JOURNAL OF COMPUTATIONAL PHYSICS 115, 245–247 (1994)

NOTE

An Approximate Time Evolution Operator to Generate the Verlet Algorithm

Approaches to the integration of the classical equations of motion based upon approximations to the classical time development operator have been applied in astrophysics, lattice gauge theory, and chemical dynamics [1, 3, 4, 6]. These methods lead to strategies for numerical integration of the classical equations of motion to any desired accuracy as well as assuring that the integrations preserve reversibility. Recently, Sexton and Weingarten [3] and Tuckerman, Berne, and Martyna [4] have shown how such methods can be applied to systems with disparate time scales in the context of the hybrid Monte Carlo approach to field theory and molecular simulations, respectively. Sexton and Weingarten are also able to present explicit error expressions for any symmetric decomposition of the time development operator.

Strangely though, one of the most fundamental integrators used in MD simulations, the Verlet algorithm [2], apparently does not fit into this framework as pointed out by Tuckerman, Berne, and Martyna. Since the Verlet algorithm is a widely used integration scheme for MD simulations, it is interesting to ask how the method may be derived within a symplectic approach to MD. The method makes use of the Poisson bracket

$$L(H)f(p, q) = \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right) \tag{1}$$

which for a function $f(t) = f[p(t), q(t)]$ allows the equations of motion to be written

$$\frac{d}{dt}f(t) = L(H)f(t). \tag{2}$$

The evolution of a variable is then given by

$$f(t) = \exp[t\,L(H)]f(0). \tag{3}$$

The observation is then made that an approximation to the exponential

$$\begin{aligned}\exp[\Delta t\,L(H)] \approx \exp[\Delta t\,L(h_n)] &\times \dots \times \exp[\Delta t\,L(h_2)]\\ &\times \exp[\Delta t\,L(h_1)]\\ &\times \exp[\Delta t\,L(h_2)]\\ &\times \dots \times \exp[\Delta t\,L(h_n)]\end{aligned} \tag{4}$$

with

$$L(H) = L(h_1) + 2\sum_{i=2}^{n} L(h_i) \tag{5}$$

has certain advantages when formulating an integration scheme [1, 3, 4, 6]. The symmetry of the factorization assures for any decomposition of $L(H)$ that the resulting time evolution is reversible. Furthermore, the scheme is measure preserving and the error to any order is easily obtained from the Baker–Hausdorff formula [3, 6].

Now let us turn to the Verlet algorithm by considering an *asymmetric* factorization of the evolution operator

$$\exp[\Delta t\,L(H)] \approx \exp[\Delta t\,L(h_2)]\exp[\Delta t\,L(h_1)] \tag{6}$$

with

$$\begin{aligned}L(h_1) &= \frac{p}{m}\frac{\partial}{\partial q}\\ L(h_2) &= -\frac{\partial U(q)}{\partial q}\frac{\partial}{\partial p}.\end{aligned} \tag{7}$$

Two things can be said about the approximation:

1. the Baker–Hausdorff formula implies an error of $\mathcal{O}[(\Delta t)^2]$ since

$$[L(h_2), L(h_1)] \neq 0, \tag{8}$$

2. time reversibility is apparently not satisfied since

$$\begin{aligned}&\exp[-\Delta t\,L(h_2)]\\ &\exp[-\Delta t\,L(h_1)]\exp[\Delta t\,L(h_2)]\exp[\Delta t\,L(h_1)] \neq 1.\end{aligned} \tag{9}$$

A position update from Eq. 6 is given by

$$\begin{aligned}q^{i+1} &= \exp[\Delta t\,L(h_2)]\exp[\Delta t\,L(h_1)]q^i\\ &= q^i + \frac{\Delta t}{m}p^i - \frac{(\Delta t)^2}{m}\frac{\partial U(q^i)}{\partial q^i}\end{aligned} \tag{10}$$

0021-9991/94 $6.00

and, similarly, the momenta are updated as

$$p^{i+1} = \exp[\Delta t\, L(h_2)] \exp[\Delta t\, L(h_1)]p^i = p^i - \Delta t \frac{\partial U(q^i)}{\partial q^i}. \tag{11}$$

Superscripts are being used to denote time increments. Note that the position update is correct only through $\mathcal{O}[(\Delta t)]$ and, likewise, the momentum update is the Taylor series expansion of p^{i+1} truncated after the first order in Δt: these errors in the positions and momenta are the errors anticipated from the Baker–Hausdorff formula. An equivalent truncated expansion for the momenta can be obtained from Eq. (10) for the updated positions as

$$m\left(\frac{q^{i+1} - q^i}{\Delta t}\right) = p^i - \Delta t \frac{\partial U(q^i)}{\partial q^i} = \vec{p}^{\,i+1} \tag{12}$$

and the forward arrow has been introduced to designate that the momentum update is for positive time propagation. Now an expression for the position updates in terms of the updated momenta equation (12) may be written as

$$q^{i+1} = 2q^i - q^{i-1} - \frac{(\Delta t)^2}{m} \frac{\partial U(q^i)}{\partial q^i} \tag{13}$$

which is the standard form of the Verlet algorithm. As is well known, the Verlet integration scheme as written is *time reversible.*[1] Also, the integration is accurate to $\mathcal{O}[(\Delta t)^4]$ [5] since if q^i, q^{i-1} are known exactly, then expanding q^{i-1} in a Taylor series results in

$$q^{i+1} = q^i + \Delta t \frac{d}{dt} q^i + \frac{(\Delta t)^2}{2!} \frac{d^2}{dt^2} q^i + \frac{(\Delta t)^3}{3!} \frac{d^3}{dt^3} q^i - \frac{(\Delta t)^4}{4!} \frac{d^4}{dt^4} q^i + \ldots \tag{14}$$

which is correct to fourth order. To start the position integrations, it is required to specify q^i, q^{i-1} exactly. The updated coordinate q^{i+1} is then predicted correctly up to $\mathcal{O}[(\Delta t)^4]$ due to the use of the *updated* momenta and a consequent fortuitous cancellation of the error.[2]

Reversibility in the Verlet algorithm arises from asymmetry in the momenta updates depending upon whether the coordinates are propagated forward or backward in time. A position update for negative time is given by

$$q^{i-1} = \exp[-\Delta t\, L(h_2)] \exp[-\Delta t\, L(h_1)]q^i = q^i - \frac{\Delta t}{m} p^i - \frac{-(\Delta t)^2}{m} \frac{\partial U(q^i)}{\partial q^i} \tag{15}$$

and the backward momenta are updated as

$$p^{i-1} = \exp[-\Delta t\, L(h_2)] \exp[-\Delta t\, L(h_1)]p^i = p^i + \Delta t \frac{\partial U(q^i)}{\partial q^i}. \tag{16}$$

As for forward time propagation, the backward momenta may be expressed in terms of the position updates:

$$m\left(\frac{q^i - q^{i-1}}{\Delta t}\right) = p^i + \Delta t \frac{\partial U(q^i)}{\partial q^i} = \overleftarrow{p}^{\,i-1} \tag{17}$$

and the backward arrow has been introduced to designate that the momentum update is for negative time propagation. For positive time propagation the approximate time development operator requires use of the backward difference operator in defining the momenta, whereas for negative time propagation the momenta are defined in terms of the forward finite difference operator. The differences in the updating scheme for forward and backward time propagation is shown in Fig. 1. This asymmetry in time gives rise to the reversibility of the Verlet algorithm,

$$q^{i-1} = 2q^i - q^{i+1} - (-\Delta t)^2 \frac{1}{m} \frac{\partial U(q^i)}{\partial q^i}, \tag{18}$$

which retraces the same trajectory generated by Eq. (13). Equivalently, the time reversibility of the algorithm can be seen directly from

$$\exp[-\Delta t\, L(h_2)] \exp[-\Delta t\, L(h_1)] \exp[\Delta t\, L(h_2)] \exp[\Delta t\, L(h_1)]q^i = q^i \tag{19}$$

if the appropriate forward and backward momenta are used for positive or negative time increments:

$$\begin{aligned} \exp[-\Delta t\, L(h_2)] \exp[-\Delta t\, L(h_1)]q^{i+1} &= q^{i+1} - \frac{\Delta t}{m}\left(\overleftarrow{p}^{\,i+1} + \Delta t \frac{\partial U(q^{i+1})}{\partial q^{i+1}}\right) \\ &= q^{i+1} - \frac{\Delta t}{m} \overleftarrow{p}^{\,i} \\ &= q^i. \end{aligned} \tag{20}$$

[1] In its simplest formulation, the Verlet algorithm is manifestly time symmetric. Newton's equation is approximated by a finite difference equation $F = m\ddot{q} = (m/\Delta t^2)\, \Delta_t \Delta_t q$. For a symmetric time difference operator, reversibility is assured.

[2] The error terms from the Baker–Hausdorff formula arising from use of the approximate time evolution operator may be compared to those in the Taylor series expansion with the replacement $d/dt \rightarrow (p/m)(\partial/\partial q) - (\partial U(q)/\partial q)(\partial/\partial p)$.

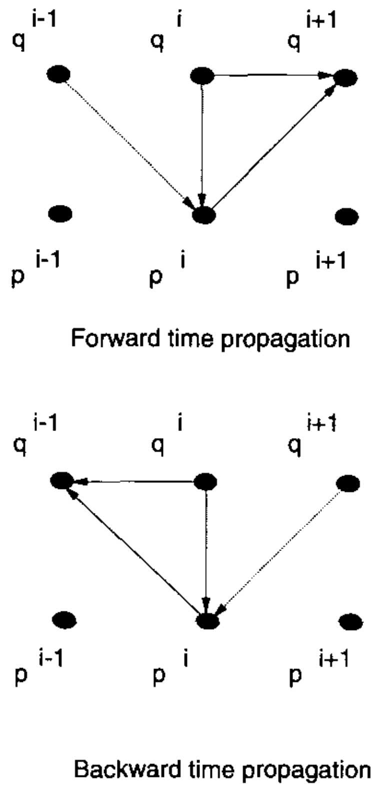

FIG. 1. Updating schemes for the Verlet algorithm for forward and backward time propagation. The dashed line shows the two coordinates necessary for a momentum update. The solid lines show the coordinate and momentum necessary for a position update. The error predicting the p^ith momenta cancels the error in predicting the q^{i+1}th positions to fourth order in the timestep.

The momentum at any given time point is ambiguous since

$$\vec{p} \neq \overleftarrow{p}, \tag{21}$$

and, hence, the energy estimation at any point

$$E^i \approx \frac{(p^i)^2}{2m} + U(q^i) \tag{22}$$

is dependent, through the kinetic energy term, upon whether time propagation is forward or backward in time. In actual practice, the energy in the Verlet algorithm is estimated by the expression

$$E^i \approx \frac{m}{2}\left(\frac{q^{i+1} - q^{i-1}}{2\,\Delta t}\right)^2 + U(q^i), \tag{23}$$

where the use of a symmetric derivative preserves the time reversal properties if the positions are calculated with Eq. (13). With this choice, the Verlet algorithm integrates positions to an accuracy of $\mathcal{O}[(\Delta t)^4]$, whereas the kinetic energy estimator in Eq. (23) is only accurate to $\mathcal{O}[(\Delta t)^2]$. In the context of the approximate time development operator used to generate the coordinate updates, the energy estimator equation (23) is obtained by defining

$$\bar{p}_i = \tfrac{1}{2}(\vec{p}^{\,i+1} + \overleftarrow{p}^{\,i-1}) \tag{24}$$

to avoid ambiguities in the energy estimation.

To summarize, some well-known properties of the Verlet algorithm have been re-derived within the context of a sympletic approach. Although the approximate time development operator used to generate the Verlet integration scheme is not time reversible and introduces an error of $\mathcal{O}[(\Delta t)^2]$, the use of momentum updates (as opposed to the exact momenta) in generating trajectories results in a time reversible algorithm with an error of $\mathcal{O}[(\Delta t)^4]$. Since the exact momenta are never known, one must resort to the use of the updated momenta in actual calculations (in the Verlet scheme this is implicit). Therefore, as has been shown, an algorithm can display significantly different characteristics in its actual implementation than predicted a priori by its operator formulation.

ACKNOWLEDGMENTS

This work was made possible by an endowment from Hitachi, Ltd. to Trinity College Dublin. I also thank Dr. J. C. Sexton for informing me of Refs. [3, 4, 6] and for several helpful discussions.

REFERENCES

1. M. Creutz, *Phys. Rev. D* **38,** 1228 (1988); M. Creutz and A. Gocksch, *Phys. Rev. Lett.* **63,** 9 (1989).
2. L. Verlet, *Phys. Rev.* **159,** 98 (1967).
3. J. C. Sexton and D. H. Weingarten, *Nucl. Phys. B* **380,** 665 (1992).
4. M. Tuckerman, B. J. Berne, and G. J. Martyna, *J. Chem. Phys.* **97,** 1990 (1992).
5. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford Univ. Press, Oxford, 1989).
6. H. Yoshida, *Celestial Mechanics and Dynamical Astronomy* **56,** 27 (1993).

Received June 17, 1993; revised December 17, 1993

J. C. Greer

Department of Chemistry and Scientific Computation Laboratory
O'Reilly Institute, Trinity College
University of Dublin
Dublin 2, Republic of Ireland