Symplectic Integration with Variable Stepsize*

Robert D. Skeel

Department of Computer Science and Beckman Institute (University of Illinois at Urbana-Champaign), 304 West Springfield Avenue, Urbana, Illinois 61801-2987, USA

Jeffrey J. Biesiadecki

Jet Propulsion Laboratory, 4800 Oak Grove Drive, M/S 301-345 Pasadena, California 91109, USA

There is considerable evidence suggesting that for Hamiltonian systems of ordinary differential equations it is better to use numerical integrators that preserve the symplectic property of the flow of the system, at least for long-time integrations. We present what we believe is a practical way of doing symplectic integration with variable stepsize. Another idea, orthogonal to variable stepsize, is the use of different stepsizes for different processes. In applications like classical molecular dynamics it has been found advantageous, because of the wide range of time-scales present, to use multiple time steps, in which different terms of the right-hand side are integrated with different time steps. It is possible to use multiple time steps so as to preserve the symplectic property. Our proposal for variable stepsize makes use of the machinery of multiple time stepping. The idea is to decompose an interaction into a sum of interactions: shorter-range interactions to be sampled at frequent intervals and smoother longer-range interactions to be sampled at less frequent intervals.

Keywords: leapfrog method, Störmer method, Verlet method, symplectic method, canonical method, multiple-time-step methods, distance class methods, symplectic integrator, molecular dynamics simulation, variable stepsize.

Subject classification: AMS(MOS):65L07,70H15 CR:G.1.3.

1. Introduction

There is considerable evidence suggesting that for Hamiltonian systems of ordinary differential equations it is better to use numerical integrators that pre-

* This work was supported in part by National Science Foundation Grant DMS 90 15533 and National Institutes of Health Grant PHS 2 P41 RR05969-03. Work of the second author was completed while at the University of Illinois.

serve the symplectic property of the flow of the system, at least for long-time integrations [8]. However, if a method that is symplectic for fixed stepsize is applied with variable stepsize, there is observed a degradation in accuracy [2, 4] (however, see [7]). Moreover, it also loses, in the most simple-minded sense, the symplectic property [9]. In this paper we present what we believe is a practical way of doing symplectic integration with variable stepsize. Some of the elements of this method are currently in use in molecular dynamics (MD). Another way of varying the stepsize, based on using a partition of unity to split the Hamiltonian, is given by [6].

It is well accepted that varying the stepsize can greatly improve performance for many problems. Another idea, orthogonal to variable stepsize, is the use of different stepsizes for different processes. If we identify processes with subsystems of the ODE system, then we have a multirate method [3]. However, it seems more appropriate to identify processes with "interaction terms" of the right-hand side of the ODE system.[1] This is an problem-dependent idea, which nonetheless seems applicable in an obvious way to many applications. For example, in MD the potential energy is a vast sum of 2-, 3-, and 4-body interactions, which provides natural decomposition of the right-hand side. In a multiple-time-step method [10], different terms would be evaluated with different frequencies. For bonded interactions a fixed stepsize may be appropriate. For nonbonded interactions the strength of the interaction drops off rapidly as the distance between particles increases, and variable stepsize is appropriate.

Our proposal for variable stepsize makes use of the machinery of multiple time stepping. For purposes of illustration we consider the use of two stepsizes h and Nh. The idea is to split an interaction into a sum of two interactions: a *short-range* interaction to be sampled at periods of h plus a *smooth* long-range interaction to be sampled at periods of Nh. The short-range interaction is constructed to be nonzero only in those parts of phase space where a stepsize of h is appropriate. Hence, if we are outside the active region of the short-range interaction, we can omit its evaluation and the stepsize is effectively Nh. As a practical matter the cost of determining whether we are in the active region needs to be considerably less than the cost of evaluating the interaction itself. Also, the cost of computing the decomposed interactions needs to be only a little more than the cost of the original interaction.

Section 2 provides more details of the proposed method, Section 3 gives some early numerical results, Section 4 presents an untested improvement and generalization, and Section 5 reports a curiosity discovered in the process of numerical testing.

[1] Nonetheless, it is true that by a change of variables multiple time stepping can often be expressed as a multi-rate method.

2. Some details

We consider the special separable Hamiltonian

$$H(R,P) = \frac{1}{2}P^{\mathrm{T}}M^{-1}P + V(R)$$

where R is the vector consisting of all position coordinates, P is the vector of momentum coordinates, M is a diagonal matrix of masses (each mass replicated three times), and $V(R)$ is the potential energy. The resulting Hamiltonian system of ODEs is

$$\frac{d}{dt}R = M^{-1}P,$$

$$\frac{d}{dt}P = F(R)$$

where the forces $F(R) = -\nabla_R V(R)$. Because the system is autonomous, there is a mapping φ_h, called the *flow*, which maps a solution value $(R(t), P(t))$ to the value $(R(t+h), P(t+h))$. This mapping is a *symplectic* transformation because its Jacobian matrix φ_h' satisfies

$$(\varphi_h')^{\mathrm{T}} \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \varphi_h' = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

The popular Encke/Störmer/leapfrog/Verlet method integrates from time nh to $(n+1)h$ as follows. We begin the step with values R_n, P_n, and $F_n = F(R_n)$ obtained from the previous step. Then we compute

$$\begin{aligned} P_{n+1/2} &= P_n + \tfrac{h}{2}F_n, \\ R_{n+1} &= R_n + hM^{-1}P_{n+1/2}, \\ F_{n+1} &= F(R_{n+1}), \\ P_{n+1} &= P_{n+1/2} + \tfrac{h}{2}F_{n+1}. \end{aligned}$$

This can be shown to define a symplectic map from (R_n, P_n) to (R_{n+1}, P_{n+1}). To do this, one decomposes the map as $(R_n, P_n) \mapsto (R_n, P_{n+1/2}) \mapsto (R_{n+1}, P_{n+1/2}) \mapsto (R_{n+1}, P_{n+1})$ and uses the fact that the composition of symplectic maps is also symplectic and the Jacobian matrix of $F(R)$ is symmetric.

The Verlet method can be generalized to multiple time steps in various ways [5], most of which destroy the symplecticness. There is a way to retain symplecticness [1], which we describe for multiple stepsizes h and Nh. Suppose we express $V = V^{\mathrm{hard}} + V^{\mathrm{soft}}$ and correspondingly partition the force vector. Then define

$$F_n = \begin{cases} F_n^{\mathrm{hard}} + N F_n^{\mathrm{soft}}, & n \text{ a multiple of N}, \\ F_n^{\mathrm{hard}}, & \text{otherwise}. \end{cases}$$

This retains the second-order accuracy of the Verlet method as well as its symplectic property. It is called the *Verlet-I* method in [5, 1].

In order to effect variable stepsize, we do an *artificial* partitioning of an interaction V into a short-range interaction and a smooth long-range interaction. For example, consider the potential energy

$$V(r) = \frac{C}{r},$$

such as might occur due to gravitational or electrostatic attraction. We can split this into

$$V^{\mathrm{soft}}(r) = \begin{cases} C(2r_{\mathrm{cut}} - r)r_{\mathrm{cut}}^{-2}, & r \le r_{\mathrm{cut}}, \\ Cr^{-1}, & r \ge r_{\mathrm{cut}}, \end{cases}$$

and

$$V^{\mathrm{hard}}(r) = \begin{cases} C(r_{\mathrm{cut}} - r)^2 r_{\mathrm{cut}}^{-2} r^{-1}, & r \le r_{\mathrm{cut}}, \\ 0, & r \ge r_{\mathrm{cut}}, \end{cases}$$

where for $r \le r_{\mathrm{cut}}$ we have chosen $V^{\mathrm{soft}}(r)$ to be the first two terms of the Taylor series expansion of $V(r)$ thus ensuring C^1 continuity and second-order accuracy. If we wish to allow for a third yet longer stepsize, we can split $V^{\mathrm{soft}}(r)$, and so on.

In practical three-dimensional simulations the potential energy is $C\|\boldsymbol{r}_B - \boldsymbol{r}_A\|^{-1}$ and the test $\|\boldsymbol{r}_B - \boldsymbol{r}_A\|^2 < r_{\mathrm{cut}}^2$ is considerably cheaper to perform than is the computation of the force, because of the square root. Moreover, when $r_{AB} \gg r_{\mathrm{cut}}$ it may be possible to limit the testing to the beginning of every *macrostep* when n is a multiple of N. The Verlet-I method has a physical interpretation, in which the forces are approximated by periodic impulses with positions changing linearly with time between impulses. Thus it may be possible with little computation to predict when the next impulse is due. If not, then it may be satisfactory to take risks based on probabilities obtained, say, from statistical mechanics.

3. Numerical experiments

We tested the idea on the Kepler problem, used by Calvo and Sanz-Serna [2] to show the degrading effect of variable stepsize. The position $R = [x, y]^{\mathrm{T}}$, $M = I$, and $V(x, y) = -(x^2 + y^2)^{-1/2}$. Initial conditions are

$$\begin{aligned} x(0) &= 1 - e, \qquad \dot{x}(0) = 0, \\ y(0) &= 0, \qquad \dot{y}(0) = \sqrt{\tfrac{1+e}{1-e}}, \end{aligned}$$

where e is a free parameter, $0 \le e < 1$, which equals the eccentricity of the orbit. The experiments use $e = 0.9$. The period of revolution is 2π.

The experiments use $r_{\mathrm{cut}} = 1$, which is a somewhat arbitrary choice that happens to encompass exactly half of the elliptical orbit. To achieve meaningful comparative results, the numerical solution was in all cases sampled at increments of $2\pi/M$ with $M = 100$ for a total simulation time of $P = 100$ periods. Figure 1 shows the numerical trajectory at sampling points for one period.

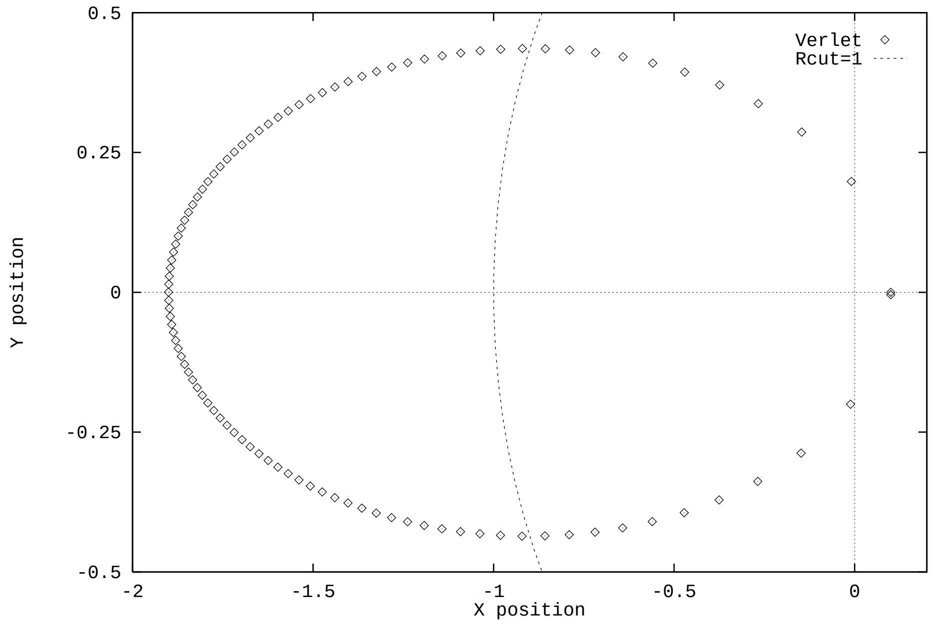

Fig. 1. Numerical trajectory.

Two measures of accuracy were used. One is the average relative error in energy, $E(nh) = \frac{1}{2}(\dot{x}_n^2 + \dot{y}_n^2) - (x_n^2 + y_n^2)^{-1/2}$, which is supposed to be conserved. The formula is

$$\frac{1}{PM} \sum_{k=1}^{PM} \left| \frac{E(k \cdot 2\pi/M) - E(0)}{E(0)} \right|.$$

The other is a measure of the deviation of the position (x, y) from the elliptical orbit $(x+e)^2 + y^2/(1-e^2) = 1$. The formula is

$$\frac{1}{PM} \sum_{k=1}^{PM} |D(k \cdot 2\pi/M)|$$

where

$$D(nh) := \sqrt{(x_n + e)^2 + y_n^2/(1-e^2)} - 1.$$

Figure 2 shows the results of using different stepsizes h ranging from $2\pi/10000$

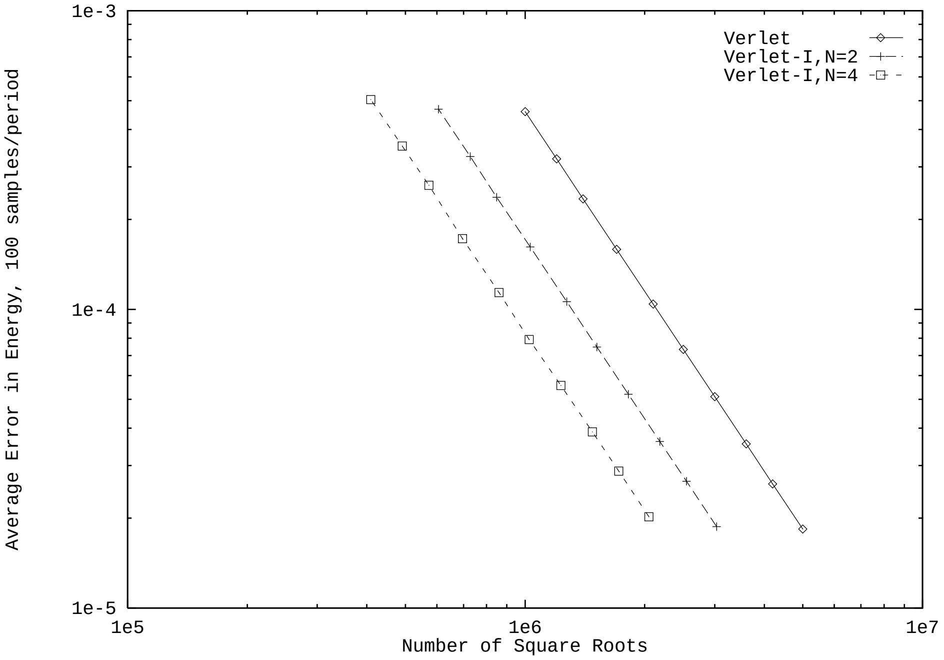

Fig. 2. Average relative error in energy.

down to $2\pi/50000$ for each of $N = 1$ (fixed stepsize), $N = 2$ (stepsizes h and $2h$), and $N = 4$ (stepsizes h and $4h$). The vertical axis measures the average relative error in energy. The horizontal axis gives the cost of an integration in terms of the number of time points at which a force evaluation is required, which equals the number of square roots needed. Figure 3 f shows the same experiments with accuracy measured by relative deviation from the orbit. We observe that for any given accuracy, $N = 4$ is most efficient followed by $N = 2$ and $N = 1$. We also deduce from the -2 slope of each curve that the methods are second-order accurate.

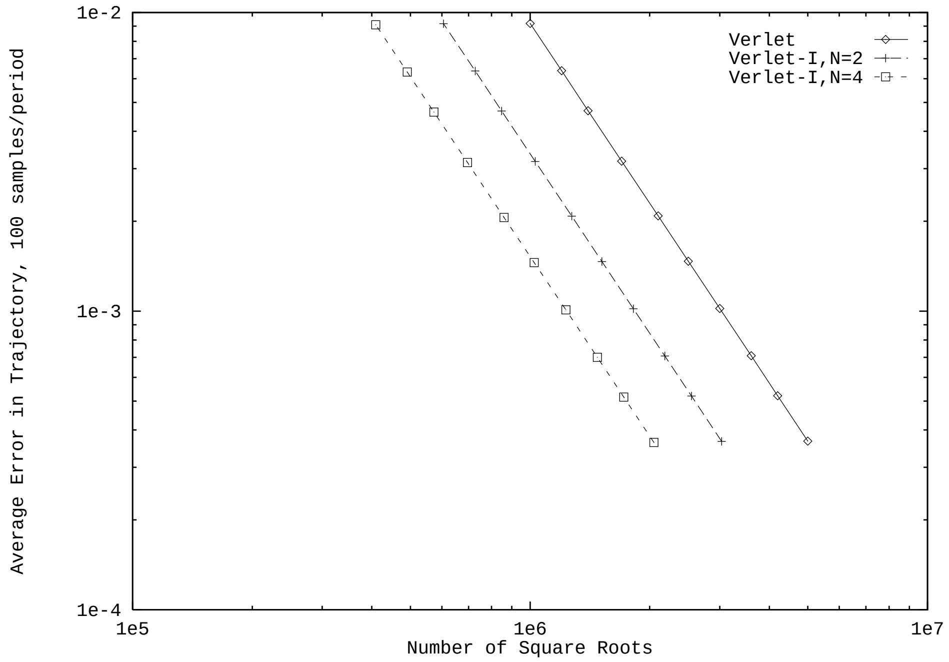

Fig. 3. Average relative error in position.

4. Possible improvement and generalization

It may be possible to improve the splitting proposed in Section 2 because the potential energy $V^{\rm soft}$ is not smooth. We would like $V^{\rm soft}\left(\sqrt{x^2+y^2}\right)$ to have bounded second derivatives with respect to x and y as $\sqrt{x^2+y^2} \to 0$, but this is not the case. To avoid this, we should instead choose $V^{\rm soft}$ so that $V^{\rm soft}(\sqrt{s})$ is smooth for $s < r_{\rm cut}^2$, which can be accomplished by using, for $s \leq r_{\rm cut}^2$, a truncated Taylor expansion for $V(\sqrt{s})$ about $s = r_{\rm cut}^2$:

$$V^{\rm soft}(\sqrt{s}) = V(r_{\rm cut}) + \left(s - r_{\rm cut}^2\right) V'(r_{\rm cut}) / (2 r_{\rm cut}),$$

hence

$$V^{\rm soft}(r) = C\left(\frac{3}{2} r_{\rm cut}^2 - \frac{1}{2} r^2\right) r_{\rm cut}^{-3}$$

and $V^{\rm hard} = V - V^{\rm soft}$.

Also, we can generalize the scheme to a set of cutoff radii $0 < r_1 < r_2 < \cdots < r_m$. Define

$$V_k(r) = \begin{cases} C\left(\frac{3}{2} r_k^2 - \frac{1}{2} r^2\right) r_k^{-3}, & r \leq r_k, \\ \frac{C}{r}, & r \geq r_k, \end{cases}$$

and use as a splitting

$$V = (V - V_1) + (V_1 - V_2) + \cdots + (V_{m-1} - V_m) + V_m,$$

where the term $V_k - V_{k+1}$ is used with stepsize $2^k h$. This means using expressions like

$$(V - V_1) + 2(V_1 - V_2) + \cdots + 2^k(V_k - V_{k+1})$$

to compute the force vector. This calculation simplifies if the r_k form a geometric progression. A truncation error analysis suggests that an appropriate ratio is $r_{k+1}/r_k = 2^{3/2}$.

5. A curiosity

In early experiments we sampled the relative error in energy only at integer multiples of the period. We observed sixth-order behavior. What was expected, based on [2], was fourth-order accuracy. In Figure 4, we show the results of an

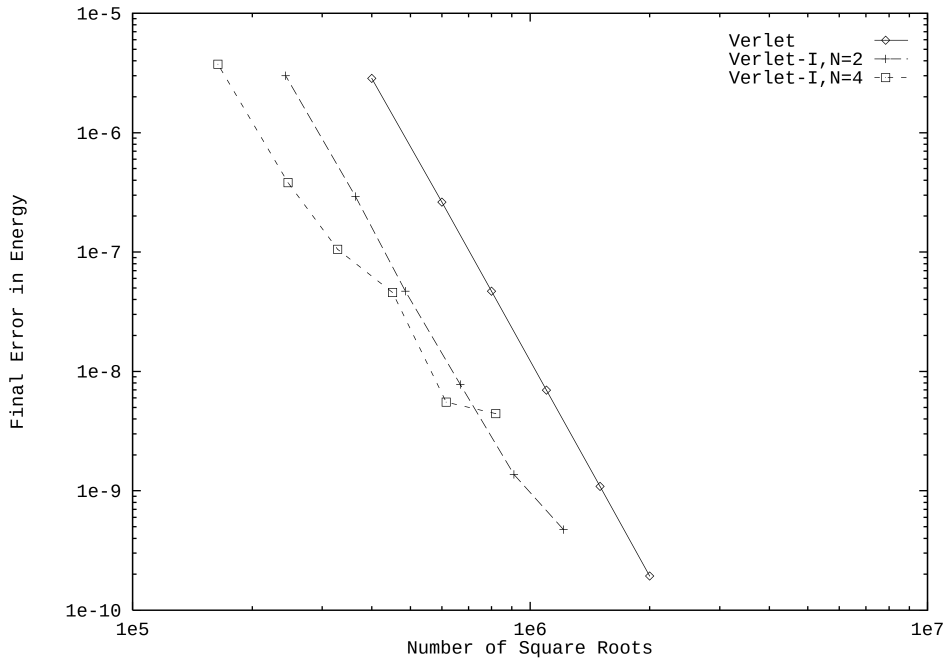

Fig. 4. Error in energy at end of simulation.

experiment with $e = 0.9$, $P = 10$, $r_{\text{cut}} = 1$, and h ranging from $2\pi/40000$ down to $2\pi/200000$. For the fixed-stepsize case $N = 1$ the slope is -6; for the cases $N = 2, 4$ the slope is -6 until the stepsize gets very small.

Acknowledgment

We are grateful to Daniel Okunbor for independently confirming the sixth-order accuracy observed in the preceding section.

References

[1] J.J. Biesiadecki and R.D. Skeel, Dangers of multiple-time-step methods, J. Comput. Phys. to appear.
[2] M.P. Calvo and J.M. Sanz-Serna, The development of variable-step symplectic integrators, with application to the two-body problem, SIAM J. Sci. Comput. 14 (1993) 936-952.
[3] C.W. Gear and D.R. Wells, Multirate linear multistep methods, BIT 24 (1984) 484-502.
[4] B. Gladman, M. Duncan, and J. Candy, Symplectic integrators for long-term integrations in celestial mechanics, Celestial Mech. Dynamical Astronomy 52 (1991) 221-240.
[5] H. Grubmüller, H. Heller, A. Windemuth, and K. Schulten, Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range interactions, Molecular Simulation 6 (1991) 121-142.
[6] W. MacEvoy and J.C. Scovel, Integrators with variable stepsize for Hamiltonian systems, technical report, Los Alamos National Lab., in preparation.
[7] D. Okunbor, Variable step size does not harm second-order integrators for Hamiltonian systems, J. Comput. Appl. Math. 47 (1993) to appear.
[8] J.M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: an overview, Acta Numerica 1 (1992) 243-286.
[9] R.D. Skeel and C.W. Gear, Does variable step size ruin a symplectic integrator?, Physica D 60 (1992) 311-313.
[10] W.B. Streett, D.J. Tildesley, and G. Saville, Multiple time step methods in molecular dynamics, Mol. Phys. 35 (1978) 639-648.