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# Explicit Variable Stepsize and Time-Reversible Integration

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**Abstract**

In [10], a variable stepsize, semi-explicit variant of the explicit Störmer-Verlet method has been suggested for the time-reversible integration of Newton's equations of motion. Here we propose a fully explicit version of this approach applicable to explicit and symmetric integration methods for general time-reversible differential equations. This approach greatly simplifies the implementation of the method while providing a straightforward approach to higher-order reversible variable timestep integration. As applications, we discuss the variable stepsize, time-reversible, and fully explicit integration of rigid body motion and the Kepler problem.

## 1 Introduction

We consider the numerical treatment of differential equations

$$\frac{d}{dt}\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}) \tag{1}$$

which we assume to satisfy a *time-reversal symmetry* [20, 19], i.e., there exists an involution[1] $\boldsymbol{S}$ such that

$$\boldsymbol{f}(\boldsymbol{x}) = -\boldsymbol{S}\boldsymbol{f}(\boldsymbol{S}\boldsymbol{x}).$$

An example of such a differential equation is provided by the Newtonian equations of motion

$$\frac{d}{dt}\boldsymbol{q} = \boldsymbol{M}^{-1}\boldsymbol{p}, \tag{2}$$

$$\frac{d}{dt}\boldsymbol{p} = -\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}) \tag{3}$$

with $\boldsymbol{M}$ a symmetric, positive-definite mass matrix and $V(\boldsymbol{q})$ a potential energy function. The equations are time-reversible under the involution $(\boldsymbol{q},\boldsymbol{p}) \to (\boldsymbol{q},-\boldsymbol{p})$. Thus a solution $(\boldsymbol{q}(t),\boldsymbol{p}(t))$ of (2)-(3) forward in time ($t \geq 0$) with initial condition $(\boldsymbol{q}_0,\boldsymbol{p}_0)$ at $t=0$ satisfies

$$(\boldsymbol{q}(t),\boldsymbol{p}(t)) = (\bar{\boldsymbol{q}}(-t), -\bar{\boldsymbol{p}}(-t)), \qquad (t \geq 0),$$

where $\bar{\boldsymbol{q}}(t),\bar{\boldsymbol{p}}(t))$ is the solution of (2)-(3) backward in time ($t \leq 0$) with initial condition $(\boldsymbol{q}_0,-\boldsymbol{p}_0)$ at $t=0$. The time-reversible symmetry implies important restrictions on the possible solution behavior of time-reversible systems (1) [19]. For that reason it seems important to preserve this symmetry under numerical discretization. In fact, any *symmetric* partitioned Runge-Kutta method [7] will respect the time-reversal symmetry of (2)-(3) when used with a *constant stepsize* [20]. In many applications, however, the use of a constant stepsize would lead to enormous computational expense that could be avoided by the application of a *variable stepsize* integrator. As first demonstrated by Stoffer [20] and Hut, Makino & McMillan [9], variable stepsize, time-reversible integration methods can be constructed. The implementation of these methods leads, in general, to implicit

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[1] An involution $\boldsymbol{S}$ is a matrix that satisfies $\boldsymbol{S} = \boldsymbol{S}^{-1}$.

methods even though the underlying constant stepsize method is explicit. Significant progress has been achieved for the Newtonian equations of motion (2)-(3) by HUANG & LEIMKUHLER [10] by deriving a semi-explicit, variable stepsize, time-reversible modification of the Störmer-Verlet discretization [23, 7]

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}_{n+1/2}, \tag{4}$$

$$\boldsymbol{p}_{n+1/2} = \boldsymbol{p}_n - \frac{\Delta t}{2}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n), \tag{5}$$

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_{n+1/2} - \frac{\Delta t}{2}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}). \tag{6}$$

In this paper, we show that fully explicit variable stepsize time-reversible methods can easily be constructed for classical mechanical systems (2)-(3) based on the Störmer-Verlet method. This idea facilitates the development of explicit higher-order reversible variable stepsize integrators. This explicit variable stepsize strategy can be applied to general time-reversible differential equations (1), not just mechanical Hamiltonian systems, and in combination with general second order symmetric methods. As examples, we discuss the numerical solution of the Euler equations describing the motion of rigid bodies [12] and give a higher-order integrator for the Kepler problem.

## 2 Time-reversible, constant stepsize integration

For compactness of notation, we discuss the essential concepts of time-reversible integration in terms of general one-step methods

$$\boldsymbol{x}_{n+1} = \boldsymbol{\Phi}_{\Delta t}(\boldsymbol{x}_n) \tag{7}$$

applied to a time-reversible differential equation (1).

Let us denote the time-$\tau$-flow map of a differential equation (1) by $\boldsymbol{\Psi}_\tau$, i.e.

$$\boldsymbol{x}(t+\tau) = \boldsymbol{\Psi}_\tau(\boldsymbol{x}(t)).$$

The time-reversibility of (1) under the involution $\boldsymbol{S}$ implies that

$$\boldsymbol{\Psi}_{-\tau}(\boldsymbol{x}) = \boldsymbol{S}\boldsymbol{\Psi}_\tau(\boldsymbol{S}\boldsymbol{x}) \tag{8}$$

for all $\tau$ and all $\boldsymbol{x}$ in the domain of definition. Furthermore, since any flow map satisfies

$$[\boldsymbol{\Psi}_\tau]^{-1} = \boldsymbol{\Psi}_{-\tau}, \tag{9}$$

it follows that time-reversible differential equations generate time-reversible flow maps, i.e.

$$[\boldsymbol{\Psi}_\tau]^{-1}(\boldsymbol{x}) = \boldsymbol{S}\boldsymbol{\Psi}_\tau(\boldsymbol{S}\boldsymbol{x}) \tag{10}$$

for all $\tau$ and all $\boldsymbol{x}$ in the domain of definition. Here $[\boldsymbol{\Psi}_\tau]^{-1}$ denotes the inverse of the map $\boldsymbol{\Psi}_\tau$ ($\tau$ fixed).

**Definition.** A one-step method (7) is said to be *time-reversible* if the map $\boldsymbol{\Phi}_{\Delta t}$ is reversible, i.e.

$$[\boldsymbol{\Phi}_{\Delta t}]^{-1}(\boldsymbol{x}) = \boldsymbol{S}\boldsymbol{\Phi}_{\Delta t}(\boldsymbol{S}\boldsymbol{x}) \tag{11}$$

for all $\Delta t$ and all $\boldsymbol{x}$ in the domain of definition.

Most one-step methods, in particular all partitioned Runge-Kutta methods, satisfy

$$\boldsymbol{\Phi}_{-\Delta t}(\boldsymbol{x}) = \boldsymbol{S}\boldsymbol{\Phi}_{\Delta t}(\boldsymbol{S}\boldsymbol{x})$$

when applied to a reversible differential equation. However, only so called *symmetric* methods also satisfy

$$[\boldsymbol{\Phi}_{\Delta t}]^{-1} = \boldsymbol{\Phi}_{-\Delta t}$$

For example, the Störmer-Verlet method is symmetric while the following first order method

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}_{n+1}, \tag{12}$$

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_n - \Delta t \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n) \tag{13}$$

is not symmetric (and thus is not time-reversible).

Given a nonsymmetric method, a symmetric method can be derived as follows [7]: First we define the *adjoint method* $\boldsymbol{\Phi}^*_{\Delta t}$ of a given method $\boldsymbol{\Phi}_{\Delta t}$ by

$$\boldsymbol{\Phi}^*_{\Delta t} := [\boldsymbol{\Phi}_{-\Delta t}]^{-1}$$

(For symmetric methods we clearly have $\boldsymbol{\Phi}^*_{\Delta t} = \boldsymbol{\Phi}_{\Delta t}$.) Then a new method $\widetilde{\boldsymbol{\Phi}}_{\Delta t}$ is defined via the concatenation

$$\widetilde{\boldsymbol{\Phi}}_{\Delta t} := \boldsymbol{\Phi}^*_{\Delta t/2} \circ \boldsymbol{\Phi}_{\Delta t/2}. \tag{14}$$

This method is symmetric as seen from

$$\begin{aligned} \widetilde{\boldsymbol{\Phi}}^*_{\Delta t} &= \left[\boldsymbol{\Phi}^*_{-\Delta t/2} \circ \boldsymbol{\Phi}_{-\Delta t/2}\right]^{-1} \\ &= \left[[\boldsymbol{\Phi}_{\Delta t/2}]^{-1} \circ [\boldsymbol{\Phi}^*_{\Delta t/2}]^{-1}\right]^{-1} \\ &= \boldsymbol{\Phi}^*_{\Delta t/2} \circ \boldsymbol{\Phi}_{\Delta t/2} \\ &= \widetilde{\boldsymbol{\Phi}}_{\Delta t}. \end{aligned}$$

For example, the adjoint method of the first oder method (12)-(13) is given by

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}_n, \tag{15}$$

$$\boldsymbol{p}_{n+1} = \boldsymbol{p}_n - \Delta t \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}), \tag{16}$$

and the corresponding method (14) is equivalent to the Störmer-Verlet method. We also point out that both methods (12)-(13) and (15)-(16) are explicit. The Störmer-Verlet method is an example of an explicit partitioned Runge-Kutta method but it can also be viewed as a second-order composition method [18]. Higher order, explicit, and symmetric composition methods can, for example, be found in [13]. All of these methods can be written as a concatenation (14) of a lower order composition method with its adjoint. This will become important in the following section when we derive variable stepsize methods.

## 3 Explicit variable stepsize methods

As shown by Stoffer & Nipp [21], general variable stepsize one-step methods reduce asymptotically to the integration of a scaled differential equation

$$\frac{d}{ds}\boldsymbol{x} = \frac{1}{U(\boldsymbol{x})}\boldsymbol{f}(\boldsymbol{x}) \tag{17}$$

with a constant stepsize $\Delta s$. However, the corresponding scaling function $U$ does, in general, not satisfy the condition

$$U(\boldsymbol{x}) = U(\boldsymbol{S}\boldsymbol{x}). \tag{18}$$

Thus the differential equation (17) is no longer time reversible and the corresponding numerical method will not be reversible either.

A natural way to avoid this problem is to start out with an appropriate scaling function $U$ that satisfies (18) and to discretize the corresponding scaled differential equation (17) by a symmetric method and with constant stepsize $\Delta s$. In terms of the original time variable $t$ this is equivalent to integrating (1) with a variable stepsize $\Delta t_n \approx \Delta s / U(\boldsymbol{x}_n)$. This approach to variable stepsize integration is appealing but leads, in general, to implicit methods even though the underlying method applied to the unscaled equation (1) is explicit. For example, consider a classical mechanical system

(2)-(3) and a scaling function $U(\boldsymbol{q})$. A proper (symmetric) modification of the Störmer-Verlet method [7] would yield

$$
\begin{aligned}
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_n + \frac{\Delta s}{2U(\boldsymbol{q}_n) + 2U(\boldsymbol{q}_{n+1})} \boldsymbol{M}^{-1} \boldsymbol{p}_{n+1/2}, \\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{p}_n - \frac{\Delta s}{2U(\boldsymbol{q}_n)} \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n), \\
\boldsymbol{p}_{n+1} &= \boldsymbol{p}_{n+1/2} - \frac{\Delta s}{2U(\boldsymbol{q}_{n+1})} \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1})
\end{aligned}
$$

which is implicit in $U(\boldsymbol{q}_{n+1})$.

It was the idea of Huang & Leimkuhler to derive a variable stepsize modification of the Störmer-Verlet method by considering an additional fictive variable $\rho$ related to the scaling function $U$. The resulting variable stepsize Störmer-Verlet method, suggested in [10], is explicit if $U$ depends only on $\boldsymbol{q}$ and semi-explicit if $U$ also depends on $\boldsymbol{p}$. The method proposed next is a generalization (and also a simplification) of the Huang & Leimkuhler approach.

We describe our method for general systems (17). We assume[2] that we have an explicit, second order, and symmetric method $\widetilde{\boldsymbol{\Phi}}_{\Delta t}$ that can be written as the concatenation (14) of a method $\boldsymbol{\Phi}_{\Delta t/2}$ and its adjoint $\boldsymbol{\Phi}^*_{\Delta t/2}$.

Then, using the fictive variable $\rho$, the following method is an explicit, symmetric, and second order discretization of the scaled differential equation (17):

$$
\begin{aligned}
\boldsymbol{x}_{n+1/2} &= \boldsymbol{\Phi}_{\frac{\Delta s}{2\rho_n}}(\boldsymbol{x}_n), && (19)\\
\rho_{n+1} + \rho_n &= 2U(\boldsymbol{x}_{n+1/2}), && (20)\\
\boldsymbol{x}_{n+1} &= \boldsymbol{\Phi}^*_{\frac{\Delta s}{2\rho_{n+1}}}(\boldsymbol{x}_{n+1/2}). && (21)
\end{aligned}
$$

If the scaled differential equation (17) is time-reversible, then (19)-(21) is a time-reversible method.

Let us write out this compact notation for the Störmer-Verlet method. Using the two first order methods (12)-(13) and (15)-(16), we obtain

$$
\begin{aligned}
\boldsymbol{q}_{n+1/2} &= \boldsymbol{q}_n + \frac{\Delta s}{2\rho_n} \boldsymbol{M}^{-1} \boldsymbol{p}_{n+1/2}, && (22)\\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{p}_n - \frac{\Delta s}{2\rho_n} \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n), && (23)\\
\rho_{n+1} + \rho_n &= 2U(\boldsymbol{q}_{n+1/2}, \boldsymbol{p}_{n+1/2}), && (24)\\
\boldsymbol{p}_{n+1} &= \boldsymbol{p}_{n+1/2} - \frac{\Delta s}{2\rho_{n+1}} \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}), && (25)\\
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_{n+1/2} + \frac{\Delta s}{2\rho_{n+1}} \boldsymbol{M}^{-1} \boldsymbol{p}_{n+1/2}. && (26)
\end{aligned}
$$

This method is fully explicit and symmetric. Thus it is time-reversible if the scaling function $U$ satisfies $U(\boldsymbol{q}, \boldsymbol{p}) = U(\boldsymbol{q}, -\boldsymbol{p})$. It can be shown to be equivalent to the variable stepsize Störmer-Verlet method suggested in [10] if $U$ depends only on $\boldsymbol{q}$. The general semi-explicit formulation of [10] is recovered from (22)-(26) by replacing the update (24) by

$$
\rho_{n+1} + \rho_n = U(\boldsymbol{q}_{n+1/2}, \boldsymbol{p}_{n+1}) + U(\boldsymbol{q}_{n+1/2}, \boldsymbol{p}_n).
$$

To start the integration, one can use $\rho_0 = U(\boldsymbol{x}_0)$ as initial value for the fictive variable $\rho$. As discussed in [4] for the variable stepsize Störmer-Verlet method, this choice of the initial $\rho_0$ might lead to "wobbles" in the numerically computed $\rho_n$'s. This can be avoided by an appropriately modified initialization of $\rho_0$ [4].

Another crucial issue is the choice of the scaling function $U$. As suggested in [10], one possibility is $U(\boldsymbol{x}) = ||\boldsymbol{f}(\boldsymbol{x})||_2$. Other choices can, for example, be found in [8]. In that article, a scaling

[2] This assumption is, for example, satisfied for symmetric composition methods based on the Strang splitting and generalizations thereof [22, 13, 18].

function, based on a local error estimator for the Störmer-Verlet method, has been derived for the Newtonian equations of motion (2)-(3); namely

$$U(\boldsymbol{q},\boldsymbol{p}) = \sqrt{V'(\boldsymbol{q})V'(\boldsymbol{q})^T + \boldsymbol{p}^T\boldsymbol{M}^{-1}V''(\boldsymbol{q})V''(\boldsymbol{q})\boldsymbol{M}^{-1}\boldsymbol{p}}$$

with $V'(\boldsymbol{q}) = \boldsymbol{\nabla}_{\boldsymbol{q}}V(\boldsymbol{q})^T$ the Jacobian and $V''(\boldsymbol{q})$ the Hessian of the potential energy $V$ at $\boldsymbol{q}$.

The original time variable $t$ is recovered from the update

$$t_{n+1} = t_n + \frac{\Delta s}{2}\left[\frac{1}{\rho_n} + \frac{1}{\rho_{n+1}}\right]$$

which is a discretization of

$$\frac{dt}{ds} = \frac{1}{U(\boldsymbol{x})}.$$

Other choices of of the scaling function have been developed in the context of integration of few-body systems with inverse power potentials [2].

Note that the suggested symmetric, variable stepsize method (19)-(21) is not restricted to second-order methods. Often higher-order methods for time-reversible differential equations are based on an appropriate concatenation of a symmetric second-order method. For example, let $\boldsymbol{\Phi}_{\Delta t}^{SV}$ denote the map defined by (4)-(6). Then, following YOSHIDA [24], the following concatenated method

$$\widetilde{\boldsymbol{\Phi}}_{\Delta t} := \boldsymbol{\Phi}_{c_1\Delta t}^{SV} \circ \boldsymbol{\Phi}_{c_2\Delta t}^{SV} \circ \boldsymbol{\Phi}_{c_1\Delta t}^{SV} \tag{27}$$

with $c_1 = (2 - 2^{1/3})^{-1}$ and $c_2 = 1 - 2c_1$ is symmetric and of fourth order in $\Delta t$. In a corresponding variable stepsize method, the symmetric, variable stepsize version of the Störmer-Verlet method (22)-(26) could be used as a building block. Thus, denoting the variable stepsize method (22)-(26) by $\boldsymbol{\Phi}_{\Delta s}^{ASV}$, the concatenated method

$$\widetilde{\boldsymbol{\Phi}}_{\Delta t} := \boldsymbol{\Phi}_{c_1\Delta s}^{ASV} \circ \boldsymbol{\Phi}_{c_2\Delta s}^{ASV} \circ \boldsymbol{\Phi}_{c_1\Delta s}^{ASV}$$

yields a symmetric and fourth-order (in $\Delta s$) discretization of the scaled differential equation (17). More generally, higher-order methods can be obtained by using the symmetric composition methods described, for example, in [13] and the second-order symmetric method (19)-(21) as the basic method.

# 4 Examples

## 4.1 Kepler problem

We consider the planar Kepler problem with Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

and initial conditions $q_1(0) = 1 - e$, $q_2(0) = 0$, $p_1(0) = 0$, $p_2(0) = \sqrt{(1+e)/(1-e)}$ corresponding to an orbit of period $2\pi$ and eccentricity $e$. This problem and its variable stepsize integration were carefully studied in [3]. It was found that the fourth order Gauss-Legendre method [7] combined with a symplectic variable stepsize strategy [6, 17] performs best among variable stepsize geometric integration methods of order two and four and that this method may also outperform standard integration software. In particular, it was also demonstrated that, despite its simplicity, the adaptive Störmer-Verlet method was not competitive due to its low (second) order accuracy.

As pointed out in §3, higher order variants of the fully explicit Störmer-Verlet method can, however, be found. We implemented a fourth order method based on Yoshida's concatenation (27) and integrated the Kepler problem over 1025 periods with an eccentricity of $e = 0.9$ using the scaling function

$$U(\boldsymbol{q}) = \left(q_1^2 + q_2^2\right)^{3/2}$$

and $\Delta s \in [0.0025, \ldots, 0.02]$. The results are shown in Fig. 1. It can be seen that the method is indeed of fourth order and that, upon comparing the result to Fig. 3 in [3], the method is competitive with the fourth-order Gauss-Legendre implementation of the symplectic variable stepsize approach. To clearly demonstrate the advantage of using a higher-order method, we also show in Fig. 1 the results for the second-order adaptive Störmer-Verlet method.

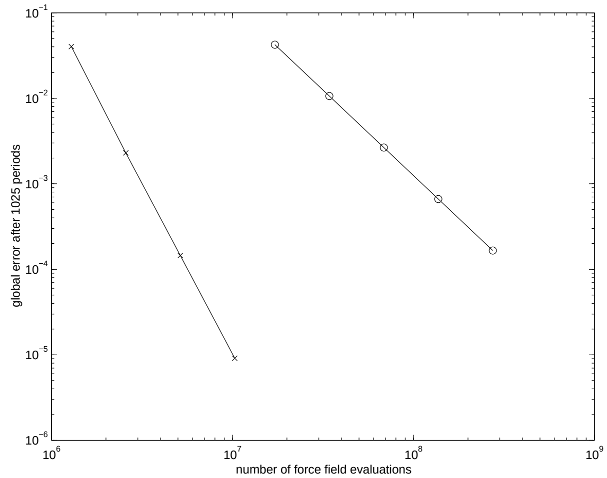


Figure 1: Error in the coordinates $\boldsymbol{q}$ after 1025 periods of eccentricity $e = 0.9$ with the fourth-order adaptive method (27) (x) and the second-order adaptive Störmer-Verlet method (o).

## 4.2 Rigid body dynamics

For classical mechanical systems, the variable stepsize Störmer-Verlet method (22)-(26) is essentially equivalent to the method of Huang & Leimkuhler. The advantage of the approach suggested in this paper becomes clear when looking at systems that cannot be discretized by the Störmer-Verlet method but which can be integrated by second-order reversible splitting methods. An example is the Euler equation [12]

$$\frac{d}{dt}\boldsymbol{\pi} = \boldsymbol{\pi} \times \boldsymbol{I}^{-1}\boldsymbol{\pi} + \boldsymbol{\tau}(\boldsymbol{Q}), \tag{28}$$

$$\frac{d}{dt}\boldsymbol{Q} = \boldsymbol{Q}\widehat{\boldsymbol{I}^{-1}\boldsymbol{\pi}} \tag{29}$$

for the rotation of a rigid body with fixed center of mass and applied torque $\boldsymbol{\tau}$. Here $\boldsymbol{\pi} \in R^3$, $\boldsymbol{Q} \in SO(3)$, $\boldsymbol{I}$ the diagonal moment of inertia matrix, and $\widehat{\boldsymbol{v}}$ the skew-symmetric $3 \times 3$-matrix associated with a vector $\boldsymbol{v} \in R^3$ such that $\boldsymbol{v} \times \boldsymbol{u} = \widehat{\boldsymbol{v}}\boldsymbol{u}$ [12].

The equations (28)-(29) are time-reversible under the involution $(\boldsymbol{Q}, \boldsymbol{\pi}) \to (\boldsymbol{Q}, -\boldsymbol{\pi})$.

An explicit second-order method based on an appropriate splitting of the equations of motion into integrable subsystems has been proposed by Reich [15] (see also Dullweber, Leimkuhler & McLachlan [5] for application to multiple rigid body molecular simulations). This method is time-reversible and preserves the orthogonality of the numerically computed matrices $\boldsymbol{Q}_n$, i.e. $\boldsymbol{Q}_n \in SO(3)$. The idea is to use a special first order integrator for the free rigid body equations

$$\frac{d}{dt}\boldsymbol{\pi} = \boldsymbol{\pi} \times \boldsymbol{I}^{-1}\boldsymbol{\pi}, \tag{30}$$

$$\frac{d}{dt}\boldsymbol{Q} = \boldsymbol{Q}\widehat{\boldsymbol{I}^{-1}\boldsymbol{\pi}} \tag{31}$$

and its adjoint method. See the Appendix for details. Let us denote these methods by $\boldsymbol{\Phi}^{RB}_{\Delta t}$, $\boldsymbol{\Phi}^{RB*}_{\Delta t}$ respectively. Then a symmetric, constant stepsize method for the equations (28)-(29) is given by

$$\begin{aligned} \bar{\boldsymbol{\pi}}_n &= \boldsymbol{\pi}_n + \frac{\Delta t}{2}\boldsymbol{\tau}(\boldsymbol{Q}_n), \\ (\bar{\boldsymbol{\pi}}_{n+1}, \boldsymbol{Q}_{n+1}) &= \boldsymbol{\Phi}^{RB*}_{\Delta t/2} \circ \boldsymbol{\Phi}^{RB}_{\Delta t/2}\,(\bar{\boldsymbol{\pi}}_n, \boldsymbol{Q}_n), \\ \boldsymbol{\pi}_{n+1} &= \bar{\boldsymbol{\pi}}_{n+1} + \frac{\Delta t}{2}\boldsymbol{\tau}(\boldsymbol{Q}_{n+1}). \end{aligned}$$

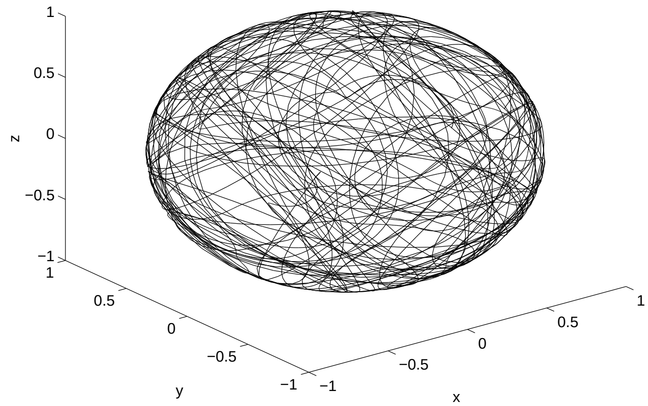


Figure 2: Motion of a material point on the rigid body over time which is "non-regularly" distributed over the unit sphere.

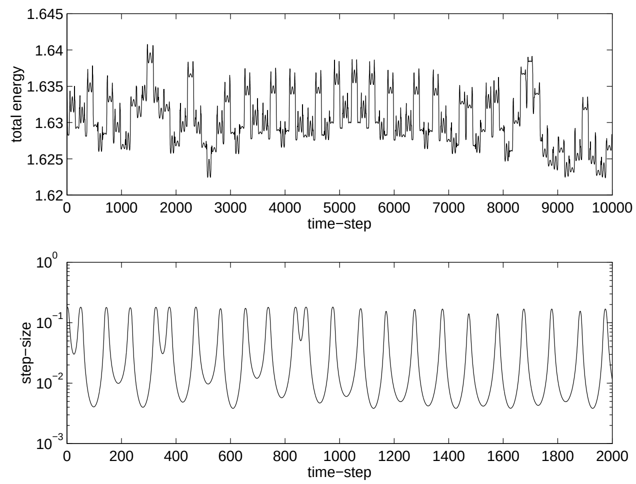


Figure 3: Top: Total energy $E$ for $\Delta s = 0.1$ (10000 integration steps). Buttom: stepsize $\Delta t$ for the variable stepsize integrator with $\Delta s = 0.1$ (2000 integration steps).

This method can be turned into a variable stepsize method. Following (19)-(21), we obtain

$$
\begin{aligned}
\bar{\boldsymbol{\pi}}_n &= \boldsymbol{\pi}_n + \frac{\Delta s}{2\rho_n}\boldsymbol{\tau}(\boldsymbol{Q}_n),\\
(\boldsymbol{\pi}_{n+1/2}, \boldsymbol{Q}_{n+1/2}) &= \boldsymbol{\Phi}^{RB}_{\frac{\Delta s}{2\rho_n}}(\bar{\boldsymbol{\pi}}_n, \boldsymbol{Q}_n),\\
\rho_{n+1} + \rho_n &= 2U(\boldsymbol{\pi}_{n+1/2}, \boldsymbol{Q}_{n+1/2}),\\
(\bar{\boldsymbol{\pi}}_{n+1}, \boldsymbol{Q}_{n+1}) &= \boldsymbol{\Phi}^{RB*}_{\frac{\Delta s}{2\rho_{n+1}}}(\boldsymbol{\pi}_{n+1/2}, \boldsymbol{Q}_{n+1/2}),\\
\boldsymbol{\pi}_{n+1} &= \bar{\boldsymbol{\pi}}_{n+1} + \frac{\Delta s}{2\rho_{n+1}}\boldsymbol{\tau}(\boldsymbol{Q}_{n+1}).
\end{aligned}
$$

In general, the equations (28)-(29) have to be supplemented by the equations for the center of mass motion [15, 5]. Since these are of type (2)-(3), they can be discretized by the variable stepsize Störmer-Verlet method (22)-(26) and the resulting variable stepsize integrator for rigid body dynamics is of second order and time-reversible.

**Numerical Example.** As an illustration, we consider the motion of a rigid body with moment of inertia matrix

$$\boldsymbol{I} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4.5 \end{bmatrix}$$

and applied torque

$$\boldsymbol{\tau}(\boldsymbol{Q}) = \mu(Q_{33}) \begin{bmatrix} -Q_{32} \\ +Q_{31} \\ 0 \end{bmatrix}$$

with

$$\mu(Q_{33}) = -(\beta + Q_{33})^{-2} + 10\sigma(\beta + Q_{33})^{-11},$$

$\beta = 1.1$, and $\sigma = 0.001$. This represents a torque coming from an attractive (Coulombic) potential coupled with a repulsive "soft" wall, relative to a plane situated just below the rigid body. The rigid body is repeatedly drawn towards the plane, then repelled sharply from the "wall".

The repelling torque has to be resolved by a relatively small stepsize and provides a good test example for the variable stepsize method. As the scaling function $U$, we chose

$$U(\boldsymbol{Q}) = 0.5 + (\beta + Q_{33})^{-4}.$$

The corresponding equations of motion possess the total energy

$$E = \frac{\boldsymbol{\pi}^T \boldsymbol{I}^{-1} \boldsymbol{\pi}}{2} - (\beta + Q_{33})^{-1} + \sigma(\beta + Q_{33})^{-10}$$

as a first integral. The initial conditions are $\boldsymbol{\pi}_0 = [2, 2, 2]$ and

$$\boldsymbol{Q}_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The computed motion of a material point on the rigid body can be found in Fig. 2. The error in the total energy $E$ and the actual stepsize $\Delta t_n = \Delta s/\rho_n$ is given in Fig. 3. The conservation of total energy is comparable to constant stepsize, time-reversible integration. However, many fewer integration steps are needed. The average stepsize $\Delta t$ in Fig. 3 is about 0.0439 while a constant stepsize implementation would have to use a stepsize of $\Delta t = 0.0038$.
Other applications of the variable stepsize method described in §3 include constrained mechanical systems [1] and regularized perturbed Kepler motion [11].

# Appendix

Since the moment of inertia matrix $\boldsymbol{I}$ in (30)-(31) is assumed to be diagonal, we can write

$$\boldsymbol{I}^{-1} = \boldsymbol{J}_1 + \boldsymbol{J}_2 + \boldsymbol{J}_3$$

with $\boldsymbol{J}_i$ having zero entries except for the diagonal element $J_{ii}$, $i = 1, 2, 3$. Thus the Euler equation (30)-(31) can be considered as the sum of the three Euler equations

$$\frac{d}{dt}\boldsymbol{\pi} = \boldsymbol{\pi} \times \boldsymbol{J}_i \boldsymbol{\pi}, \quad (32)$$

$$\frac{d}{dt}\boldsymbol{Q} = \boldsymbol{Q}\widehat{\boldsymbol{J}_i \boldsymbol{\pi}}, \quad (33)$$

$i = 1, 2, 3$, each of which can be solved exactly and corresponds to a planar rotation over a fixed axis. As suggested in [14, 16], a first order approximation $\boldsymbol{\Phi}_{\Delta t}^{RB}$ to the time-$\Delta t$-flow map of (30)-(31) is now given by concatenation of the time-$\Delta t$-flow maps of (32)-(33) using the sequence $i = 1, 2, 3$. Its adjoint method $\boldsymbol{\Phi}_{\Delta t}^{RB*}$ is obtained by using the reverse sequence $i = 3, 2, 1$.

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