CMST 23(4) 299–303 (2017) DOI:10.12921/cmst.2017.0000031

Bit-Reversible Version of Milne's Fourth-Order Time-Reversible Integrator for Molecular Dynamics

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Received: 28 June 2017; accepted: 29 June 2017; published online: 17 August 2017

Abstract: We point out that two of Milne's fourth-order integrators are well-suited to bit-reversible simulations. The fourth-order method improves on the accuracy of Levesque and Verlet's algorithm and simplifies the definition of the velocity v and energy $e = (q^2 + v^2)/2$. (We use this one-dimensional oscillator problem as an illustration throughout this paper). Milne's integrator is particularly useful for the analysis of Lyapunov (exponential) instability in dynamical systems, including manybody molecular dynamics. We include the details necessary to the implementation of Milne's Algorithms.

Key words: bit-reversible molecular dynamics, Lyapunov instability, chaotic dynamical systems

I. INTRODUCTION

William Milne's 1949 work *Numerical Calculus* [1] was republished by the Princeton University Press in 2015. The book is a particularly valuable source of clear and direct numerical methods. Research workers in statistical mechanics, molecular dynamics, and dynamical systems will find his approach to what is our own research interest, solving and analyzing differential equations for chaotic systems small and large, reliable and useful. Writing about a decade prior to the computer revolution Milne had no particular interest in "reversible computing" and the "bit-reversible" algorithms which make it possible to extend sequences of coordinates forward and backward in time stably and reversibly *ad infinitum*. Nevertheless his work is directly applicable to such finite-difference applications.

In 1993 Dominique Levesque and Loup Verlet used an *integer* algorithm to solve problems in Newtonian mechanics with perfect time reversibility [2]. Loup had popularized Størmer and Newton's Leapfrog Algorithm a quarter century earlier, in the early days of molecular dynamics [3],

$$q_{t+dt} - 2q_t + q_{t-dt} = a_t(dt)^2.$$

"Verlet's algorithm" appears on page 140 of Reference 1. If the righthand side of this finite-difference algorithm is truncated to an integer the resulting acceleration is precisely the same (to the very last computational "bit") in either direction of time. Because this algorithm conserves phase volume when written in a "symplectic" centered-difference form:

$$q_{t+(dt/2)} = q_t + v_t(dt/2);\ v_{t+dt} = v_t + a_{t+(dt/2)}dt;$$

$$q_{t+dt} = q_{t+(dt/2)} + v_{t+dt}(dt/2),$$

there is no tendency for energy drift. The errors in the velocity and energy in the leapfrog algorithm are unnecessarily large, so that two of Milne's algorithms (both of them also on page 140 of Reference 1) can provide better accuracy for longer runs:

$$q_{t+2dt} - q_{t+dt} - q_{t-dt} + q_{t-2dt} =$$

$$= [5a_{t+dt} + 2a_t + 5a_{t-dt}](dt^2/4).$$

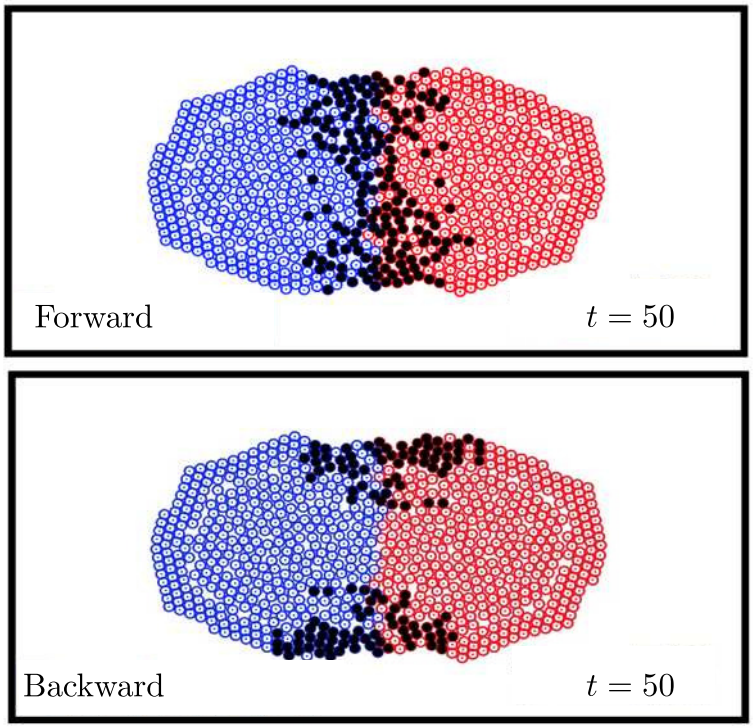

Fig. 1. Shows the important particles evaluated both forward and backward in time at a time of 50. The important particles are blacked in in the figure. The two colliding balls are inverted images of each other. We used the Levesque-Verlet algorithm to reverse the motion at time 100 and analyze the trajectory "backward" in time to the pre-collision state at time 0. The bit-reversible algorithm makes it unnecessary to store a forward trajectory in order to process it backward. Notice in the reversed trajectory, where the coalesced balls are beginning to "neck" in order to separate, that the important particles are on the periphery, where the strain is greatest, rather than at the interface. Although the motion reverses perfectly the stability does not. It is remarkable that the two directions of time differ so much (162 important particles forward *versus* 120 important particles backward) in this measure of chaos. For additional snapshots in this series see Reference 10

The error, $\simeq (17/240)dt^6$, is quite tolerable relative to the Størmer error, $\simeq (1/12)dt^4$. Milne also gives an even better corrector formula with an error $\simeq (-1/240)dt^6$.

$$q_{t+2dt} - 2q_{t+dt} + q_t = [\ a_{t+2dt} + 10a_{t+dt} + a_t\ ](dt^2/12).$$

II. APPLICATIONS

For several years now [4, 5] we have been exploring the differences in Lyapunov spectra forward and backward in time in order to get insight into the Second Law of Thermodynamics. The fractal structures which arise in nonequilibrium deterministic and time-reversible steady-state problems provide explanations to both Loschmidt's Reversibility paradox and Zermélo's Recurrence paradox [6]. Levesque and Verlet's integer algorithm has proved to be a useful tool in these studies despite its relatively coarse description of particle trajectories.

Integer algorithms are also useful in studies of the effects of finite precision (single, double, quadruple, ...) on phase-space distributions generated by flows and maps [7, 8]. Mauricio Romero-Bastida [9] suggested the use of the integer-based leapfrog algorithm for generating a reversible reference trajectory of arbitrary length in his studies of the "covariant" Lyapunov exponents. In 2013 we were able to see a qualitative difference between the "important particles" (those making above-average contributions to the Lyapunov instability) forward and backward in time in the example inelastic-collision problem of **Figure 1** [10]. Continuing progress in low-cost computation caused us to revisit these problems in connection with a lecture course delivered at Kharagpur's Indian Institute of Technology in December 2016 [11]. We were very pleased to find that Milne's work offers an improvement in the precision and accuracy of these Lyapunov studies and believe that others will find this approach useful to their own work. Although these improvements are not at all "new" we do expect that this work will accelerate progress in understanding the time-reversible simulation of irreversible processes.

Figure 1 illustrates the important particles (those making above-average contributions to the largest Lyapunov exponent) forward and backward in time for the collision of two 400-particle balls. The 162 important particles forward in time are those blacked in along the interface between the balls while the 120 important particles backward in time are those blacked in in the necking regions where the plastic strain is greatest as the balls are separating. This simulation

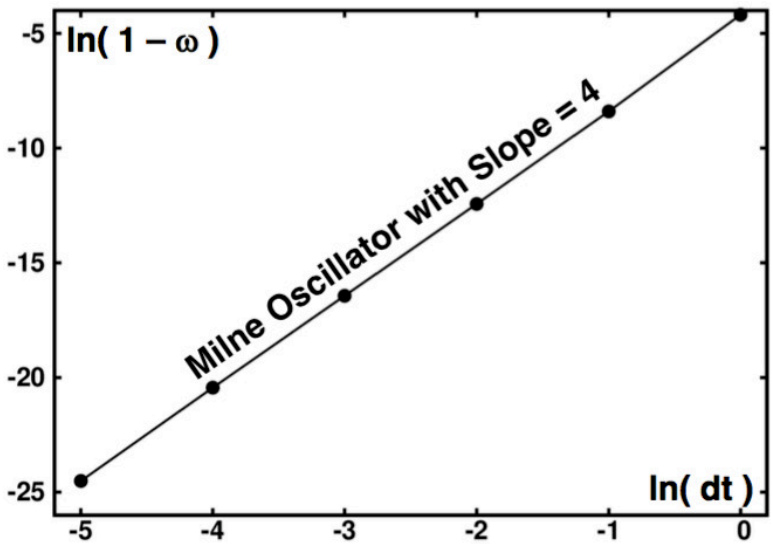

Fig. 2. Analysis of the oscillator motion equation confirms the stability of Milne's method

employed the Levesque-Verlet algorithm for the reference trajectory and a Runge-Kutta fourth-order algorithm for the two satellite trajectories (one forward and another backward) as is described in Reference 10.

III. NUMERICAL IMPLEMENTATION OF MILNE'S ALGORITHMS

To illustrate the application of Milne's Algorithms we consider an integer version of the simpler of his two fourth-order algorithms. We describe a harmonic oscillator with $\ddot{q} = -q$. The preliminaries, which we give at the top of the following page, provide integer forms for five previous coordinates and the corresponding contributions to the acceleration, all of them multiplied by 10^{15}. We select an example timestep of $(\pi/50)$ in the Fortran instructions so that an oscillator period corresponds to one hundred timesteps.

We carried out two kinds of tests for the Milne integrator, reversibility, confirming that reversing the four prereversal coordinates exactly reverses the sequence of integers back to the initial value of 10^{15}. It is easy to show that the algorithm is exactly reversible in this way. Stability can be confirmed by solving for the dependence of the oscillation frequency on the timestep. Numerical work consistent with the linear analysis for the oscillator (given in more detail as the nearly straight line in **Figure 2**) shows that the dependence of the phase shift is quartic in the timestep for the range $0 < dt < 1$.

The stability analysis for Milne's algorithm is straightforward. If we substitute the trial solution $q \propto e^{i\omega t}$ into the wholly linear algorithm the result is:

$$\cos(2\omega dt) - \cos(\omega dt) + (dt^2/4)[\, 5\cos(\omega dt) + 1\,] = 0.$$

This simplifies to a quadratic equation in $\cos(\omega dt)$:

$$2C^2 + [\,(5dt^2/4) - 1\,]C + (dt^2/4) - 1 = 0,$$

$$\text{where } C \equiv \cos(\omega dt).$$

Figure 2 shows that the dependence of the frequency error on the timestep is quartic, $(1 - \omega) \propto dt^4$, confirming the stability of the algorithm.

A direct simulation of the integer version of the algorithm, using two billion timesteps with $dt = 0.2$, showed no tendency toward damping or instability. Similar results can be obtained by solving the floating-point version of the problem, where precise reversibility has to be abandoned (because roundoff error will spoil it). These results establish that the Milne algorithm is both reversible and stable for the oscillator. We recommend it to our colleagues for their use.

The implementation of the algorithm is to some extent hardware dependent. On our various Mac computers using the free gnu compiler we had no trouble using 16-byte integers, giving roughly 15 digits for arithmetical operations. The following extract from the setup of the computation generates the inital data (in this case four points from a cosine curve) as well as the three integers, proportional to $dt^2 \times 10^{15}$, and needed for the accelerations. On the following page we summarize the time-stepping loop where the three accelerations are expressed as integers $\{$`IAP`, `IAO`, `IAM`$\}$. We include at the end an indication of the coordinate reversal procedure needed to integrate backward.

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER*16 IQMM,IQM,IQ0,IQP,IQPP  ! Contiguous integer coordinates
      INTEGER*16 IAP,IA0,IAM            ! Ingredients of the accelerations
      INTEGER*16 I1,I2,I3,I4            ! Storage for coordinate reversal
      ITMAX = 100
      TWOPI = 2.D0*3.141592653589793D0
      DT = TWOPI/ITMAX
      QMM  =  DCOS(-2.D0*DT)
      QM   =  DCOS(-1.D0*DT)
      Q0   =  DCOS( 0.D0*DT)
      QP   =  DCOS(+1.D0*DT)
CONVERT COORDINATES TO 15-DIGIT INTEGERS
      IQMM   = QMM*(10.D0**15)
      IQM    = QM *(10.D0**15)
      IQ0    = Q0 *(10.D0**15)
      IQP    = QP *(10.D0**15)          ! Finish of the preliminaries
```

Here follows a bare-bones evolution loop for the integer coordinates. After `ITMAX` iterations the coordinate reversal steps make it possible to return precisely to, and beyond, the beginning. In the event that the velocities are to be calculated from Milne's fifth-order interpolation (which is one order of overkill) it is necessary to compute the integer coordinates to include `IQPPP` and `IQMMM`, getting `IQPPP` from the "step" `IQPPP = IQPP + IQ0 - IQM - (IAPP + IAP + IA0)`.

```
      DO IT = 1,ITMAX
      TIME = IT*DT
COMPUTE INGREDIENTS OF THREE  ACCELERATIONS
      IAP  = 0.25D00*DT*DT*(5.D0*IQP)
      IA0  = 0.25D00*DT*DT*(2.D0*IQ0)
      IAM  = 0.25D00*DT*DT*(5.D0*IQM)
COORDINATE UPDATES FOR FIVE SUCCESSIVE TIMES
      IQPP = IQP + IQM - IQMM - (IAP + IA0 + IAM)  ! This is the "step".
      IQMM = IQM
      IQM  = IQ0
      IQ0  = IQP
      IQP  = IQPP
      END DO
COORDINATE REVERSAL
      I1 = IQMM
      I2 = IQM
      I3 = IQ0
      I4 = IQP
      IQMM  = I4
      IQM   = I3
      IQ0   = I2
      IQP   = I1
      DO IT = 1,ITMAX
CONTINUE REVERSAL WITH SAME STATEMENTS AS IN THE FORWARD LOOP
      END DO
```

There is no difficulty in computing an accurate velocity with Milne's page 99 formula using six centered coordinates. This fifth-order interpolation gives not only good velocities, but also an accurate energy. Accurate values of these phase variables are a real advantage of the Milne algorithm over that of Levesque and Verlet.

Acknowledgement

We gratefully acknowledge the interest and support of Harald Posch (Universität Wien), Clint Sprott (University of Wisconsin-Madison), and Karl Travis (University of Sheffield). It is a pleasure to thank Artur Pozniak for his help in the composition of this article.

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