Journal of Statistical Physics, Vol. 76, Nos. 3/4, 1994

Time-Reversible Continuum Mechanics

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Received December 31, 1993

Levesque and Verlet developed a time-reversible and "bit-reversible" computational leapfrog algorithm. Their algorithm uses integer arithmetic and is exactly time reversible to the last computational bit describing the particle coordinates. We generalize their idea, developed for atomistic molecular dynamics, to smoothed-particle continuum mechanics. In the special case of a two-dimensional isentropic ideal gas, these two approaches, one microscopic and the other macroscopic, are isomorphic. In the more general nonadiabatic case, but still without dissipative terms, our continuum extension of the leapfrog scheme remains stable and also exhibits the exact time and bit reversibility associated with Levesque and Verlet's atomistic approach.

KEY WORDS: Time-reversible; smoothed-particle; continuum mechanics; chaotic.

1. INTRODUCTION

The "leapfrog algorithm" of atomistic molecular dynamics[1]

$$\{r_+ - 2r_0 + r_- \equiv dt^2(F/m)_0\}$$

is patently time reversible. Any "trajectory," a selection of discrete time-ordered coordinates $\{r\{n\,dt\}\}$, going forward in time, is mathematically equivalent to a time-reversed trajectory $\{r\{-n\,dt\}\}$ obeying the same motion equations. But ordinarily computer roundoff errors lead to small errors in the last decimal place. Such errors grow in time, with *Lyapunov instability*, as $\exp(\lambda t)$, restricting the effective time reversibility of trajectories to just a few "Lyapunov times," that is, a few times $1/\lambda$. For a description of Lyapunov instability in many-body systems see ref. 2.

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0022-4715/94/0800-1075$07.00/0

Levesque and Verlet[1] showed that the irreversible effect due to round-off error plus Lyapunov instability can be eliminated entirely by using an integer representation of coordinate space $\{r\}$. Here we explore that same idea from the standpoint of macroscopic continuum mechanics, employing a version of continuum mechanics, smoothed-particle applied mechanics, which closely resembles microscopic molecular dynamics, but which extends the state space to include densities $\{\rho\}$ and internal energies $\{e\}$ for each particle.

In Section 2 we describe smoothed-particle continuum mechanics and point out the special case in which this approach becomes isomorphic to molecular dynamics. In Section 3 we apply an extension of Levesque and Verlet's bit-reversible algorithm to a more general smoothed-particle situation, still without dissipation, and demonstrate, by computer simulation, that both numerical stability and exact time reversibility hold for the extension. Section 4 contains a short summary as well as a conjecture, suggested by this work, concerning the possibility of further extensions.

2. SMOOTHED-PARTICLE APPLIED MECHANICS

Monaghan[3] and Lucy[4] developed a convergent finite-difference approximation to the solutions of the continuity, motion, and energy equations of continuum mechanics. Their finite-difference equations arise by interpolation of the field variables onto an irregular grid of relatively moving points. The interpolation involves a smoothing or weighting function $w(r)$ with a finite range equal to a few times the interparticle spacing. In the usual case w has no angle dependence. By interpolating the hydrodynamic velocity and internal energy onto the moving grid points, the "smoothed" hydrodynamic partial *differential* equations are transformed into *ordinary* differential equations for the motion of the points. This simplification is a key advantage of the method. In brief, the value of any point function f (a field variable such as velocity or internal energy) can be represented by a sum of weighted contributions from all nearby grid points:

$$f(r) \equiv \sum m_j f_j w(r - r_j)/\rho_j$$

The motivation for this definition is the simple form which gradients take:

$$\nabla_r f(r) \equiv \sum (m_j f_j/\rho_j) \nabla_r w(r - r_j)$$

In the simplest case the weighting function w and its gradient ∇w have a fixed finite range (so as to include several points in the average). Many forms have been used. Here we consider points in two space dimensions

with unit mass and with a weighting function[2] $w(r)$ which vanishes for $r > 1$:

$$w(0 < r < 1/2) = (40/7\pi)(1 - 6r^2 + 6r^3)$$
$$w(1/2 < r < 1) = (80/7\pi)(1 - r)^3$$

The weighting function can be thought of as describing the smearing out or *smoothing* of the mass associated with each point to a neighborhood with unit radius. The integral of w is normalized to unity:

$$\int_0^1 2\pi r w \, dr \equiv 1$$

In smoothed-particle mechanics it is usual to compute the density at each point by superposing the contributions from all nearby points (rather than by integration of the continuity equation). At location i, for instance,

$$\rho_i \equiv \sum m_j w_{ij} \tag{1a}$$

where the sum over j includes the term $i = j$. The usual continuum equation of motion,

$$dv/dt \equiv (1/\rho)\nabla \cdot \sigma$$

in the comoving frame, is rewritten using the identity

$$(1/\rho)\nabla \cdot \sigma \equiv (\sigma/\rho^2) \cdot \nabla\rho + \nabla \cdot (\sigma/\rho)$$

in the symmetric form:

$$d^2 r_i/dt^2 \equiv dv_i/dt \equiv \sum [(m\sigma/\rho^2)_i + (m\sigma/\rho^2)_j] \cdot \nabla_i w_{ij} \tag{1b}$$

In the absence of heat conduction the comoving energy equation takes a similar form:

$$de_i/dt \equiv -\tfrac{1}{2} \sum [(m\sigma/\rho^2)_i + (m\sigma/\rho^2)_j] : v_{ij} \nabla_i w_{ij}; \qquad v_{ij} \equiv v_i - v_j \tag{1c}$$

The set of ordinary differential equations (1a)–(1c) can then be solved, using Runge-Kutta integration, for the motion of all the particles together with the time development of their densities and energies. For some recent applications of this approach see ref. 5. We have recently applied this approach to the chaotic Rayleigh–Bénard problem,[6] the simulation of gravitationally excited unstable convection in a system heated from below and cooled above.

The equations of motion (1b) become isomorphic to the equations of molecular dynamics in the special case that the stress is that of a two-dimensional isentropic ideal gas, $\sigma = -(\mathbf{I}/2)\rho^2$, where $\mathbf{I}$ is the unit tensor. In this special case $w(r)$ behaves as a pair potential function $\phi(r)$, with the equations of motion for particles of unit mass:

$$\left\{ d^2 r_i/dt^2 \equiv dv_i/dt \equiv \sum -\nabla_i \phi_{ij} \right\}$$

The continuum energy equation likewise corresponds exactly to atomistic conservation of energy in this case. In the next section we consider a finite-difference approximation to a more general, nonisentropic case in which the stress depends separately on both density and energy.

3. TIME-REVERSIBLE CONTINUUM MECHANICS

The leapfrog representation of the continuum particles' equations of motion can be combined with a time-symmetric energy equation to give the following explicit algorithm:

$$r_+ - 2r_0 + r_- \equiv dt^2 \sum ([(m\sigma/\rho^2)_i + (m\sigma/\rho^2)_j] \cdot \nabla_i w_{ij})_0$$

$$e_+ - e_- \equiv -dt \sum [(m\sigma/\rho^2)_i + (m\sigma/\rho^2)_j]_0 : v_{ij}(\nabla_i w_{ij})_0$$

$$2dtv_{ij} \equiv (r_+ - r_-)_i - (r_+ - r_-)_j$$

The initial values required are coordinates and energies at two successive times, $t = -dt$ and $t = 0$, for instance. Numerical tests indicate that this scheme is stable, with local errors which are third order in the timestep dt and global errors which are second order. That the scheme is stable is by no means obvious *a priori*. For example, a similar difference scheme for the first-order differential equations of molecular dynamics, taken from Milne's text,[7]

$$r_+ - r_- \equiv 2dtv_0; \qquad v_+ - v_- \equiv 2dt(F/m)_0$$

though formally equivalent to the leapfrog scheme for a doubled timestep of $2dt$, turns out to be unstable for molecular dynamics.[8]

After our successful trials in one dimension suggested the possibility of stability for this approach, we tested this scheme in two space dimensions with the hydrostatic nonlinear equation of state

$$P \equiv -\sigma \equiv \rho^2 - 1 + e$$

containing both tensile and compressive parts as well as thermal expansion. The numerical results for 25 particles of unit mass in a 2.5×2.5 periodic container with initial internal and kinetic energies of 25 and 25 conserved energy well with timesteps of 0.01 and 0.02, showing the expected second-order global errors. The energy errors are plotted in Fig. 1. The overall density in this case is 4, around which the smoothed-particle sum fluctuates. The particles were initially arranged in a square lattice with random velocities summing to zero. The ordered arrangement gives way to disordered fluid arrangements of the type shown in Fig. 2.

Following Levesque and Verlet,[1] we replaced the coordinates and energies by 32-bit integers, carrying out intermediate operations in floating point arithmetic and then truncating the results for the $\{r\}$ and $\{e\}$ to integers. Tests showed bit-perfect time reversibility (as would be expected from the time symmetry of the difference equations) over computations of tens of thousands of timesteps. We conclude that the same reversibility properties which apply to molecular dynamics can be extended to the Euler equations of continuum mechanics by using the smoothed-particle approach.

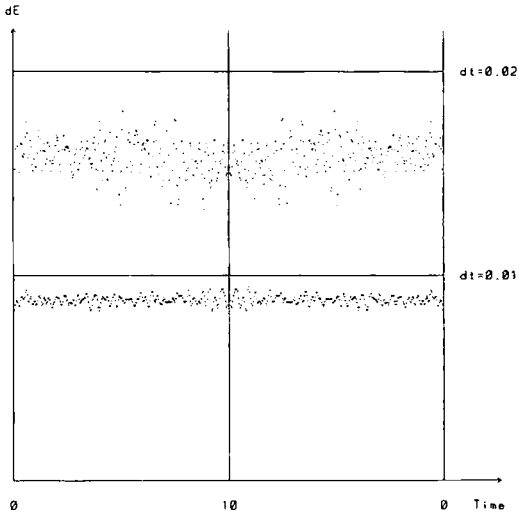

Fig. 1. Time development of the 25-particle energy error (with a total energy fluctuating about 50.0) using generalized leapfrog timesteps of 0.01 (below) and 0.02 (above) to solve Eqs. (1a)–(1c) of the text. A timestep of 0.04 is unstable. At time 10 the velocities were reversed and the simulations returned *exactly* ("bit reversibly") to the initial condition shown in Fig. 2.

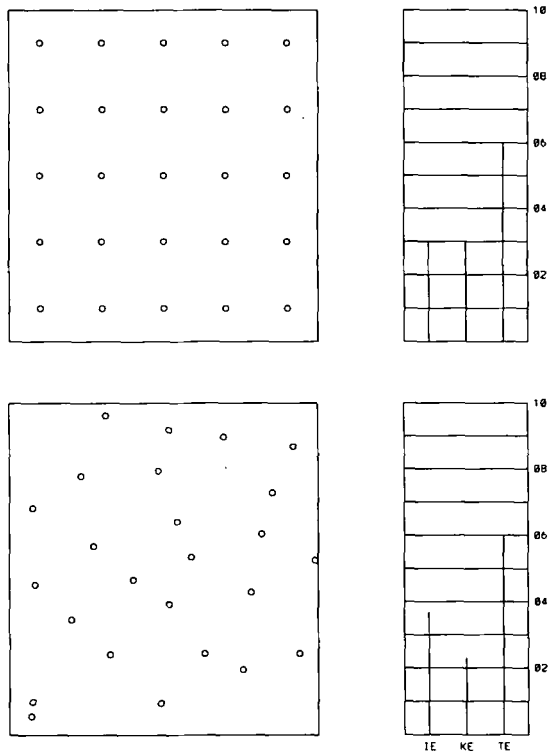

Fig. 2. Initial and final configuration (time 1000, with timestep 0.01) for 25 periodic continuum particles with the equation of state $P = \rho^2 - 1 + e$. The time-averaged internal and kinetic energies are 33.94 and 16.05. The vertical bars indicate (from left to right) internal, kinetic, and total energy.

4. SUMMARY

A time-symmetric difference scheme extending Levesque and Verlet's atomistic algorithm to continuum problems is stable and precisely time-reversible (bit-reversible for an integer state space). In the special case of an isentropic ideal gas, the smoothed-particle approach to the continuum simulation produces trajectories identical to those found in molecular dynamics, so that the continuum weight function $w(r)$ is equivalent to an atomistic potential function $\phi(r)$. We were unable to find a similar time-symmetric stable formulation in the *continuum* case when dissipation is present. We were also unable to extend Levesque and Verlet's approach to the *atomistic* case with a *constrained kinetic energy*[8, 9]:

$$\{dr/dt \equiv v;\ dv/dt \equiv (F/m) - \zeta v\}$$

$$\zeta \equiv (1/2K) \sum F \cdot v; \qquad K \equiv (m/2) \sum v^2; \qquad dK/dt \equiv 0$$

We conjecture that a stable time-symmetric bit-reversible algorithm for these atomistic *isokinetic* equations *cannot* be found. From the physical standpoint, this might be expected, because such thermostatted equations can be used to drive steady nonequilibrium heat currents, producing multifractal strange attractor and repellor objects in the phase space.[8, 9] These fractal structures are the antithesis of the conserved phase volume which characterizes equilibrium flows.

ACKNOWLEDGMENTS

This work was supported in part by the Lawrence Livermore National Laboratory through Contract W-7504-Eng-48, in part by a grant from the Agency for Defense Development, Korea, and in part through an Inter-university Transfer Agreement for the support of O.K.

REFERENCES

1. D. Levesque and L. Verlet, Molecular dynamics and time reversibility, *J. Stat. Phys.* **72**:519 (1993).
2. H. A. Posch and W. G. Hoover, Equilibrium and nonequilibrium Lyapunov spectra for dense fluids and solids, *Phys. Rev. A* **38**:473 (1988).
3. J. J. Monaghan, Smoothed particle hydrodynamics, *Ann. Rev. Astron. Astrophys.* **30**:543 (1992).
4. L. B. Lucy, A numerical approach to the testing of the fission hypothesis, *Astron. J.* **82**:1013 (1977).
5. H. E. Trease, M. J. Fritts, and W. P. Crowley, eds., *Advances in the Free-Lagrange Method* (Springer-Verlag, Berlin, 1991).
6. W. G. Hoover, C. G. Hoover, A. J. De Groot, and T. G. Pierce, Microscopic and macroscopic dynamics, in *Parallel Computation*, Jens Vokert, ed. (Springer-Verlag, Berlin, 1993).
7. W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, New Jersey, 1949).
8. W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1991).
9. D. J. Evans and G. P. Morriss, *Nonequilibrium Liquids* (Academic Press, New York, 1990).

Communicated by J. L. Lebowitz