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Explicit Variable Step-Size and Time-Reversible Integration

Preprint SC 98-17 (July 1998)

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3rd July 1998

Abstract

In [9], a variable step-size, semi-explicit variant of the explicit Störmer-Verlet method has been proposed 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. As applications, we discuss the variable step-size, time-reversible, and fully explicit integration of rigid body motion and reversible Nosé-Hoover dynamics.

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* [19, 18], 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) [18]. For that reason it seems important to preserve this symmetry under numerical discretization. In fact, any *symmetric* partitioned Runge-Kutta method [4] will respect the time-reversal symmetry of (2)-(3) when used with a *constant step-size* [19]. In many applications, however, the use of a constant step-size would lead to enormous computational expense that could be avoided by the application of a *variable step-size* integrator. As first demonstrated by Stoffer [19] and Hut, Makino & McMillan [8], variable step-size, time-reversible integration methods can be devised. The implementation of these methods leads, in general, to implicit methods even though the underlying constant step-size method is explicit. Significant progress has been

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

achieved for the Newtonian equations of motion (2)-(3) by HUANG & LEIMKUHLER [9] by deriving a semi-explicit, variable step-size, time-reversible modification of the Störmer-Verlet discretization [22, 4]

$$
\begin{aligned}
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}_{n+1/2}, && (4)\\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{q}_n - \frac{\Delta t}{2}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n), && (5)\\
\boldsymbol{p}_{n+1} &= \boldsymbol{p}_{n+1/2} - \frac{\Delta t}{2}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}). && (6)
\end{aligned}
$$

The purpose of this paper is twofold. First we derive a fully explicit, variable step-size, and time-reversible methods for classical mechanical systems (2)-(3) based on the Störmer-Verlet method. Second we discuss our approach in the context of general time-reversible differential equations (1) and second order symmetric methods. We also show how to obtain higher order, variable step-size, and time-reversible methods.

As examples, we discuss the Euler equations describing the motion of rigid bodies [11] and the Nosé-Hoover formulation for constant temperature molecular dynamics [7].

2 Time-reversible, constant step-size 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-τ-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 τ 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 τ and all $\boldsymbol{x}$ in the domain of definition. Here $[\boldsymbol{\Psi}_\tau]^{-1}$ denotes the inverse of the map $\boldsymbol{\Psi}_\tau$ (τ 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 Δt and all $\boldsymbol{x}$ in the domain of definition.

Most numerical 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 not time-reversible).

Given a non-symmetric method, a symmetric method can be derived as follows [4]: 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 like to 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 [17]. Higher order, explicit, and symmetric composition methods can, for example, be found in [12]. All 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 step-size methods.

3 Explicit variable step-size methods

As shown by Stoffer & Nipp [20], general variable step-size 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 step-size Δs. 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 step-size Δs. In terms of the original time variable t this is equivalent to integrating (1) with a variable step-size $\Delta t_n \approx \Delta s / U(\boldsymbol{x}_n)$. This approach to variable step-size 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 [4] 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 step-size modification of the Störmer-Verlet method by considering an additional fictive variable ρ related to the scaling function U. The resulting variable step-size Störmer-Verlet method, suggested in [9], 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 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 $\boldsymbol{\Phi}_{\Delta t}$ and its adjoint $\boldsymbol{\Phi}^*_{\Delta t}$.

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

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

Here

$$
\boldsymbol{\Phi}_{\frac{\Delta s}{2\rho_n}}(\boldsymbol{x}_n) = \boldsymbol{\Phi}_{\frac{1}{2}\Delta t_n}(\boldsymbol{x}_n), \qquad \text{with} \qquad \Delta t_n := \frac{\Delta s}{\rho_n} \tag{22}
$$

and

$$
\boldsymbol{\Phi}^*_{\frac{\Delta s}{2\rho_{n+1}}}(\boldsymbol{x}_{n+1/2}) = \boldsymbol{\Phi}^*_{\frac{1}{2}\Delta t_{n+1}}(\boldsymbol{x}_{n+1/2}), \qquad \text{with} \qquad \Delta t_{n+1} := \frac{\Delta s}{\rho_{n+1}}
$$

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

$$
\begin{aligned}
\boldsymbol{q}_{n+1/2} &= \boldsymbol{q}_n + \frac{\Delta s}{2\rho_n}\boldsymbol{M}^{-1}\boldsymbol{p}_{n+1/2}, && (23) \\
\boldsymbol{p}_{n+1/2} &= \boldsymbol{p}_n - \frac{\Delta s}{2\rho_n}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_n), && (24) \\
\rho_{n+1} + \rho_n &= 2U(\boldsymbol{q}_{n+1/2}, \boldsymbol{p}_{n+1/2}), && (25) \\
\boldsymbol{p}_{n+1} &= \boldsymbol{p}_{n+1/2} - \frac{\Delta s}{2\rho_{n+1}}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_{n+1}), && (26) \\
\boldsymbol{q}_{n+1} &= \boldsymbol{q}_{n+1/2} + \frac{\Delta s}{2\rho_{n+1}}\boldsymbol{M}^{-1}\boldsymbol{p}_{n+1/2}. && (27)
\end{aligned}
$$

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 step-size Störmer-Verlet method suggested in [9] if U depends only on $\boldsymbol{q}$. The general semi-explicit formulation of [9] is recovered from (23)-(27) by replacing the update (25) by

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

[2]This assumption is, for example, satisfied for symmetric composition methods based on the Strang splitting and generalizations thereof [21, 12, 17].

To start the integration, one can use $\rho_0 = U(\boldsymbol{x}_0)$ as initial value for the fictive variable ρ. As discussed in [2] for the variable step-size Störmer-Verlet method, this choice of the initial ρ_0 might lead to "wobbles" in the numerically computed ρ_n's. This can be avoided by an appropriately modified initialization of ρ_0 [2].

Another crucial issue is the choice of the scaling function U. As suggested in [9], one possibility is $U(\boldsymbol{x}) = ||\boldsymbol{f}(\boldsymbol{x})||_2$. Other choices can, for example, be found in [5]. In particular, a scaling 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 $V'(\boldsymbol{q}) = \boldsymbol{\nabla_q} V(\boldsymbol{q})^T$ 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

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

which is a discretization of

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

Note that the suggested symmetric, variable step-size 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 [23], the following concatenated method

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

with $c_1 = (2 - 2^{3/2})^{-1}$ and $c_2 = 1 - 2c_1$ is symmetric and of fourth order in Δt. In a corresponding variable step-size method, the symmetric, variable step-size variant of the Störmer-Verlet method (23)-(27) could be used as a building block. Thus, denoting the variable step-size method (23)-(27) 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 Δs) 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 [12] and the second order symmetric method (19)-(21) as the basic method.

4 Examples

4.1 Rigid body dynamics

For classical mechanical systems, the variable step-size Störmer-Verlet method (23)-(27) is basically equivalent to the method of Huang & Leimkuhler. The advantage of the approach suggested in this paper becomes clear when looking at systems that cannot (or should not) be discretized by the Störmer-Verlet method. An example is the Euler equation [11]

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

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

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 3×3-matrix associated with a vector $\boldsymbol{v} \in R^3$ such that $\boldsymbol{v} \times \boldsymbol{u} = \widehat{\boldsymbol{v}}\boldsymbol{u}$ [11].

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] and DULLWEBER, LEIMKUHLER &

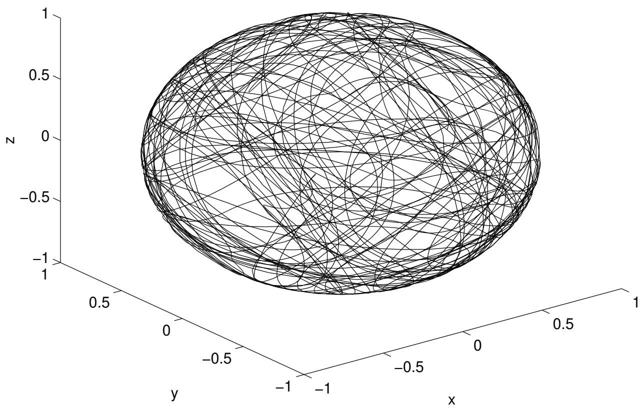

Figure 1: Motion of a material point on the rigid body over time which is "non-regularly" distributed over the unit sphere.

McLachlan [3]. This method is also time-reversible and preserves the orthogonality of the numerically computed matrices $\boldsymbol{Q}_n$, i.e. $\boldsymbol{Q}_n \in SO(3)$. The basic idea is to use a special first order integrator for the free rigid body equations

$$\begin{aligned} \frac{d}{dt}\boldsymbol{\pi} &= \boldsymbol{\pi} \times \boldsymbol{I}^{-1}\boldsymbol{\pi}, && (30) \\ \frac{d}{dt}\boldsymbol{Q} &= \boldsymbol{Q}\widehat{\boldsymbol{I}^{-1}\boldsymbol{\pi}} && (31) \end{aligned}$$

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 step-size method for the equations (28)-(29) is given by

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

This method can be turned into a variable step-size 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, 3]. Since these are of type (2)-(3), they can be discretized by the variable step-size Störmer-Verlet method (23)-(27) and the overall variable step-size integrator for rigid body dynamics is second order and time-reversible.

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

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

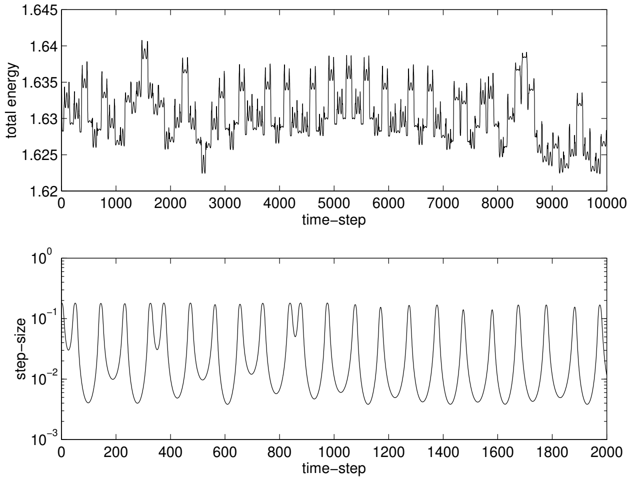

Figure 2: Top: Total energy E for $\Delta s = 0.1$ (10000 integration steps). Buttom: Step-size Δt for the variable step-size integrator with $\Delta s = 0.1$ (2000 integration steps).

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 step-size and provides a good test example for the variable step-size 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. 1. The error in the total energy E and the actual step-size $\Delta t_n = \Delta s/\rho_n$ is given in Fig. 2. The conservation of total energy is comparable to constant step-size, time-reversible integration. However, many fewer integration steps are needed. The average step-size Δt in Fig. 2 is about 0.0439 while a constant step-size implementation would have to use a step-size of $\Delta t = 0.0038$.

4.2 Reversible Nosé-Hoover Dynamics

Often, molecular dynamics is treated in the so-called constant temperature ensemble. The equations of motion are given in a time-reversible formulation due to Nosé and Hoover.

The derivation begins with the canonical Nosé extended Hamiltonian which, for a system of particles, takes the form[3] [14]:

$$\mathcal{H}_{\text{Nosé}} = \frac{1}{2z^2}\boldsymbol{p}^T\boldsymbol{M}^{-1}\boldsymbol{p} + V(\boldsymbol{q}) + \frac{1}{2Q}\pi_z^2 + \frac{g}{\beta}\ln z.$$

The equations of motion are thus

$$\begin{aligned}
\frac{d}{dt}\boldsymbol{q} &= \frac{1}{z^2}\boldsymbol{M}^{-1}\boldsymbol{p},\\
\frac{d}{dt}\hat{\boldsymbol{p}} &= -\boldsymbol{\nabla}\boldsymbol{V}(\boldsymbol{q}),\\
\frac{dz}{dt} &= \pi_z/Q,\\
\frac{d\pi_z}{dt} &= \frac{1}{z}\left(\frac{1}{z^2}\boldsymbol{p}^T\boldsymbol{M}^{-1}\boldsymbol{p} - \frac{g}{\beta}\right).
\end{aligned}$$

The Hoover formulation is typically derived via a time-transformation followed by a coordinate transformation. We begin here instead with a coordinate transformation:

$$\xi = \frac{1}{Q}\pi_z, \qquad \hat{\boldsymbol{p}} = \frac{\boldsymbol{p}}{z}.$$

The definition of ξ appears to have a slightly different form at this point than that used by Hoover, since the time and coordinate transformation do not commute. In these new variables, the equations of motion become

$$\begin{aligned}
\frac{d}{dt}\boldsymbol{q} &= \frac{1}{z}\boldsymbol{M}^{-1}\hat{\boldsymbol{p}}, && (32)\\
\frac{d}{dt}\hat{\boldsymbol{p}} &= -\frac{1}{z}\boldsymbol{\nabla}\boldsymbol{V}(\boldsymbol{q}) - \frac{1}{z}\xi\hat{\boldsymbol{p}}, && (33)\\
\frac{dz}{dt} &= \xi, && (34)\\
\frac{d\xi}{dt} &= \dot{\pi}_z/Q, &&\\
&= (\frac{1}{z^2}\boldsymbol{p}^T\boldsymbol{M}^{-1}\boldsymbol{p} - \frac{g}{\beta})/(Qz), &&\\
&= (\hat{\boldsymbol{p}}^T\boldsymbol{M}^{-1}\hat{\boldsymbol{p}} - \frac{g}{\beta})/(Qz). && (35)
\end{aligned}$$

Finally a time transformation $dt/d\tau = z$ results in the system

$$\begin{aligned}
\frac{d}{d\tau}\boldsymbol{q} &= \boldsymbol{M}^{-1}\hat{\boldsymbol{p}}, && (36)\\
\frac{d}{d\tau}\hat{\boldsymbol{p}} &= -\boldsymbol{\nabla}\boldsymbol{V}(\boldsymbol{q}) - \xi\hat{\boldsymbol{p}}, && (37)\\
\frac{d\xi}{d\tau} &= (\hat{\boldsymbol{p}}^T\boldsymbol{M}^{-1}\hat{\boldsymbol{p}} - \frac{g}{\beta})/Q, && (38)\\
\frac{dz}{d\tau} &= \xi z, && (39)
\end{aligned}$$

which are identical to the equations arrived at in [7]. A symmetric second order discretization has been suggested in [6].

The system (36)-(39) is time-reversible under the involution

$$\boldsymbol{S}\left(\begin{bmatrix}\boldsymbol{q}\\ \hat{\boldsymbol{p}}\\ z\\ \xi\end{bmatrix}\right) = \left(\begin{bmatrix}\boldsymbol{q}\\ -\hat{\boldsymbol{p}}\\ z\\ -\xi\end{bmatrix}\right).$$

[3] The variable z is equivalent to the variable s in [14, 7].

and the time-transformation $dt/d\tau = z$ obviously preserves the symmetry.

In analogy to rigid body motion, a fully explicit, symmetric, and second order discretization of the equations (36)-(39) can be obtained by an appropriate splitting of the differential equation into integrable subproblems. For example, one could use the splitting

$$\begin{aligned}
\frac{d}{d\tau}\boldsymbol{q} &= \boldsymbol{M}^{-1}\hat{\boldsymbol{p}}, \\
\frac{d}{d\tau}\hat{\boldsymbol{p}} &= \boldsymbol{0}, \\
\frac{d\xi}{d\tau} &= (\hat{\boldsymbol{p}}^T\boldsymbol{M}^{-1}\hat{\boldsymbol{p}} - \frac{g}{\beta})/Q, \\
\frac{dz}{d\tau} &= 0,
\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{d\tau}\boldsymbol{q} &= \boldsymbol{0}, \\
\frac{d}{d\tau}\hat{\boldsymbol{p}} &= -\boldsymbol{\nabla V}(\boldsymbol{q}) - \xi\hat{\boldsymbol{p}}, \\
\frac{d\xi}{d\tau} &= 0, \\
\frac{dz}{d\tau} &= \xi z,
\end{aligned}$$

A first order approximation $\boldsymbol{\Psi}_{\Delta\tau}$ to the time-$\Delta\tau$-flow map of (36)-(39) is now given by the concatenation of the exact time-$\Delta\tau$-flow maps of these two differential equations. Its adjoint method $\boldsymbol{\Psi}^*_{\Delta\tau}$ is obtained by reversing the order in the concatenation of these two exact flow maps.

Using these two methods and a scaling function $U(\boldsymbol{q}, z)$, i.e. a time transformation $d\tau/ds = U(\boldsymbol{q}, z)$, a time-reversible and variable step-size method for the Nosé-Hoover dynamics (36)-(39) can now be constructed using the general recipe (19)-(21). Note that Δt has to be replaced by $\Delta\tau$, i.e. $\Delta\tau_n := \Delta s/\rho_n$ in (22). In particular, a second order method for the equations (32)-(35) is obtained upon using $U(\boldsymbol{q}, z) = z$.

Other applications of the variable step-size method described in §3 include constrained mechanical systems [1] and regularized perturbed Kepler motion [10].

Acknowledgements. We thank Peter Deuflhard for his interest and stimulating remarks.

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

$$\frac{d}{dt}\boldsymbol{\pi} = \boldsymbol{\pi} \times \boldsymbol{J}_i\boldsymbol{\pi}, \tag{40}$$

$$\frac{d}{dt}\boldsymbol{Q} = \boldsymbol{Q}\widehat{\boldsymbol{J}_i\boldsymbol{\pi}}, \tag{41}$$

$i = 1, 2, 3$, each of which can be solved exactly and corresponds to a planar rotation over a fixed axis. As suggested in [13, 16], a first order approximation $\boldsymbol{\Phi}^{RB}_{\Delta t}$ to the time-Δt-flow map of (30)-(31) is now given by concatenation of the time-Δt-flow maps of (40)-(41) using the sequence $i = 1, 2, 3$. Its adjoint method $\boldsymbol{\Phi}^{RB*}_{\Delta t}$ is obtained by using the reverse sequence $i = 3, 2, 1$.

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