Accurate symplectic integrators via random sampling

William G. Hoover, Oyeon Kum, and Nancy E. Owens
Department of Applied Science, University of California at Davis and Lawrence Livermore National Laboratory, Livermore, California 94551-7808

(Received 14 February 1995; accepted 20 April 1995)

We develop a random-sampling method for finding accurate symplectic integrators which best match the exact trajectory of a one-dimensional harmonic oscillator. We recover several well-known algorithms. We demonstrate the usefulness of the random sampling method by finding and validating a new integrator, applying it to the classical many-body problem. © *1994 American Institute of Physics.*

I. INTRODUCTION

Very recently Gray *et al.*[1] compared and applied seven symplectic integrators and two nonsymplectic integrators to the harmonic-oscillator problem. The oscillator furnishes a simple and robust test of integrator accuracy, as is elaborated in the comprehensive list of references cited by Gray *et al.* Symplectic integrators have a desirable property. They exactly maintain the comoving phase-space volume $\Delta q \Delta p$ in accordance with the requirement of Liouville's theorem. This special phase-space property applies only to systems obeying Hamiltonian mechanics, though generalizations of it are useful in introducing heat transfer into mechanics.[2,3]

Because the analytic derivation of symplectic integration rules is relatively arduous we sought a simpler automatic approach, leaving the brunt of the work to a fast computer. We accomplished this by optimizing *randomly chosen* integration rules applied to the harmonic oscillator. We discuss and apply this idea in Sec. II. In Sec. III we establish the validity of our approach by deriving a new symplectic and time-reversible integration rule and applying it to a classical chaotic many-body problem. Our conclusions make up Sec. IV.

II. METHOD

For a harmonic oscillator, Hamilton's equations of motion are linear in the coordinate q and the momentum p:

$$\dot{q} = +p; \quad \dot{p} = -q.$$

We choose here the simplest model, an oscillator with unit mass, and the simplest solution of the motion equations: $q = \cos t$; $p = -\sin t$. *Symplectic* integrators, though they do reproduce the comoving phase volume $\Delta q \Delta p$ exactly, do not preserve the total energy, $H = (q^2 + p^2)/2$. The kinetic and potential energy errors in any approximate scheme, such as the second-order "*si2.a*" integrator of Ref. 1 (equivalent to the Verlet–Störmer leapfrog scheme[4,5]):

$$dq = +a_1 p\, dt; \quad a_1 = 0.500\ 00;$$

$$dp = -b_1 q\, dt; \quad b_1 = 1.000\ 00;$$

$$dq = +a_2 p\, dt; \quad a_2 = 0.500\ 00$$

depend on the time step dt and the chosen numerical coefficients $\{a_1, b_1, a_2\}$ in the integrator. Integrators of this type, in which the coordinate change pdt is independent of q and the momentum change $a(q)dt$ is independent of p obviously keep the phase volume unchanged:

$$\partial \ln(\Delta q \Delta p)/\partial t = p(\partial \ln dq/\partial q) + a(\partial \ln dp/\partial p)$$

$$= 0 + 0 \equiv 0.$$

With $dt = 2\pi/32(2\pi/64)$, this integrator has a maximum total energy error of 0.0049(0.0012) in the 32(64) steps required to trace out one orbit. If the coefficients $\{a\} = \{0.500\ 00, 0.500\ 00\}$ for the two coordinate advances, $\{a_i dtp\}$ are allowed to vary, with the sum held fixed,

$$a_1 + a_2 \equiv 1.000\ 00,$$

then it is easy to develop a simple Monte Carlo scheme, based on selecting the coefficient a_1 randomly, to minimize an error criterion. Such a procedure converges easily to the $\{a_i\}$ values $\{1/2, 1/2\}$ with an error of order 0.0001 or less. As a criterion for the acceptance of a Monte Carlo change in the $\{a_i\}$ it is useful to sum the rms errors in coordinate and momentum, $\Delta_q + \Delta_p$:

$$\Delta_q^2 \equiv (q - \cos t)^2; \quad \Delta_p^2 \equiv (p + \sin t)^2.$$

Other choices might work equally well, or better. Because the variation of the error near a minimum is at least quadratic, errors in the fourth digit of the coefficients lead to insignificant effects on the single-orbit maximum energy errors of 0.0049 and 0.0012.

The symmetric three-stage third-order integrator[6] "*si3.b*" from Ref. 1:

$$dp = -0.268\ 3301 q\, dt; \quad dq = +0.919\ 6615 p\, dt;$$

$$dp = +0.187\ 9916 q\, dt; \quad dq = -0.187\ 9916 p\, dt;$$

$$dp = -0.919\ 6615 q\, dt; \quad dq = +0.268\ 3301 p\, dt$$

has smaller energy errors, for the same time steps, $dt = 2\pi/32(2\pi/64)$. The maximum energy errors are 0.000 045 (0.0000056) during a single orbit. Choosing two of the three coefficients randomly (with the third fixed by the sum rule, $a_1 + a_2 + a_3 \equiv 1.000\ 00$) again reproduces the accurate coefficients listed above with an accuracy of order 0.000 002 or less. An example four-digit approximation:

$$dp = -0.2683 q\, dt; \quad dq = +0.9197 p\, dt;$$

 0021-9606/95/103(4)/1530/3/$6.00

$$dp=+0.1880q\,dt;\quad dq=-0.1880p\,dt;$$

$$dp=-0.9197q\,dt;\quad dq=+0.2683p\,dt$$

has maximum energy errors of 0.000 049 (0.000 0076) during the first orbit.

The time-reversible four-stage fourth-order integrator[7] "*si4.a*":

$$dq=+0.675\ 6036p\,dt;\quad dp=-1.351\ 2072q\,dt;$$

$$dq=-0.175\ 6036p\,dt;\quad dp=+1.702\ 4144q\,dt;$$

$$dq=-0.175\ 6036p\,dt;\quad dp=-1.351\ 2072q\,dt;$$

$$dq=+0.675\ 6036p\,dt$$

incurs energy errors of 0.000 058 (0.000 0036), which do not increase significantly for either time step if all the coefficients are rounded off to the closest value in the fourth digit. It is quite easy to obtain these fourth digits by Monte Carlo refinement of preliminary guesses based on a coefficient mesh with spacing 0.25.

Without such a preliminary investigation, the Monte Carlo program can sometimes become trapped in a relative minimum. To verify that the integrators found in this way are accurate for nonlinear problems, the oscillator equation of motion can be changed to the pendulum equation:

$$\dot{p}=-q\rightarrow\dot{p}=-\sin q.$$

A more severe and convincing test is the chaotic many-body fluid problem discussed in the following Section.

III. MANY-BODY MECHANICS WITH A SYMPLECTIC INTEGRATOR

To verify the utility of the Monte Carlo scheme in a case *without* a known answer, we sought to find a relatively complicated *time-reversible* integrator with four undetermined coefficients. The result

$$dq=+0.005\ 904p\,dt;\quad dp=-0.171\ 669q\,dt;$$

$$dq=+0.515\ 669p\,dt;\quad dp=+0.516\ 595q\,dt;$$

$$dq=-0.021\ 573p\,dt;\quad dp=-1.689\ 852q\,dt;$$

$$dq=-0.021\ 573p\,dt;\quad dp=+0.516\ 595q\,dt;$$

$$dq=+0.515\ 669p\,dt;\quad dp=-0.171\ 669q\,dt;$$

$$dq=+0.005\ 904p\,dt$$

has a maximum energy error of about 10^{-9} with a time step of $2\pi/100$. Errors with 32 and 64 time steps are 0.000 0016 and 0.000 0001. Monte Carlo iteration of the coefficients can further reduce this small error.

We applied this same algorithm to the 256 equations describing a periodic square 64-atom two-dimensional system of particles interacting with Lucy's specially smooth pair potential;[5] the potential was specially chosen so as to minimize errors resulting from the cutoff at $r=3$:

$$\phi_{\mathrm{LUCY}}(r)=(5/9\pi)(1+r)[1-(r/3)]^3;\quad r<3.$$

The 64 particles were initially arranged in a square lattice, with total potential energy 26.435 and a kinetic energy equal to 24. For a total simulation time of 50 the *maximum* energy excursions, $H_{\mathrm{MAX}}-H_{\mathrm{MIN}}=(\Phi+K)_{\mathrm{MAX}}-(\Phi+K)_{\mathrm{MIN}}$, were {0.000 000 62; 0.000 003 7; 0.000 018 75} for time steps of {0.01; 0.02; 0.04}. Thus the oscillator-based algorithms are quite well suited to solving the classical chaotic many-body problem.

IV. CONCLUSIONS

It is feasible to use fast computers to discover efficient algorithms for numerical integration. Our present work is very much in the spirit of Sprott's recent effort.[8,9] He discovered the simplest possible sets of chaotic differential equations by the expedient of examining numerical solutions of *tens of millions* of sets of ordinary differential equations.

If there is a basis for the popular custom of quoting the coefficients in integration rules to many significant figures, it is at best aesthetic. The accuracy of integration rules with coefficients specified to four or five figures is, in many cases, operationally indistinguishable from rules given to the full machine accuracy.

It is not apparent that symplecticity is the best test of utility for integrators. Such a test cannot be applied to non-Hamiltonian systems (though extensions of our Monte Carlo schemes can be used to develop accurate integration schemes). The lack of energy drift in symplectic integrators might favor them, though energy conservation can also be, and has often been,[2,3] imposed by the use of energy-based feedback forces.

Finally, the common practice, in molecular dynamics, of using discontinuous or linear force cutoffs makes a discussion of higher-order integrators in such work somewhat academic. Until such discontinuous simulations encounter a significant criterion for accuracy which they are unable to meet, low-order approximate integrators, such as the Verlet–Störmer scheme and the fourth-order Runge–Kutta integrator, are unlikely to be displaced by their more nearly accurate competitors.

ACKNOWLEDGMENTS

We thank Steve Gray for helpful conversations and for furnishing his computer program for cross checking our results with those of Ref. 1. Nancy Owens thanks the Academy of Applied Science (Concord, New Hampshire) for support during the summer and fall quarters of 1994. Oyeon Kum was supported in part through a University of California Interuniversity Transfer Agreement and in part through a grant from the Agency for Defense Development, Korea. Work at the Lawrence Livermore National Laboratory was carried out under the auspices of the United States Department of Energy as specified by Contract W-7405-Eng-48 with the University of California.

[1] S. K. Gray, D. W. Noid, and B. G. Sumpter, J. Chem. Phys. **101**, 4062 (1994).
[2] W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, New York, 1991).

[3]D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, New York, 1990).
[4]D. Levesque and L. Verlet, J. Stat. Phys. **72**, 519 (1993).
[5]O. Kum and W. G. Hoover, J. Stat. Phys. **76**, 1075 (1994).
[6]R. I. McLachlan and P. Atela, Nonlinearity **5**, 541 (1992).
[7]J. Candy and W. Rozmus, J. Comput. Phys. **92**, 230 (1991).
[8]J. C. Sprott, Phys. Rev. E **50**, R647 (1994).
[9]W. G. Hoover, Phys. Rev. E **51**, 759 (1995).