \,. \end{aligned}$$

Therefore, an integrator (31) is symplectic if and only if

$$\mathrm{d}a \wedge (\mathrm{d}x + \tau \mathrm{d}v) = 0 \,. \tag{32}$$

In the case of (20) we have

$$\mathrm{d}a = \frac{V'(x + \tau(v - \Delta v), t + \tau) - V'(x + \tau(v + \Delta v), t + \tau)}{2\tau \Delta v m} (dx + \tau \mathrm{d}v) \,, \tag{33}$$

so that (32) is satisfied, and (20) is a symplectic integrator. That it is of second order can be seen from

$$\Phi^1{}_{2\Delta t, \Delta v}(v, x, t) - \Phi^1{}_{\Delta t, \Delta v}(\Phi^1{}_{\Delta t, \Delta v}(v, x, t)) = (O(\Delta t^3), O(\Delta t^3), 0) \,. \tag{34}$$

If V depends on time only through t^2, this integrator is also invariant with respect to *motion reversal*:

$$\left(\mathcal{T} \circ \Phi^1{}_{\Delta t,\Delta v} \circ \mathcal{T} \circ \Phi^1{}_{\Delta t,\Delta v}\right)(v,x,t) = (v,x,t) \ , \tag{35}$$

where the motion reversal operation is $\mathcal{T} : (v,x,t) \mapsto (-v,x,-t)$. Both relations involve lengthy calculations and are conveniently verified using a symbolic manipulation package such as *Mathematica*.

After having seen how the method works, let us look back to the logic in selecting expression (3). The point of view suggested so far was to consider (3) the most simple expression that can be proposed for the action along a short path from which we only know that it starts at (x,t), reaches the point (x',t'), and ends at $(\underline{x},\underline{t})$. Since the expression is 'algebraic' we don't need to know about differentiation and integration to define it. The action for longer paths can be obtained equally well by summation of expressions (3) or by integration of the Lagrangian with v replaced by the derivative $\dot{x}$. It should also be noted that $S(x,t;x',t';\underline{x},\underline{t})$ can be expressed in terms of L alone, not making use of the separation into T and V. There is, however, a more conventional interpretation of expression (3): It is the exact value of the traditional action associated with a piecewise rectilinear path connecting the given triplet of points and a modified Lagrangian in which V is changed into an impulse potential, active only at time t'.

It is instructive to replace (3) by an expression based on integrating the actual (non-impulsive) Lagrangian (1) along differentiable paths: We consider the parabolic paths which are uniquely determined by the initial point (x,t), the initial velocities v_p, and the condition that they merge at the point $(\underline{x},\underline{t})$. Since we want the paths to be differentiable, there is no ambiguity in updating the velocities: The final velocities from one time step have to be taken for the initial velocities of the next time step. We calculate the action along a path, exactly for the kinetic part, and by Simpson's rule for the potential part:

$$\begin{aligned} S_p &= \tfrac{1}{3}\tau m \left(v_p^2 - 2v_p \tfrac{\underline{x}-x}{2\tau} + 2\left|\tfrac{\underline{x}-x}{2\tau}\right|^2\right) - \\ &\quad \tfrac{1}{3}\tau\left(V(x,t) + 4V(x'_p,t') + V(\underline{x},\underline{t})\right) \ . \end{aligned} \tag{36}$$

The point x'_p, as before, is the position at time t' on path p. Since the path is parabolic now, this point is not simply given as $x+\tau v_p$. After some algebra we get

$$S_1 - S_2 = \tfrac{1}{3}m(v_1 - v_2)\left(x - \underline{x} + 2\tau v + 2\tau^2 a\right) \ , \tag{37}$$

where, again, a is given by (11). The intermediate points x'_p also depend on a :

$$x'_p = x + \frac{\tau}{2}(v + v_p + \tau a) , \tag{38}$$

thus creating an implicit system of equations for determining a. It can be shown that equation $S_1 - S_2 = 0$, together with differentiability of paths yields equations (15)–(19). This defines a time-stepping scheme denoted

$$(\underline{v}, \underline{x}, \underline{t}) = \Phi^2{}_{\Delta t, \Delta v}(v, x, t) . \tag{39}$$

The equations (11) and (38) are most conveniently solved for a by iteration [6]:

$$\begin{aligned} a_0 &:= 0 , \\ y_1 &:= x + \frac{\tau}{2}(v + v_1 + \tau a_n) , \\ y_2 &:= x + \frac{\tau}{2}(v + v_2 + \tau a_n) , \\ a_{n+1} &:= \frac{V(y_2, t+\tau) - V(y_1, t+\tau)}{m(y_1 - y_2)} . \end{aligned} \tag{40}$$

The value a_1 in this scheme coincides with the result of the original method (20). It is interesting that the implicit nature of the defining equations neither is a serious obstacle for an effective solution nor for a proof of symplecticity. From (11) and (38) we have

$$a = \frac{V(x + \tau(v - \frac{\Delta v}{2} + \tau a), t+\tau) - V(x + \tau(v + \frac{\Delta v}{2} + \tau a), t+\tau)}{2\tau \Delta v m} . \tag{41}$$

Thus

$$\mathrm{d}a = g\,(\,\mathrm{d}x + \tau\,\mathrm{d}v + \tfrac{1}{2}\tau^2\,\mathrm{d}a) , \tag{42}$$

where

$$g = \frac{V'(x + \tau(v - \frac{\Delta v}{2} + \tau a), t+\tau) - V'(x + \tau(v + \frac{\Delta v}{2} + \tau a), t+\tau)}{2\tau \Delta v m} . \tag{43}$$

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[6] Although the iteration step for solving $x = f(x)$ is written as $x_{n+1} = f(x_n)$, in numerical examples I always use $x_* = f(x_n), x_{**} = f(x_*), x_{n+1} = \frac{1}{2}(x_* + x_{**})$, which is much more stable.

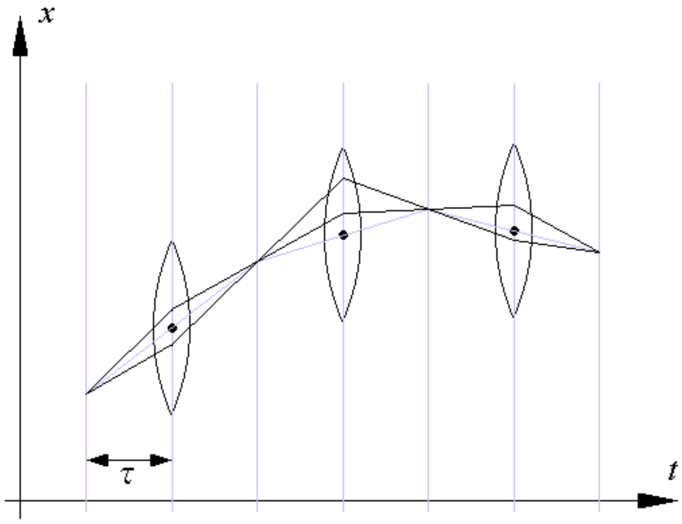


Figure 1: Optical analogy to path geometry

Therefore

$$\mathrm{d}a = \frac{g}{1 - \frac{1}{2}g\tau^2}\left(\mathrm{d}x + \tau \mathrm{d}v\right), \tag{44}$$

so that (32) is satisfied and (39) is a symplectic integrator. As for the integrator (20), we can form the limit $\Delta v \to 0$, and get an ordinary integrator $\Phi^2_{\Delta t}$. As is easily seen from (41), this is just the implicit midpoint integrator (29).

Integrators for differentiable paths will not be pursued in this paper[7]. Although they may be capable of increasing the accuracy for sufficiently regular potentials, they certainly are less intuitive and simple than the method using piecewise rectilinear paths.

A series of consecutive evolution steps creates two polygonal space-time paths such that the kinks of each (and maximum separation between the two paths) occur at half steps, and intersection of the paths occurs at full steps. A concise visualization of such a geometry is given by two light rays in a plane which run through a system of equi-spaced thin lenses which all have the same focal length equal to a fourth of the lens spacing, as indicated in figure 1.

This optical analogy suggests a physical characterization of the state

[7] Method (39) will be included in the examples in the next section, though.

changes during the course of time[8]. In the intersection points (full steps) we have well defined positions and maximum spread of velocity, whereas at the lens position (half steps) we have maximum spread of position and a well defined direction of propagation: in a more realistic representation of the light rays inside the lenses those would be parallel (and parallel to the auxiliary lines in figure 1 which pass through the lens centers). Thus the system oscillates between two states, which in quantum mechanics would be called *complementary*. The duality of these states allows to group the process differently: So far we counted steps from focal point to focal point. We also may count from lens plane to lens plane. Then the roles of positions and velocities in determining an initial state are reversed, and one may arrive at a formulation which reflects the symmetry between positions and momenta in mechanics.

If the time step tends to zero, the two paths get closer and closer together so that in this limit the conventional one-path representation is retained. In spaces of dimension higher than one, we will need more than two paths, so that *multiple path method* (MPM) is an indicative name for the method under consideration.

It is clear that after each full step, we are free to change the time step; this is essential for practical applications where the time step should be adjusted such that no relevant detail of the trajectory remains unresolved. This can be done by comparing the result of a single Δt step with the result of two consecutive $\frac{1}{2}\Delta t$ steps.

3 A numerical example

We consider the radial motion in the Kepler problem, since it is a nontrivial, natural, and exactly solvable problem with one degree of freedom. As we have seen from (21), the harmonic oscillator would not be a good example since the influence of the velocity spread parameter Δv cancels out in this case. The harmonic oscillator is covered, however, since the radial Kepler motion approximates harmonic oscillation for the numerical eccentricity ε tending to zero. What would be denoted $(\dot{r}, r)$ in the context of the Kepler problem will be denoted (v, x) here, in order to have the same notation as in the previous section. Restricting ourselves to orbits of non-vanishing angular momentum and choosing

[8]notice that only the initial and final state allow an interpretation in terms of a classical trajectory

suitable units we get the following Lagrangian of the system:

$$L(v,x) = T(v) - V(x) = \tfrac{1}{2}v^2 - \tfrac{1}{x}\left(\tfrac{1}{2x} - 1\right) . \tag{45}$$

Although the exact solution of the corresponding equation of motion is well known for all initial values, we restrict ourselves here to the bound states, which perform an oscillatory motion. These states are characterized by having negative total energy: $T(v)+V(x) < 0$. Let the state (v,x) for $t=0$ satisfy this condition. Then the state $(v_t,x_t) = \phi_t(v,x)$ for any other time t can be computed from the following chain of formulae, which essentially goes back to Kepler. Here, it also defines the functions $a(\cdot,\cdot)$ and $M(\cdot,\cdot)$ which are useful in comparing the exact solution to the various discrete approximations.

$$\begin{aligned}
a(v,x) &= a = -\frac{1}{2(T(v)+V(x))} , \\
E &= \arg\left(1 - \frac{x}{a} + \mathrm{i}\frac{vx}{\sqrt{a}}\right) , \\
\varepsilon &= \sqrt{1-\frac{1}{a}} , \\
M(v,x) &= M = E - \varepsilon \sin E , \\
n &= a^{-3/2} , \\
M_t &= M + nt , \\
E_t &= \text{solution of} \quad E_t = M_t + \varepsilon \sin E_t , \\
x_t &= a(1-\varepsilon \cos E_t) , \\
v_t &= \varepsilon \frac{a^2}{x_t} n \sin E_t .
\end{aligned} \tag{46}$$

The method for solving Kepler's equation $E = M + \varepsilon \sin E$ for E, which will be used in the numerical example, is iteration (see footnote 6)

$$E_0 = M , \quad E_{n+1} = M + \varepsilon \sin E_n . \tag{47}$$

As can be seen from the previous equations, the function $t \mapsto a(v_t,x_t)$ is constant, and $t \mapsto M(v_t,x_t)$ is linear (up to jumps of height 2π). Replacing the exact solution by an approximate solution generated by successively applying a numerical integrator, defines a family of evolution operators $\hat{\phi}_t$ for which we write $(\hat{v}_t,\hat{x}_t) = \hat{\phi}_t(v,x)$. The deviation of $\hat{\phi}$ from the exact evolution ϕ, results in $t \mapsto a(\hat{v}_t,\hat{x}_t)$ being no longer constant and $t \mapsto M(\hat{v}_t,\hat{x}_t)$ deviating from the linear function of the exact solution.

Figures 2 and 3 show this deviation for the four integration methods to be considered in this section. These are three symplectic methods: Störmer (St) (28), MPM1 (20), MPM2 (39), and the non-symplectic second-order Runge-Kutta method (RK2) (27). The following measures will be used in the figures for comparing computed with and exact trajectories: *Absolute error*

$$\sqrt{(\hat{v}_t - v_t)^2 + (\hat{x}_t - v_t)^2}\ ,$$

relative amplitude error

$$\log \left| \frac{a(\hat{v}_t, \hat{x}_t) - a(v,x)}{a(v,x)} \right|\ ,$$

and *phase error*

$$\arg \mathrm{e}^{\mathrm{i}(M(\hat{v}_t, \hat{x}_t) - M(v_t, x_t))}\ .$$

All figures deal with the same trajectory of the system: In the language of the Kepler problem, we consider an orbit of numeric eccentricity $\varepsilon = 0.3$, start the integration at perihelion ($v_0 = 0$, $x_0 =$ minimum) and extend it over 8 revolutions.

For all diagrams except of figure 5, the number of steps per revolution is 32. For all diagrams except of figure 4, the parameter Δv is 10^{-4} times the mean velocity $v_{\mathrm{mean}} = 4a/t_{\mathrm{period}}$. For the symplectic integrators the curves in figures 2 and 3 follow an interesting pattern. The amplitude error seems to be periodic, and the phase error shows a weak linear trend with some periodic modulation on top. This means that the discretized trajectory has a slightly different frequency than the exact one. One should be able to calculate this frequency shift.

Figure 4 shows the dependence of the method MPM1 on the velocity spread parameter Δv. The four curves corresponding to $\Delta v = 10^{-2}, \ldots, 10^{-8}$ coincide within the resolution of the graphics, and the same holds true for the amplitude error. So the trajectory is virtually independent of this parameter over at least six orders of magnitude. For Δv approaching the relative accuracy of the computer's number representation, the results become increasingly affected by roundoff errors and attain the random walk nature seen in the upper curve. For Δv becoming too large, the situation is similar to having the time step Δt chosen too large: the dynamics described by the discrete integrator and the exact dynamics become increasingly unrelated.

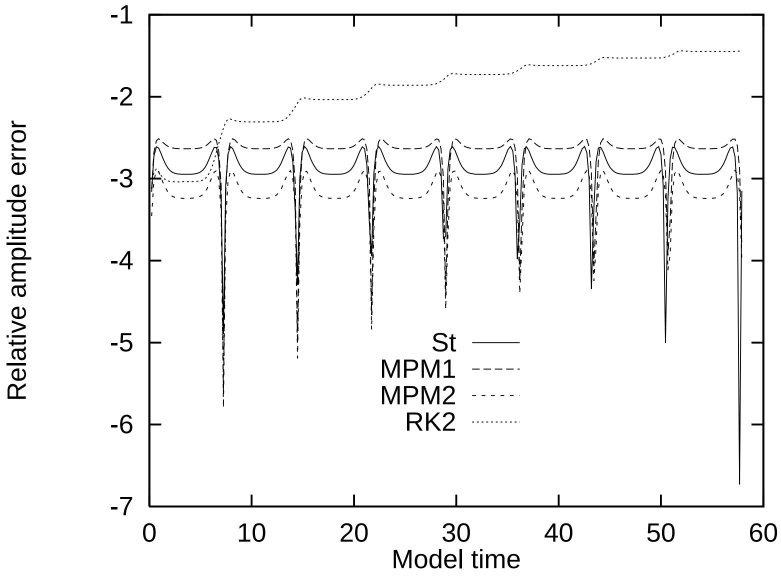


Figure 2: Relative amplitude error versus time

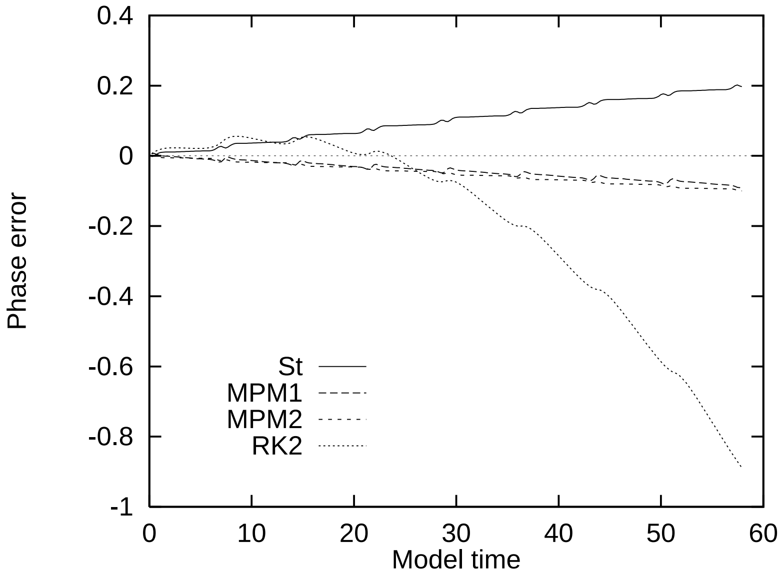


Figure 3: Phase error versus time

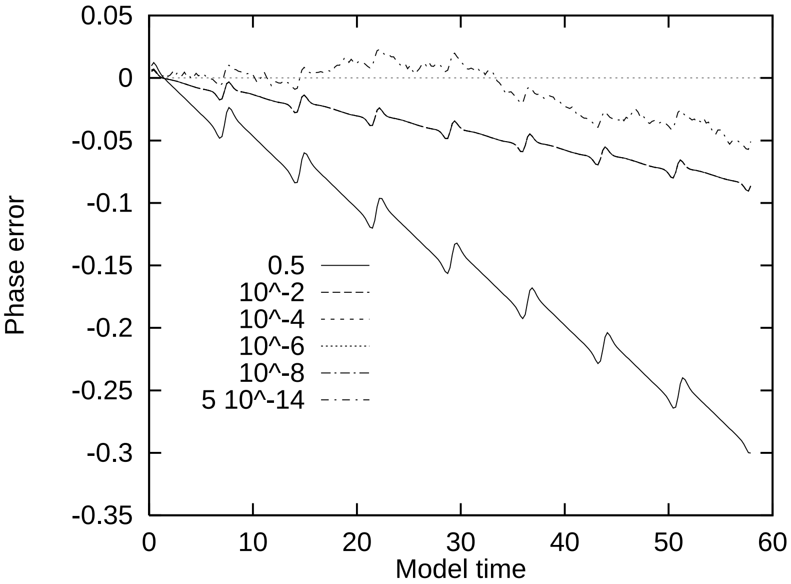


Figure 4: Phase error versus time for MPM1 and various values of Δv.

Figure 5 shows how the absolute error after eight revolutions declines if the number of integration steps increases. If the absolute error and the step number both are shown on a logarithmic scale, as is done here, the *order* of an integrator is closely related to the slope of a straight line shown in such a diagram. So the indication is that all methods are of the same order, which thus is 2. This is surprising at least at a first glance, since one could imagine that going from polygon paths to piecewise parabolic paths in approximating the action integral would make MPM2 higher order than MPM1.

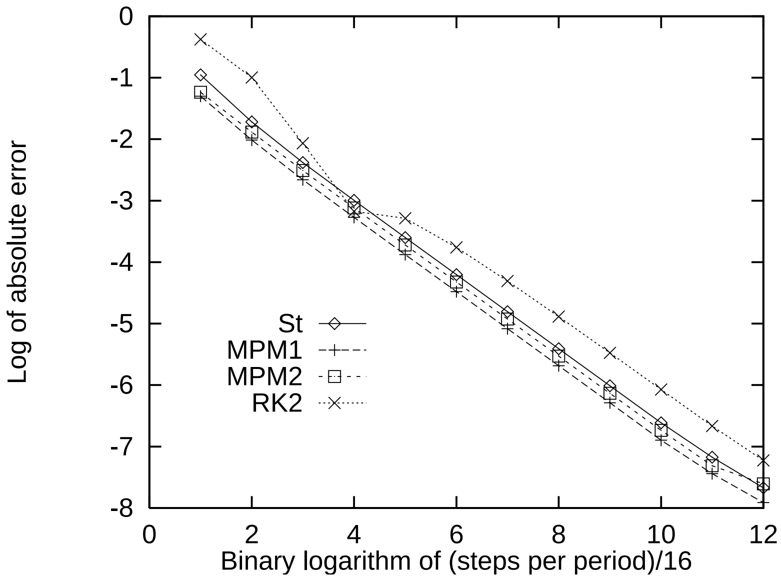


Figure 5: Total error versus step number

4 A more general holonomic mechanical system

In this section we extend the method to many-particle systems including friction to make collisions inelastic—the kind of problems for which I developed the method and for which I still use it heavily. The emphasis here is on obtaining an economic system of equations for the time step and not on the structural properties of the method. These are only exemplified in the next section.

We assume the configuration space X of the system as a Cartesian product of n subsystems each having a d-dimensional configuration space X_i [9]. This allows an easy application to systems of point particles for $d = 3$, or systems of rigid bodies for $d = 6$. For a system which doesn't fall into subsystems, one can use all following formulas for $n = 1$ and d equal to the number of degrees of freedom of the system. In a first reading it might be helpful to take the forces F as zero and to assume the dependence of the kinetic energy T on x and t to be trivial. Then one has a familiar text-book situation and the following derivations become smooth generalizations of those in section 2. Let us call this the *special case*.

We shall assume the following form for the Lagrangian

$$\begin{aligned}
L(v,x,t) &= T(v,x,t) - V(x,t)\ , \qquad (48)\\
x &= (x_1,\ldots,x_n), \quad x_i = (x_{i1},\ldots,x_{id}) \in X_i\ ,\\
v &= (v_1,\ldots,v_n), \quad v_i = (v_{i1},\ldots,v_{id}) \in \mathbb{R}^d\ ,\\
T(v,x,t) &= \sum_{i=1}^{n} T_i(v_i,x_i,t)\ ,
\end{aligned}$$

where $T_i(v_i,x_i,t)$ depends on its argument v_i as a non-degenerate quadratic form:

$$T_i(\xi,x_i,t) = \sum_{a,b=1}^{d} \xi_a M_i(x_i,t)_{ab}\xi_b\ . \qquad (49)$$

[9] These spaces are manifolds of system configurations, each structured by a choice of a global system of generalized coordinates. Operationally, this implies (i) that points of X_i and elements of $\mathbb{R}^d$ can be added to give points in X_i, and (ii) points of X_i can be subtracted from points of X_i to give elements of $\mathbb{R}^d$. An unambiguous physical meaning of these operations and the validity of affine geometry rules for them are given only approximately—the closer the points together and the shorter the numerical vectors the better.

We use the same name for the corresponding bilinear form:

$$T(v,w,x,t) = \sum_{i=1}^{n} T_i(v_i,w_i,x_i,t) = \sum_{i=1}^{n} \sum_{a,b=1}^{d} v_{ia} M_i(x_i,t)_{ab} w_{ib} \,. \tag{50}$$

Such a form of T allows the subsystems to be rigid bodies (orientation described by Euler angles), which change their geometry under the influence of a slow external process, such as solid spheres that change their moment of inertia through thermal expansion in an externally controlled heat bath.

Further, we allow for forces which are not represented by the potential V and which may or may not be conservative:

$$F_{ia}(v,x,t) \,. \tag{51}$$

Then the equations of motion are

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v_{ia}} - \frac{\partial L}{\partial x_{ia}} = F_{ia} \,, \quad i \in \{1,\ldots,n\} \,, \quad a \in \{1,\ldots,d\} \,. \tag{52}$$

Due to the F's, the usual action integral is no longer stationary around the physical path but shows a first order dependence on the path shift given by the forces [3]. This allows to form a new expression which is stationary and replaces the action in the formulation of maximum constructive interference of paths: For a path which is obtained from a physical trajectory by a variation δx, satisfying $\delta x(t_1) = \delta x(t_2) = 0$, we get

$$\begin{aligned} &\int_{t_1}^{t_2} L(v + \tfrac{\mathrm{d}}{\mathrm{d}t}\delta x, x + \delta x, t)\,\mathrm{d}t = \\ &\quad \int_{t_1}^{t_2} L(v,x,t)\,\mathrm{d}t + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v}\right) \mathrm{d}x\,\mathrm{d}t = \\ &\quad \int_{t_1}^{t_2} L(v,x,t)\,\mathrm{d}t - \int_{t_1}^{t_2} F(v,x,t)\delta x\,\mathrm{d}t \,. \end{aligned} \tag{53}$$

Thus the values of the following expressions are stationary at $\delta x = 0$:

$$\int_{t_1}^{t_2} \Big(L(v + \tfrac{\mathrm{d}}{\mathrm{d}t}\delta x, x + \delta x, t) + F(v,x,t)\delta x \Big)\,\mathrm{d}t \,, \tag{54}$$

$$\int_{t_1}^{t_2} \Big(L(v + \tfrac{\mathrm{d}}{\mathrm{d}t}\delta x, x + \delta x, t) + F(v + \tfrac{\mathrm{d}}{\mathrm{d}t}\delta x, x + \delta x, t)\delta x \Big)\,\mathrm{d}t \,. \tag{55}$$

For $\delta x \to 0$, they both tend to the action integral $\int_{t_1}^{t_2} L(v,x,t)\,\mathrm{d}t$. For the present purpose, (55) is more suitable, since it minimizes the reference to the physical trajectory. The physical trajectory only enters as the 'starting point' of δx (since $\delta x = (x+\delta x) - x$) and will cancel out in the expressions to be considered.

In close analogy to section 2 we represent expression (55) along a short path

$$(x,t) \to (x',t') \to (\underline{x},\underline{t}) \tag{56}$$

by

$$\begin{aligned} &S(x,t;x',t';\underline{x},\underline{t}) := \\ &\quad (t'-t)L(\tfrac{x'-x}{t'-t},x',t') + (\underline{t}-t')L(\tfrac{\underline{x}-x'}{\underline{t}-t'},x',t') + \\ &\quad (\underline{t}-t)F(\tfrac{x'-x}{t'-t},x',t')(x' - x'_{\text{exact}})\,. \end{aligned} \tag{57}$$

The effect of F has to be considered as an impulse at time t' in order to make the description of conservative forces by either a potential or a force term equivalent. Therefore δx comes in only as $\delta x(t')$. Describing even conservative forces that way, offers a speed advantage. One gets an integrator which evaluates the force term only once per step and, therefore, is nearly as fast as the Euler method (see method MPMF in the next section).

Given a position x (in configuration space) of the initial state, we have to consider a system of paths which allows to determine the $n \cdot d$ components of the end position $\underline{x}$ after a time step. We will see that a sufficient set of paths can be constructed by prescribing $N := d+1$ velocities for each subsystem. As in section 2, the time step algorithm will update these velocities after each step. Therefore, it is only once, at the beginning of a trajectory, that we have to assign values to these velocities. This shall be done as follows: We choose a family $\eta = (\eta^1, \ldots, \eta^N)$ of unit vectors in $\mathbb{R}^d$ such that

$$\sum_{p=1}^{N} \eta^p = 0\,, \tag{58}$$

and each subsystem of d vectors is linearly independent. These vectors, together with a family $v = (v_1, \ldots, v_n), v_i \in \mathbb{R}^d$, of initial (mean) velocities of the subsystems, and a family $\Delta v = (\Delta v_1, \ldots, \Delta v_n), \Delta v_i \in \mathbb{R}$, of velocity spread parameters, will be used to define $n \cdot N$ paths

$$\Pi^{ip} \quad i \in \{1, \ldots, n\}\,, \quad p \in \{1, \ldots, N\}\,.$$

First we define the start velocities v^{ip} of Π^{ip} :

$$v^{ip} := v + \Delta v^{ip} , \quad \text{where} \quad (\Delta v^{ip})_j := \delta_{ij} \eta^p \Delta v_i \tag{59}$$

and the corresponding intermediate positions

$$y := x + \tau v , \quad y^{ip} := x + \tau v^{ip} = y + \tau \Delta v^{ip} . \tag{60}$$

The $n \cdot N$ paths then unite in a single end position $(\underline{x}, \underline{t})$.

$$\Pi^{ip} : (x,t) \to (y^{ip}, t') \to (\underline{x}, \underline{t}) , \quad t' := t + \tau , \quad \underline{t} := t' + \tau . \tag{61}$$

These paths reflect the subsystem structure. On path Π^{ip} every subsystem j with $j \neq i$ follows a path which is independent of p. The action along Π^{ip} is given by (compare (9))

$$S^{ip} := S(x,t; y^{ip}, t'; \underline{x}, \underline{t}) = \tag{62}$$

$$\tau T(v^{ip}, y^{ip}, t') + \tau T(\tfrac{\underline{x}-x}{\tau} - v^{ip}, y^{ip}, t') -$$
$$-2\tau V(y^{ip}, t') + 2\tau (y^{ip} - y_{\text{exact}}) F(v^{ip}, y^{ip}, t') . \tag{63}$$

Stated generally, the principle for selecting the end configuration $\underline{x}$ is to minimize the variation of S^{ip} from path to path. If we characterize the spread of the S^{ip} by a suitable function of merit, we can use numerical minimization methods for selecting $\underline{x}$. In that case, we easily take into account constraints of the system (even non-holonomic ones) by simply imposing them to the search space for $\underline{x}$ without changing the function of merit. This will, however, not be carried out here. We shall rather look for an analytical solution of a simple concrete version of the general principle. The first step is an approximation, which in the *special case* is an identity, and which keeps in p-dependent terms the lowest order in τ only.

$$\begin{aligned} S^{ip} \;\approx\; & \tau T(v^{ip}, y, t') + \tau T(\tfrac{\underline{x}-x}{\tau} - v^{ip}, y, t') - \\ & 2\tau V(y^{ip}, t') + 2\tau (y^{ip} - y_{\text{exact}}) F(v, y, t') =: \tau W^{ip} . \end{aligned} \tag{64}$$

Instead of the unknown $\underline{x}$, we introduce the velocity gain

$$u := \frac{\underline{x} - x}{\tau} - 2v \tag{65}$$

which equals zero if there is no interaction. Then we get

$$\begin{aligned} W^{ip} \;=\; & T(v + \Delta v^{ip}, y, t') + T(v + u - \Delta v^{ip}, y, t') - \\ & 2V(y^{ip}, t') + 2(y^{ip} - y_{\text{exact}}) F(v, y, t') \\ =\; & 2\big(T(\Delta v^{ip}, y, t') - T(\Delta v^{ip}, u, y, t') - V(y^{ip}, t')\big) + \\ & T(v + u, y, t') + T(v, y, t') + 2(y^{ip} - y_{\text{exact}}) F(v, y, t') . \end{aligned} \tag{66}$$

As stated above, we aim at determining u such that the values of W^{ip} vary as little as possible from path to path. To get simple equations, we stipulate for each i the quantity W^{ip} to be strictly constant as a function of p. This step corresponds to (8). To formulate p-independence, we introduce a notation for removing the mean value of a list $(A^p)_{p\in\{1,\ldots,N\}}$

$$\delta^p A^p := A^p - \frac{1}{N}\sum_{q=1}^{N} A^q \,. \tag{67}$$

Obviously, the condition that A is constant, can be written as

$$\delta^p A^p = 0 \quad \text{for all } p \,. \tag{68}$$

Posing this constancy condition for the W^{ip} eliminates the dependence on y_{exact}, and replaces most quantities by their subsystem components:

$$\begin{aligned} 0 = {} & \tfrac{1}{2}\delta^p W^{ip} = \\ & -\Delta v_i\, T_i(\eta^p, u_i, y_i, t') + \\ & \delta^p \left(\Delta v_i^2\, T_i(\eta^p, y_i, t') - V(y^{ip}, t')\right) + \tau \Delta v_i\, \eta^p F_i(v, y, t') \,. \end{aligned} \tag{69}$$

Therefore,

$$\begin{aligned} & \sum_{a,b=1}^{d} M_i(y_i, t')_{ab} (\eta^p)_a u_{ib} = \\ & \qquad \delta^p \left(\Delta v_i\, T_i(\eta^p, y_i, t') - \frac{V(y^{ip}, t')}{\Delta v_i}\right) + \tau \eta^p F_i(v, y, t') \,. \end{aligned} \tag{70}$$

Introducing the abbreviations

$$h_{ia} := \sum_{b=1}^{d} M_i(y_i, t')_{ab} u_{ib} \,, \tag{71}$$

and

$$g_{ip} := \delta^p \left(\Delta v_i\, T_i(\eta^p, y_i, t') - \frac{V(y^{ip}, t')}{\Delta v_i}\right) + \tau \eta^p F_i(v, y, t') \,, \tag{72}$$

and defining the (N, d)-matrix

$$\mathbf{H}_{pa} := (\eta^p)_a \tag{73}$$

we write equation (70) in the form

$$\sum_{a=1}^{d} \mathbf{H}_{pa} h_{ia} = g_{ip} \,. \tag{74}$$

This has the unique solution

$$h_{ib} = \sum_{p=1}^{d} \left(S^{-1}\right)_{bp} g_{ip} \,, \tag{75}$$

where the square matrix **S** is obtained from **H** by cancelling the last row. Let the generalized inverse [6] of **H**, which is a (d,N)- matrix, be denoted by $\mathbf{H}^{*}$. Then we have the more symmetrical representation

$$h_{ib} = \sum_{p=1}^{N} H^{*}{}_{bp}\, g_{ip} \tag{76}$$

which remains meaningful for more general prescriptions of N and η. Finally, we get u from (71) by inverting the matrix M_i of the quadratic form T_i :

$$u_{ia} = \sum_{b=1}^{d} \left(M_i(y_i,t')^{-1}\right)_{ab} h_{ib} \,. \tag{77}$$

The rest of the evolution step results easily as

$$\underline{v} := v + u \,, \quad \underline{x} := x + \tau(v + \underline{v}) \,, \quad \Delta\underline{v}^{ip} := -\Delta v^{ip} \,, \quad \underline{v}^{ip} := \underline{v} + \Delta\underline{v}^{ip} \,. \tag{78}$$

This corresponds to equations (15)–(19) from section 2 with the identification

$$a\Delta t = u. \tag{79}$$

Let us recapitulate the algorithm for the proposed integrator for Lagrangian (48):

1. Independent of the initial conditions we choose the family η (58), define matrix **H** (73) and calculate the generalized inverse $\mathbf{H}^{*}$.

2. Take the families $x, v, \Delta v$ from the initial conditions and calculate the path descriptors in (59) and (60).

3. Using (67), evaluate expression (72). Evaluate (76), (77).

4. Complete the step by calculating the quantities in (78).

5 A numerical Solar System example

The system under consideration consists of the sun and the nine (major) planets, described by non-relativistic mechanics and gravitation of point masses as the only forces. Values for positions and velocities of these bodies with respect to an inertial system of reference were derived from the heliocentric values for MJD 500120 and MJD 500320 in [9] and from the masses given there.

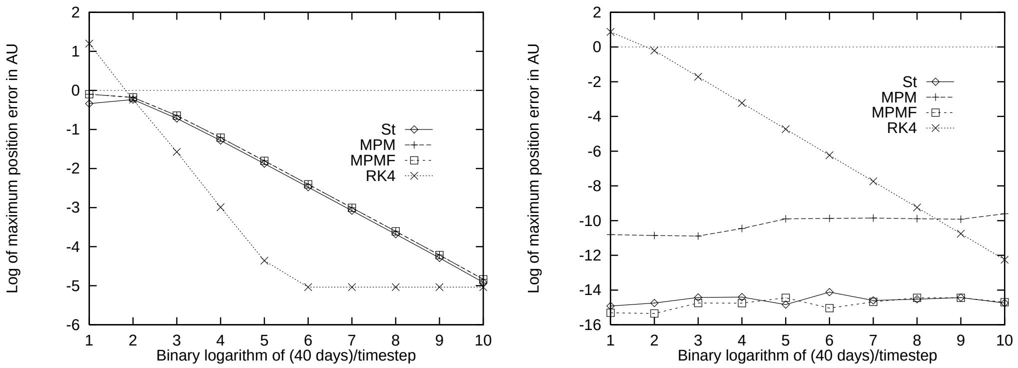
We compare three integration methods: The same Störmer method as in section 2 (St), method of section 4 with interaction described by potentials (MPM), and method of section 4 with interaction described by forces (MPMF), and the fourth order Runge-Kutta method for control purposes (RK4).

The velocity spread Δv for the MPM methods is set equal for all bodies and is determined by

$$\sum_{i=1}^{n} \frac{m_i}{2} \Delta v^2 = \alpha(T(v_0) + |V(x_0)|) \ , \tag{80}$$

where α is a dimension-less parameter, set to $\alpha = 10^{-4}$, and (v_0, x_0) is the initial state.

Figure 6(a) shows the decrease of the integration error from MJD 500120 to MJD 500320 as a function of increasing step number. The ordinate is the integration error, measured as $\log_{10}$ of the maximum separation of a computed planet position from the Almanac position in Astronomical Units. Not a surprise, the critical planet is always Mercury, who does 2.3 orbital revolutions in 200 day. We should not expect to get the end data exactly from the initial data since both data sets are rounded to the same number of digits and we would need more digits for the initial conditions. Also, the data in [9] include small effects such as those from relativity, which are not built into the present computations. Here the Störmer method is slightly more accurate than the MPM-methods. The latter give indistinguishable curves. The fourth order Runge-Kutta method reaches the final accuracy much faster than the second order methods. As a rough estimate of the computational complexity of the methods under consideration, these are my present computation times for an integration step in units of the corresponding Euler step: St 1.9, MPM 2.6, MPMF 1.24, and RK4 4.5. MPMF corresponds to (23), which also needs only as many force evaluation as the Euler method.



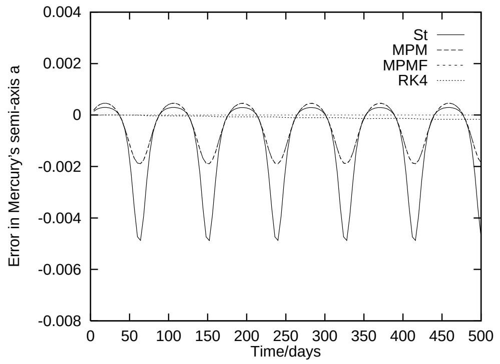
(a) Integration over 200 days

(b) Integration over 200 days with motion reversal after 100 days

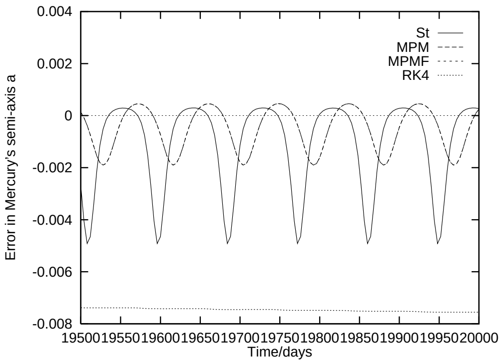
Figure 6: Behavior for successive reduction of the time step

Figure 6(b) shows the corresponding data for the artificial situation that the system evolves for 100 days, then is subjected to a motion reversal (all velocities get a minus sign), and evolves for further 100 days. An exact integration method would reproduce exactly the initial condition. The failure to do so is quantified by the same measure as in figure 6(a). Except of RK4 the methods are motion reversal invariant: the trajectory comes back rather precisely to the initial values even if the accuracy in forward direction is rather poor due to a large step size. The difference between the MPM-methods reflects different roundoff behavior.

To assess the stability of the methods, we extend the integration of our ten-particle system from 200 to 20000 days. We monitor Mercury, the fastest planet, who will be the first to suffer from instabilities. Figure 7 shows the (osculating) semi axis a of Mercury (actually, $(a-a_0)/a_0$, $a_0 = 0.387099$ AU) versus time. The time step is 2 days for integration and 4 days for data points. The subfigures show the beginning and the end of the integration. The correct value of the quantity is constantly zero far beyond drawing accuracy; the RK4-curve agrees with this for the first 100 days. Later, only the other methods show this constancy, apart from small deviations which are periodic with the revolution period of the computed planet. The RK4-value falls with increasing speed; a different integration with a time step of 3.5 days resulted in a Runge Kutta trajectory of Mercury impacting the sun and subsequently leaving the Solar System 30890 days after start. The two



(a) The first 500 days



(b) The last 500 days

Figure 7: Osculating semi-axis of Mercury as a stability test

MPM-curves are, again, indistinguishable. The phase shift between the St curve and the MPM curve is as suggested by the figure: It did not yet rise to more than a fraction of a full revolution. That the MPM curve comes closer to constancy than the Störmer curve is not sufficient evidence for a general ranking of the methods.

6 Outlook

The following topics seem to be within the range of the present method:

1. Practical dynamics for rigid bodies in contact.
2. Symmetric formulation with respect to position and momentum.
3. Extension to continuous systems.
4. Calculation of quantum corrections to classical mechanics.
5. Inclusion of relativity and retardation.
6. Extension to higher order.

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