JOURNAL OF COMPUTATIONAL PHYSICS 1, 517-535 (1967)

Time-Reversible Difference Procedures

O. BUNEMAN

Institute for Plasma Research, Stanford University, Stanford, California 94305

ABSTRACT

The computer simulation of microdynamical processes often demands that the principle of reversibility be observed strictly. Five examples are presented to show how such reversibility can be achieved in fast integrations, in spite of the presence of first-order time derivatives. The examples are: the Lorentz equation, relativistic orbits, orbits in central coordinates, gyrocenter motion, and continuity equations.

INTRODUCTION

In classical physics, irreversibility is the result of coarse-graining our description of nature; it is not intrinsic to the laws of nature. Irreversibility, or increase of entropy, can be identified directly with loss of information [1].

When one programs classical physics, and especially when one aims at reproducing apparently irreversible phenomena (such as turbulent heating, growth of instabilities, transport phenomena, anomalous diffusion), it is essential that the program itself be reversible and that any increase of entropy be introduced only by the reduction of the information extracted from the computer, not by deleting information from the memory while it simulates the processes.

Indeed, such programs ought to allow, by a change of sign of the time variable, for the exact tracing of a system back from the final state to the initial conditions [2]. Any lack of perfection of such reversal should be due to rounding-off errors only, not to the program. There is only one point at which microscopic classical physics contains irreversibility: While Maxwell's field equations themselves are time-reversible, the boundary and initial conditions must be formulated in such a manner as to represent outgoing signals only. A backward run, in order to reproduce the initial state, would have to be based on a record of the radiation which has escaped across the boundaries of the simulated volume, and this record would have to be fed in across the boundaries of the return run [3].

In sequential runs, the time is usually discretized and it is here that we need to watch for accidental irreversibility. While macroscopic equations, such as the diffusion equation, may involve a first-order time derivative, $\partial\psi/\partial t$, of a field variable ψ, this does not happen in microscopic equations. These only contain the

second-order operator $\partial^2/\partial t^2$, readily turned into a finite-difference form which is symmetric in time: One uses the central-difference equivalent,

$$\partial^2\psi/\partial t^2 \to \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{(\Delta t)^2}. \tag{1}$$

However, one must not be over-zealous and improve on the second-difference operator by adding higher-difference corrections. These corrections can, in a practical fast run, only be based upon past information. They are therefore biased. Only by going round several loops of iterations can one make sure that one's fourth-difference correction is a fair compromise between past and future data (predictor–corrector routine).

To become the basis for good statistics, a calculation which is intended to reproduce macroscopically irreversible phenomena from reversible microscopic dynamical equations, would normally involve a large number of identical elements or operations.

Computer experiments such as those in [2], [4]–[9] are in this category. The individual operations have to be repeated so often that speed is at a premium. Only the simplest difference formulas are acceptable and nothing so slow as predictor–corrector procedures or planetary orbit routines can be used when one traces out the behavior of thousands of electrons in a tube, thousands of stars in galactic evolution, or thousands of charged particles in a plasma.

Actually, there are many occasions when the use of such higher-order differences is not justified since the input (the sources, accelerations, etc.) is not as ideally smooth and differentiable as implied in the derivation of fourth-order difference coefficients. When one integrates the wave equation with a charge-current input, a lump of charge with a sharp boundary may suddenly and discontinuously sweep across a given spot and then cause "wild" fourth-differences of potential. (Again, only by laborious iteration of interval subdivision can one diagnose and treat a discontinuity with precision.)

It is principally in the dynamical equations for classical particles or fluids that one runs into problems of keeping the finite-difference form of time differentials symmetric with respect to time reversal. We give here a few examples of occasions where reversibility posed a problem, and of how the problem could be resolved.

I. The Lorentz Force

The regular acceleration of a particle by a space-dependent force $F(\mathbf{x})$ can be dealt with symmetrically, just as explained in connection with the field equation, by using central differences:

$$\frac{d^2\mathbf{x}}{dt^2} \to \frac{\mathbf{x}_{n+1} - 2\mathbf{x}_n + \mathbf{x}_{n-1}}{(\Delta t)^2} \approx \frac{1}{M}\mathbf{F}(\mathbf{x}_n). \tag{2}$$

However, already the incorporation of a Lorentz force, or Coriolis forces in rotating frames of reference, raises a difficulty: How is one to represent the velocity symmetrically in the cross-product $\mathbf{v} \times \mathbf{B}$?

The presence of a first derivative in the Lorentz equation does not constitute irreversibility. It is well known that electrodynamics is symmetric with regard to time reversal, provided one changes the sign of the magnetic field along with the sign of the time [10].

The representation

$$\mathbf{v} = \frac{d\mathbf{x}}{dt} \to \frac{\mathbf{x}_{n+1} - \mathbf{x}_{n-1}}{2\Delta t} \tag{3}$$

springs to mind but has two disadvantages:

(i) It refers only to alternate time steps and may lead to the build-up of discrepancies between even and odd sequences of points, i.e., between data at

$$t = 0, \quad 2\Delta t, \quad 4\Delta t \ldots$$

on the one hand and

$$t = \Delta t, \quad 3\Delta t, \quad 5\Delta t \ldots$$

on the other.

(ii) It implies prior knowledge of the next position $\mathbf{x}_{n+1}$.

Regarding the second point, one can resolve the difficulty readily by virtue of the linearity of the Lorentz equation in finite-difference form:

$$\frac{\mathbf{x}_{n+1} - 2\mathbf{x}_n + \mathbf{x}_{n-1}}{(\Delta t)^2} = \frac{q}{M}\left\{\mathbf{E}(\mathbf{x}_n) + \frac{\mathbf{x}_{n+1} - \mathbf{x}_{n-1}}{2\Delta t} \times \mathbf{B}(\mathbf{x}_n)\right\}. \tag{4}$$

Here $\mathbf{x}_{n+1}$ appears on both sides, but linearly, and a unique solution for $\mathbf{x}_{n+1}$ can be obtained. The presence of $\mathbf{x}_n$ on the left is sufficient to prevent the build-up of odd-even discrepancies as feared in (i).

The algebraic solution of Eq. (4) for the three components of $\mathbf{x}_{n+1}$ is not difficult. It is given explicitly in Section 4, Eq. (50) with definitions (36) and (37). Under conditions where $\mathbf{E}$ and $\mathbf{B}$ are constant along the orbit (independent of $\mathbf{x}_n$) one can solve the recursion formula between three successive $\mathbf{x}_n$ analytically. One obtains a sequence of points along a cycloidal orbit, as expected in constant fields. This cycloid, however, deviates from the true cycloid to an extent which gets worse with increasing Δt. (More precisely, it is the projection normal to $\mathbf{B}$ which is a proper cycloid. Along $\mathbf{B}$, one has free fall under steady acceleration, quadratic in t, and the difference equation gives exact answers.)

Cycloids play a role in some slightly more sophisticated methods for developing

a reversible numerical integration of the Lorentz equation. The principle of not biassing one's information at the nth step in favor of the past, and one's ignorance of the future, restrict one to the assumption that **E** and **B** do not depart from their present values during a step centered on the position $\mathbf{x}_n$, and this is the best permissable assumption. One would wish to choose the best process of integration subject to this, albeit very restricted, information, and one would hope to avoid the deviations mentioned at the end of the previous paragraph.

Constancy of **E** and **B** results in predicting intervals of cycloidal motion during a step centered at $t = t_n$. The known present values of **E** and **B** define a certain class of cycloids and the known present position $\mathbf{x}_n$ narrows down the possible cycloids further. It remains to decide with what velocity $\mathbf{v}_n$ to launch the cycloid.

One might think of this cycloid as a close approximation to the accurate orbit between $t_n - \Delta t/2$ and $t_n + \Delta t/_2$. But since one wants to reach the position a full step ahead at $t_{n+1} = t_n + \Delta t$, one must, from symmetry considerations, also look back as far as $t_n - \Delta t$. This suggests the following procedure: One can choose that cycloid which, at time t_n, passes through $\mathbf{x}_n$ and has the curvature and other properties dictated by $\mathbf{E}(\mathbf{x}_n)$, $\mathbf{B}(\mathbf{x}_n)$, but which also passes through $\mathbf{x}_{n-1}$ at t_{n-1}. On this cycloid, one then predicts the position $\mathbf{x}_{n+1}$ at t_{n+1}. There, and then, the process is repeated with new field values. Each step is thus covered by two, possibly slightly different, cycloidal orbits through common termini. The resulting recurrence formula is given by Eq. (38) of Section IV.

A more general interpretation of this procedure is given in [8]. At t_n, solve the differential orbit equation analytically assuming constant fields $\mathbf{E}(\mathbf{x}_n)$, $(\mathbf{B}(\mathbf{x}_n)$ and initial position $\mathbf{x}_n$. Treat the initial velocities as open variables. Apply the solution first at $t = t_n - \Delta t$ and determine the velocities which yield the known position $\mathbf{x}_{n-1}$. Use these velocities for advancing the general solution to $t_n + \Delta t$. The velocities which are used at the next step, at t_{n+1}, are, however, not identical with the velocities of arrival in the previous step.

The cycloid-fitting procedure gives absolutely accurate results under constant field conditions, no matter how large a step is taken. Hockney [7] has made rapid progress and obtained useful results with steps as large as one-fifth of a complete gyro-revolution. The steps taken by Yu [8] *et al.* are nearly as large. These references demonstrate the speed and success of time-symmetric cycloid fitting when tracing several thousand charged particles through a constant magnetic field and the self-consistent time-dependent electric field. Hockney reproduces, in his "computer experiments", the physically observed but mysterious phenomenon of anomalous diffusion of a plasma across a magnetic field. Yu *et al.* predict exact operating conditions of crossed-field electron tubes whose functioning had previously been understood at best only qualitatively. Yu's program is now being used to check out new tube designs for their performance on the computer before beginning construction in the workshop.

II. Relativistic Orbits

Under relativistic conditions, the mass M in the Lorentz equation

$$\frac{d}{dt}\left(M\frac{d\mathbf{x}}{dt}\right) = q\left(\mathbf{E} + \frac{d\mathbf{x}}{dt} \times \mathbf{B}\right) \tag{5}$$

must be treated as time-dependent, its variation being given by the energy equation

$$\frac{d}{dt}(Mc^2) = q\mathbf{E} \cdot \frac{d\mathbf{x}}{dt}. \tag{6}$$

Again, the appearance of first derivatives does not spoil the symmetry overall with respect to time reversal.

One might try to apply the method of Yu, described in the preceding section: In constant fields **E**, **B**, Eqs. (5) and (6) possess exact solutions [11] which involve sines and cosines of $qB\tau/M^*$ and hyperbolic functions of $qE\tau/M^*$. Here τ is proper time along the orbit and M^* is the rest mass. One gets the solutions in this form after Lorentz-transforming to a frame of reference in which **E** and **B** appear parallel. Such a transformation is almost always possible by choosing the correct velocity at right angles to the plane which **E** and **B** defined prior to transformation. There is one exception, the case where **E** and **B** are perpendicular and of equal magnitude (Gaussian units). In this latter case [12], the orbit coordinates become cubic functions of τ.

Yu's method, then, would be to fit successive branches of these generalized cycloids or cubics together, always determining the available orbit parameters from present and previous positions. This method would be practical if one could progress in equal intervals of proper time τ. However, such progression does not, in general, lead to equal intervals in observer's time t and the method is thus restricted to situations where a prepared record of the field is available in advance, allowing easy interpolation to any value of t.

More commonly, and more realistically, a record of the electromagnetic field has to be built up as the positions of the particles become known, and a field equation—essentially the wave equation with sources—calls for integration in equal steps of t. In principle, one therefore has to extend the spirit of Yu's method to the determination of the step size $\Delta\tau^-$ (in addition to the orbit velocities), which will lead to the correct t_{n-1} starting back from t_n. Furthermore, the next step $\Delta\tau^+$ must be chosen to give the preset value of t_{n+1}. In each case a cubic, or a transcendental equation involving hyperbolic and circular functions, has to be solved and the method is likely to become uneconomically slow.

Instead, the following finite-difference versions of (5) and (6) can be tried:

The left in (5) may be written

$$M\frac{d^2\mathbf{x}}{dt^2}+\frac{q\mathbf{E}}{c^2}\cdot\frac{d\mathbf{x}}{dt}\frac{d\mathbf{x}}{dt} \tag{7}$$

after substitution from (6). The acceleration and the velocity can be replaced as in (2) and (3), which leads to

$$M_n\frac{\mathbf{x}_{n+1}-2\mathbf{x}_n+\mathbf{x}_{n-1}}{(\Delta t)^2}+\frac{q\mathbf{E}_n}{c^2}\cdot\frac{\mathbf{x}_{n+1}-\mathbf{x}_{n-1}}{2\Delta t}\frac{\mathbf{x}_{n+1}-\mathbf{x}_{n-1}}{2\Delta t}$$
$$=q\left(\mathbf{E}_n+\frac{\mathbf{x}_{n+1}-\mathbf{x}_{n-1}}{2\Delta t}\times\mathbf{B}_n\right). \tag{8}$$

For Eq. (6) one can write

$$M_{n+1}-M_n=\frac{q}{c^2}\frac{\mathbf{E}_{n+1}+\mathbf{E}_n}{2}\cdot(\mathbf{x}_{n+1}-\mathbf{x}_n), \tag{9}$$

which is preferable to

$$M_{n+1}-M_{n-1}=\frac{q}{c^2}\mathbf{E}_n\cdot(\mathbf{x}_{n+1}-\mathbf{x}_{n-1}) \tag{10}$$

since this last recursion formula may lead to divergence between odd and even mass values. The sequential procedure for solving the acceleration and mass equations is to treat (8) as a quadratic equation for $\mathbf{x}_{n+1}$, assuming that the fields and the mass had been advanced as far as t_n, then to determine $\mathbf{E}_{n+1}$ from the particle data at t_{n+1} and to advance M to t_{n+1} by means of (9). Such a procedure has been employed successfully by Burn [13] in a computer simulation of sheet pinch dynamics. The calculations of Burn involved only variations with time and with one space component, x, but x- and t-dependent y- and z-velocities were taken into account in the Lorentz term. Solving the quadratic presented no serious problems since the relativistic effects were small; iterations, starting with initial neglect of the quadratic term, converged rapidly and left no doubt regarding the choice of a sign for the square roots.

To avoid the appearance of quadratic terms in the unknown x_{n+1}, the dyadic $(d\mathbf{x}/dt)\,(d\mathbf{x}/dt)$ in (7) can be replaced by

$$\frac{1}{2}\frac{\mathbf{x}_{n+1}-\mathbf{x}_n}{\Delta t}\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}+\frac{1}{2}\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\frac{\mathbf{x}_{n+1}-\mathbf{x}_n}{\Delta t} \tag{11}$$

With this replacement, the Lorentz equation becomes linear in $\mathbf{x}_{n+1}$. Burn has tested such a linearized version of the procedure and found it somewhat faster than solving the quadratic.

Summarizing, the time-symmetric finite difference replacements of derivatives are given by (3) in the $\mathbf{v} \times \mathbf{B}$ term, by (2) in the first term of expression (7), by (11) in the second term of expression (7), and by (9) in the energy Eq. (6). Results obtained by this method will be published, when enough runs on "sheet pinches" have been completed, in the plasma literature. Here we only present the results of some accuracy and stability tests, namely runs with constant electric and zero magnetic field.

For these test conditions the problem is one-dimensional, displacement measured from a suitable origin becomes proportional to the mass according to Eq. (9), and the finite-difference version of (5), with substitutions as indicated by (7), (2), and (11) becomes

$$M_n(M_{n+1} - 2M_n + M_{n-1}) + (M_{n+1} - M_n)(M_n - M_{n-1}) = q^2E^2(\Delta t)^2/c^2$$

The corresponding differential equation has the solution

$$M = [M^{*2} + q^2E^2(t - t^*)^2/c^2]^{1/2}$$

with M^* identifiable as the rest mass, and t^* another initial-value constant.

The recurrence relation was run in steps giving approximately one-quarter rest-mass increments ($qE\,\Delta t/c \sim \frac{1}{4}M^*$). Some fifty steps in the deceleration phase permitted fitting the (M, t)-relation by a hyperbola with an error in M^2 of less then $0.0007M^{*2}$. Fifty subsequent steps in the accelerating phase could be fitted similarly and the fitted rest mass turned out to be the same. A displacement in t^* occurred during the few steps near the turn-around, amounting to "jolt" of the hyperbola by $0.15\,\Delta t$. During turn-around, the rest mass, calculated by fitting a rectangular hyperbola to two neighboring (Mc, qEt) values, undergoes a temporary $\frac{3}{4}\%$ increase which corrects itself in the next few steps. A similar test with twice the step size gave hyperbolic (M, t) graphs with an M^2 error of $0.003M^{*2}$ and a "jolt" of $0.3\Delta t$, and again the same "best" M^* for acceleration and deceleration.

III. Orbits in Cylindrical Coordinates

In an r, θ geometry, the centrifugal as well as the Coriolis forces introduce first derivatives into the dynamical equations and one has to find a time-symmetric finite-difference representation of these derivatives.

An r, θ coordinate system is desirable whenever the dominant symmetry of the field of force is cylindrical or spherical, such as in planetary motion. Moreover, the condition of field decay towards infinity is more readily applied in these central coordinate systems than in an (x, y), or (x, y, z) geometry.

Dodging the centrifugal term by reverting to Cartesian coordinates for the orbit calculation, after having obtained the field in central coordinates, is an ugly and time-consuming method. We must remember the importance of speed in the programming of multiparticle problems.

Indeed, it pays to go the opposite way and to take one's cue from the field calculation for introducing an even better coordinate system than r and θ, namely

$$l = \ln r \tag{12}$$

and θ. Conformal mapping theory leads to the Laplace operator representation:

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = e^{-2l}\left(\frac{\partial^2}{\partial l^2} + \frac{\partial^2}{\partial \theta^2}\right) \tag{13}$$

and Poisson's equation, for instance, looks just the same in l, θ coordinates as it does in x, y coordinates:

$$\frac{\partial^2 \Phi}{\partial l^2} + \frac{\partial^2 \Phi}{\partial \theta^2} = -4\pi r^{-2}\rho \tag{14}$$

$$= -4\pi \times \text{charge per unit cell in the } l, \theta \text{ domain} \tag{15}$$

(since $r\,dr\,d\theta = r^2\,dl\,d\theta$ is the area element).

As in conformal mapping, one can use

$$z = x + iy, \tag{16}$$

$$\zeta = \ln z = l + i\theta \tag{17}$$

to advantage, at least for the derivation of the procedures, even if one eventually decides against the use of complex-number routines in the computer.

The dynamical equations

$$\ddot{r} - r\dot{\theta}^2 = b_r\,, \qquad \frac{d(r^2\dot{\theta})}{dt} = rb_\theta\,, \tag{18}$$

where b_r and b_θ are the radial and azimuthal accelerations, combine into

$$\ddot{\zeta} + \dot{\zeta}^2 = r^{-1}(b_r + ib_\theta) \equiv a \tag{19}$$

The simplicity of this equation proves the value of the chosen coordinates.

The square of a first derivative, somewhat like that appearing in the relativistic problem [Eq. (7)], can be replaced symmetrically as in the expression (11). More precisely, we use the following definitions:

$$\Delta \equiv \Delta t, \tag{20}$$

$$\Delta_{\text{new}} \equiv \zeta_{n+1} - \zeta_n\,, \tag{21}$$

$$\Delta_{\text{old}} \equiv \zeta_n - \zeta_{n-1}\,. \tag{22}$$

Then the recommended finite difference form of (19) becomes

$$\Delta_{\text{new}} - \Delta_{\text{old}} + \Delta_{\text{new}}\,\Delta_{\text{old}} = a\Delta^2, \tag{23}$$

symmetric in time and linear in Δ_{new}.

Cylindrical coordinates provide a simple method for incorporation of the Lorentz force due to a uniform, constant magnetic field parallel to the cylinder axis. One uses the Larmor frame of reference, rotating at angular velocity $qB/2M$, in which the Lorentz force is canceled by the Coriolis force. However a spurious centrifugal force appears in this frame and has to be corrected for by subtracting the constant $(qB/2M)^2$ from "a".

To test the algorithm (23) which advances the particles through a field of force, we have considered the case of no fields, $a = 0$. This ought to give straight orbits, constant Δz. From (23), on dividing by $\Delta_{\text{new}}\,\Delta_{\text{old}}$,

$$\Delta_{\text{new}}^{-1} = 1 + \Delta_{\text{old}}^{-1}. \tag{24}$$

Hence, by induction,

$$\Delta_{\text{old}}^{-1} = n + \text{const}, \tag{25}$$

and

$$\zeta_n = \zeta_{n-1} + (n + q)^{-1} \tag{26}$$

where

$$q \equiv (\zeta_0 - \zeta_{-1})^{-1}. \tag{27}$$

(26) is the recursion formula for the Ψ-function [14]

$$\zeta_n = \Psi(n + q). \tag{28}$$

An arbitrary constant, representing a scale, has been suppressed.

For large positive n,

$$\Psi(n + q) = \ln(n + q + \tfrac{1}{2}) + O\,(n + q + \tfrac{1}{2})^{-2} \tag{29}$$

(see [14]), so that

$$z_n = e^{\zeta_n} = n + q + \tfrac{1}{2} + O\,(n + q + \tfrac{1}{2})^{-1} \tag{30}$$

and the spacing becomes uniform, as hoped for.

For large negative $n = -|\,n\,|$, one must use the reflection formula [14]

$$\Psi(-\tfrac{1}{2} - [|\,n\,| - q - \tfrac{1}{2}]) = \Psi(-\tfrac{1}{2} + [|\,n\,| - q - \tfrac{1}{2}]) - \pi \tan \pi(|\,n\,| - q - \tfrac{1}{2}), \tag{31}$$

showing that

$$z_{-|n|} \to (|\,n\,| - q - \tfrac{1}{2}) \exp[-\pi \tan \pi(|\,n\,| - q - \tfrac{1}{2})] \\ = (|\,n\,| - q - \tfrac{1}{2}) \exp[+\pi \tan \pi(q + \tfrac{1}{2})]. \tag{32}$$

Comparing with (30), one sees that for a general complex q, both amplitude and phase of orbits steps will be different in past and future: There has been some inelastic scattering from the coordinate center.

Take q in the form

$$q = q_r + iq_i\,, \tag{33}$$

[redacted]

$$= i\frac{1 - \exp[-2\pi q_1 + 2\pi i(q_r + \tfrac{1}{2})]}{1 + \exp[-2\pi q_1 + 2\pi i(q_r + \tfrac{1}{2})]} \\ \approx i - 2i \exp[-2\pi q_1 + 2\pi i(q_r + \tfrac{1}{2})] \tag{34}$$

when q_i is at all appreciable, say greater than $\frac{1}{2}$. Taking out the factor $e^{i\pi}$ separately in (32), we find

$$z_{-|n|} = (-|\,n\,| + q + \tfrac{1}{2})\{1 - 2\pi i \exp[2\pi i(q_r + \tfrac{1}{2})]\, e^{-2\pi q_1}\}, \tag{35}$$

representing an amplitude or angle correction (which it is, or what mixture of both, is determined by q_r) of magnitude $2\pi e^{-2\pi q_1}$. In other words, for an orbit which misses the origin by a step size at least ($q_1 \geqslant 1$) the change is no larger than 0.012, meaning 1.2% in speed or 0.7° in direction. When the orbit misses by two step sizes, the change is less than 2×10^{-5}.

For close approaches, one gets severe deflections, calculable from cot πq as shown in formula (32). A nonvanishing but bounded acceleration "a" is not expected to change these estimates significantly since the "numerical" deflections are almost entirely attributable to the one step which brings the particle within a step size from the origin. For a singular central force one would have to perform some test runs in order to learn to distinguish between scattering of physical and numerical origin.

It is interesting that the scattering, as in atomic scattering theory, is associated with a "Stokes Phenomenon" of the Ψ-function shown in formula (31), meaning that the asymptotic expansion for large positive argument is *not* valid for large negative argument.

While the suggested time-symmetric algorithm (23) has not yet been tested on

a computer, the analytical study of errors due to scattering shows that one may approach the new procedure with optimism. The coordinate center ($l = -\infty$) has to be treated as singular in other parts of the calculation (field integration) and precautions against scattering can be installed readily. As regards the speed of integration, the cylindrical routine (23), while certainly slower than the planar routine (absence of the product term on the left) is unlikely to become a bottleneck.

IV. Gyrocenter Motion

As a fourth example we study a problem similar to the first, but in the limit of very slow field changes, measured on the scale of the gyroperiod $2\pi/\omega$, where

$$\omega = eB/m, \tag{36}$$

and also ignoring any forces or motion along the magnetic field. The magnetic field is uniform in direction, but we shall eventually allow a particle which traverses it to see a changing magnetic intensity. The electric field $\mathbf{E}$ is always perpendicular to $\mathbf{B}$.

In the first place, we record the formulas for cycloid fitting (described in Section I) as appropriate in this case [8]:

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t} = \mathbf{v}_{\text{new}}, \qquad \frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t} = \mathbf{v}_{\text{old}}, \tag{37}$$

$$\mathbf{v}_{\text{new}} - \frac{\mathbf{E} \times \mathbf{B}}{\mathbf{B}^2} = \left(\mathbf{v}_{\text{old}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right) \cos \omega \Delta t - \frac{\mathbf{B}}{B} \times \left(\mathbf{v}_{\text{old}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right) \sin \omega \Delta t. \tag{38}$$

One sees how the velocity relative to a "guiding" center is turned through an angle $\omega \Delta t$ at every step. The guiding center moves at velocity

$$\mathbf{v}_g = \mathbf{E} \times \mathbf{B}/B^2 \tag{39}$$

and when this vector does not change between steps, the points $\mathbf{x}_n - \mathbf{v}_g n \, \Delta t$ mark the corners of a polygon inscribed in a circle so that the points $\mathbf{x}_n$ lie on a perfect cycloid, exactly where an analytical integration places them at the times $t = n\Delta t$.

Suppose, however, that there is a very slow change of $\mathbf{E}$ and/or B, perceptible only over many gyroperiods $2\pi/\omega$. Do the points $\mathbf{x}_n$ then trace out the ideal orbit, or at least an orbit which does not deviate secularly from the ideal?

In general, for arbitrary step size Δt and turning angle $\omega \Delta t$, there will be increasing discrepancies between the ideal orbit and the points $\mathbf{x}_n$. Particularly for large step sizes, i.e., large angles $\omega \Delta t$, the discrepancies become increasingly

severe. This would prevent one from sampling the slowly varying field only infrequently and making each cycloidal stretch last for many gyroperiods.

To get some quantitative data for this effect, we study a case which permits explicit elementary integration of the dynamical equations and also elementary solution of the recurrence relation (38). This is the case of an electric field varying linearly with time while B remains constant. It is convenient to study this case in a frame of reference in which the electric field appears to pass through zero at the time $t = 0$ (the linear relation between coordinates in the original and the new frame of reference would be reproduced accurately in the finite-difference procedure).

In such a frame, one has $\mathbf{E} = \dot{\mathbf{E}}t$ where $\dot{\mathbf{E}}$ is constant, or $\mathbf{E} = \dot{\mathbf{E}}n\Delta t$ for finite-difference calculations. Placing the x-axis along $\dot{\mathbf{E}}$, one obtains

$$\ddot{x} + \omega^2 x = e\dot{E}t \tag{40}$$

after eliminating $\dot{y}$ from

$$\ddot{y} = \omega\dot{x}, \tag{41}$$

taking the origin $x = 0$ where $\dot{y} = 0$. A particular integral of (40) and (41) is

$$x = e\dot{E}t/\omega^2, \tag{42}$$

$$\dot{x} = e\dot{E}/\omega^2, \tag{43}$$

$$\dot{y} = e\dot{E}t/w, \tag{44}$$

and a complementary solution in the form of a vector rotating steadily at angular velocity ω, may be added to (43), (44).

The velocity $\dot{y} = e\dot{E}t/\omega$ represents gyrocenter motion according to the simple law $\mathbf{v}_g = \mathbf{E} \times \mathbf{B}/B^2$ which is sound when $\mathbf{E}$ is constant. The velocity component $\dot{x} = e\dot{E}/\omega^2$ represents a correction, equal in magnitude to the change of the simple v_g during one gyro-radian period. The resultant of $\dot{y}$ and $\dot{x}$ gives the true gyrocenter motion.

One can now ask: does the recursion formula (38), obtained from cycloid fitting, yield true gyrocenter motion, including the correction, when $\mathbf{E}_n = \dot{\mathbf{E}}n\Delta t$ is used for $\mathbf{E}$ at each step?

Going to components in (38), and trying a solution in the form

$$\dot{y}_{\text{new}} = e\dot{E}(n + \tfrac{1}{2})\,\Delta t/\omega, \tag{45}$$

$$\dot{y}_{\text{old}} = e\dot{E}(n - \tfrac{1}{2})\,\Delta t/\omega, \tag{46}$$

$$\dot{x}_{\text{new}} = \dot{x}_{\text{old}} = \text{const}, \tag{47}$$

one finds that such a solution does exist and one concludes that the most general solution of the recursion formula is obtained by adding the steadily rotating "polygon" solution. However, while the values of $\dot{y}_{\text{new}}$ and $\dot{y}_{\text{old}}$ are exactly those required to fit the analytic solution (44), the constant value of $\dot{x}$ is not in agreement with (43), but is, instead,

$$\dot{x}_{\text{new}} = \dot{x}_{\text{old}} = \frac{e\dot{E}\Delta t}{2\omega} \cot \frac{\omega \Delta t}{2}. \tag{48}$$

For moderate values of $\omega\Delta t/2$, permitting the cotangent to be replaced by the inverse, the drift corrections (43) and (48) agree. However, for certain choices of the time increment, namely for $\omega\Delta t = 2\pi, 4\pi, 6\pi$ etc., the drift correction (48) becomes infinite and cycloid fitting gives an erroneous description of the secular behavior. Indeed, we see immediately that (38) yields the absurd result $\mathbf{v}_{\text{new}} = \mathbf{v}_{\text{old}}$ for these choices of time increment.

Nevertheless, the recursion formula (38) can be salvaged. When one tries to take large steps—the motivation being that the slowly varying field need only be sampled infrequently—and when there are no other cogent considerations to fix a definite step size Δt, a choice can be made such that (43) and (48) agree exactly. It means that $\omega\Delta t/2$ must be identified with one of the solutions $\theta_1, \theta_2 \cdots$ of the transcendental equation:

$$\theta = \tan \theta. \tag{49}$$

There is one such solution within every interval of length π. Thus one can always pick a value Δt as close as half a gyroperiod to any step size $\Delta t'$ which may be desirable from other considerations.

For these restricted Δt-s, one can use the usual substitutions for sine and cosine in (38) in terms of half-angle tangents. This allows one to replace (38) by

$$\left(\mathbf{v}_{\text{new}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right)(1 + \omega^2 \Delta t^2/4) = \left(\mathbf{v}_{\text{old}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right)(1 - \omega^2 \Delta t^2/4) - \frac{\mathbf{B}}{B} \times \left(\mathbf{v}_{\text{old}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right) \omega \Delta t \tag{50}$$

and here we have a useful general formula, to be recommended for all orbit integrations in a magnetic field. It has the following features:

(1) it is strictly time-reversible;

(2) it leads to points on exact cycloids whenever **E** and **B** are constant;

(3) for small and moderate $\omega\Delta t$, it agrees with (38), thus associating the cycloidally arranged points with the correct time intervals between successive points;

(4) for linearly varying **E** and constant **B** it will reproduce the correct secular drifts of the gyrocenter, no matter what value of $\omega\Delta t$ is used;

(5) for large $\omega\Delta t$, useful in the case of arbitrarily but slowly varying fields, it reproduces the gyrocenter motion correctly; specifically,

(6) as $\omega\Delta t \to \infty$ it reduces to the lowest gyrocenter approximation,

$$(1/2\Delta t)(\mathbf{x}_{n+1} - \mathbf{x}_{n-1}) = \tfrac{1}{2}(\mathbf{v}_{\text{new}} + \mathbf{v}_{\text{old}}) = \mathbf{E} \times \mathbf{B}/B^2 \tag{51}$$

in manifestly time-reversible form, but if the odd–even discrepancy is encountered with this approximation, a large finite $\omega\Delta t$ may be used in (50), to anchor the recursion procedure at $\mathbf{x}_n$;

(7) when B varies (as well as **E**) and when Δt is kept fixed at a value rather larger than the range covered by $1/\omega$, the coefficients in (50) vary smoothly, unlike those in (38) which would vary erratically;

(8) ironically—and not trivially—formula (50), constructed with the objective of getting good answer for very large steps, is exactly the solution of the original finite-difference form of the Lorentz equation (4) which was based on the assumption that steps remain small!

The recursion formula (50) has been tested for speed and reliability in recent work by Hockney and Levy on the instability and breakup of certain crossed-field beam configurations. This work will be published shortly in the regular Physics literature but its history is of computational interest: Hockney and Levy began their computer experiments with the biassed irreversible guiding-center formula $\mathbf{v}_{\text{new}} = \mathbf{E} \times \mathbf{B}/B^2$. They found exceptionally poor energy conservation and this was traced by Hockney to one-way effects arising from the biassed formula. Hockney then tried the time-symmetric equation (51) and found an odd–even discrepancy which became steadily worse. Eventually, he used (50) and obtained stability, adequate energy conservation, and performance of the system which agrees with certain physical observations.

V. Continuity Equations

An Eulerian description of the dynamics of a continuous medium (or distribution) can contain first derivatives even under strictly reversible conditions (absence of dissipation). As examples, we quote the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \tag{52}$$

and the "collisionless" Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} + \frac{\partial (af)}{\partial v} = 0, \tag{53}$$

where a is the acceleration. Only one space dimension is being considered here for the sake of simplicity.

Partial differential equations of this type have received considerable attention already, largely because there is a preference for Eulerian (as against Lagrangian) descriptions of fluid and aerodynamics. In a survey of recent publications, the author found heavy concentration on questions of stability and precision, but little attention to the physical principle of reversibility.

In aerodynamical studies, which take into account dissipative processes such as diffusion, viscosity, and heat conduction, reversibility *per se* does not apply. Nevertheless, one ought to make sure that the diffusion, etc., observed in any computation is of truly physical and not of numerical origin, in the same way as one likes to check that numerical procedures do not introduce unphysical sources of mass, energy or momentum. Thus some attention to the symmetrical representation of the operator $\partial/\partial t$ is called for even in these studies. An unwanted "diffusion" is alluded to by Killeen and Rompel [15] in their integration of the collisionless Boltzmann equation when they use a manifestly unsymmetric difference operator, subsequently discarded in favor of a symmetric one [the equation following their Eq. (38)]. Their final routine, however, is essentially Leith's [16] unsymmetrical scheme. Harlow [17] discusses entropy, but not in relation to difference methods.

The classical account by Richtmyer [18] lists only three stable time-symmetric representations of $\partial/\partial t$ (out of thirteen), namely his case "2", used by Crank and Nicholson [19] (the symmetry was inspired by Hartree in this case), the beautiful scheme "8" by Dufort and Frankel and scheme "12". Incidentally, one finds that time-symmetric procedures, while not of themselves stable, are more easily analyzed for stability than unsymmetric procedures. This is borne out by Williamson's survey [21] in which only scheme 1.7 and C.5 are symmetric. The articles by Gentry, Martin, and Daly [22] and Arakawa [23] appear to be concerned with unsymmetric (forward) difference schemes only.

Numerical procedures would employ some mesh in x and t for (52) and a mesh in x, v, t for (53). A finite-difference version of (52) which is symmetric in x and t would state

$$\frac{\rho_{\text{after}} - \rho_{\text{before}}}{2\Delta t} + \frac{j_{\text{right}} - j_{\text{left}}}{2\Delta x} = 0 \tag{54}$$

at each mesh point. The "present" value of ρ would not be referred to, nor would

the "central" value of j enter. Similar considerations apply to the Boltzmann equation,

$$\frac{f_{\text{after}} - f_{\text{before}}}{2\Delta t} + \frac{(vf)_{\text{right}} - (vf)_{\text{left}}}{2\Delta x} + \frac{(af)_{\text{fast}} - (af)_{\text{slow}}}{2\Delta v} = 0 \qquad (55)$$

(here v is an independent, discretized variable, values at neighboring velocities being characterized by the subscripts "fast" and "slow").

The danger of "odd" and "even" mesh points getting out of step arises in these cases. As a precaution one can adopt the policy of simply ignoring odd x-values at even time steps and vice versa, working solely on the remaining mesh points. In other words, the x-mesh is "staggered" for alternate time steps, for the purposes of the continuity equation at least. In the Boltzmann equation, one can employ an "octahedral" lattice in x, v, t-space. "Leap-frogging" and the use of "interlaced" grids are not uncommon: see for instance Fromm's [24] time-symmetric schemes.

The feasibility of this procedure depends upon whether, in the case of the continuity equation, the j-data are available in just the cells where they are needed, or whether the ρ-data are needed in just the cells where they are supplied. If the entire dynamical calculation is carried out in the Eulerian mode, and provided there is no dissipation, then one usually finds that supply and demand of data for various quantities is just in keeping with this staggering. Indeed, one suspects that it should be possible to state some general theorem along these lines and prove it from a Hamiltonian describing the entire system. There is probably also some connection with the "Hermiticity" of matrices describing reversible evolution of systems.

As a simple example, consider a cold collisionless charged fluid governed by (52) with $j = \rho v$ and the Eulerian dynamical equation

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}\frac{v^2}{2} = \frac{q}{M}E, \qquad (56)$$

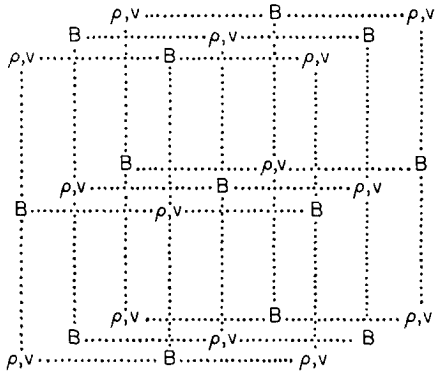
where

$$\epsilon_0(\partial E/\partial x) = \rho. \qquad (57)$$

Records of ρ and v over a diamond-shaped grid in space–time, together with a record of E at the midpoints of the diamonds, allow progressive determination of all quantities using simple central differences for space and time derivatives. A pressure related to ρ by a simple equation of state can also be incorporated and has to be recorded at the same points as ρ and v. The scheme is stable when $(\Delta t)^{-1}$ exceeds $\omega_p + |v|/\Delta x$ where ω_p is the plasma frequency $(\rho q/m\epsilon_0)^{1/2}$.

In three dimensions, a cold charged fluid whose canonical momentum $\mathbf{p} + q\mathbf{A}$ is irrotational can be dealt with similarly, and the whole set of Maxwell's equations

can be integrated simultaneously provided one records and processes the data as follows:

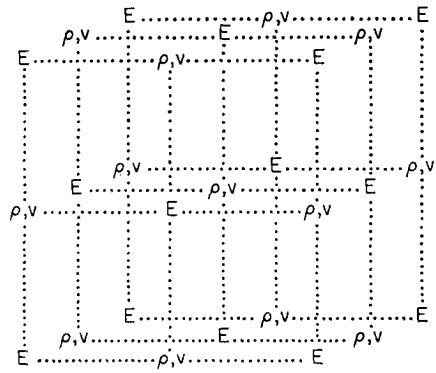


Shown here is the record at even time steps. **B**-values and ρ, **v**-values are staggered like Na and Cl in salt. From these data one calculates div $\rho\mathbf{v}$ at the **B**-lattice points, permitting one to update the odd-time ρ-values in the table below. One also forms curl **B** at the ρ, **v**-lattice points to update **E** in the table below from Maxwell's

$$\frac{\partial \mathbf{E}}{\partial t} = c \operatorname{curl} \mathbf{B} - \rho\mathbf{v}/\epsilon_0 \,. \tag{58}$$

Unbiassed values of $\langle \mathbf{E} \rangle$ are then formed at the **B**-lattice points as averages of the six previous nearest **E**-data and the six subsequent nearest **E**-data just calculated. $\langle \mathbf{E} \rangle$ need not be retained in memory, it is only needed locally for the updating of **v** in the table below from grad($\frac{1}{2}v^2$)-values at the **B**-lattice in the table above, using

$$\frac{\partial \mathbf{v}}{\partial t} = -\operatorname{grad}(\tfrac{1}{2}v^2) - \frac{q}{M}\langle \mathbf{E} \rangle. \tag{59}$$



Shown here is the record at odd time steps from which div $\rho\mathbf{v}$ can be formed at the **E**-lattice points to update ρ in the table above, curl **E** can be formed at the ρ, **v**-lattice points for the updating of **B** by Maxwell's

$$\partial\mathbf{B}/\partial t = -\text{curl}\,\mathbf{E} \tag{60}$$

and grad $(\frac{1}{2}v^2)$ is obtained at the **E**-lattice to update **v** in the scheme above, using the available **E** rather than the average as in (59).

Since a hot plasma can be described as a superposition of a large number of cold irrotational streams [25], or since the indicated data arrangement, with additional staggering in velocity space, can also be used for the integration of Boltzmann's equation, one has strong evidence of the universality of this scheme.

SUMMARY

In conclusion, we observe that in five specific examples the requirements of time-symmetric programming has raised interesting but surmountable problems. In all cases, it has been possible to develop techniques which are not only time-reversible but also aesthetically more pleasing, even simpler, than the objectionable, biased, forward-difference procedures.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation under Grant GK-625.

REFERENCES

1. L. BRILLOUIN, "Science and Information Theory." Academic Press, New York (1963).
2. J. DAWSON, *Phys. Fluids* **5**, 445 (1962); section headed "Checks on the Calculations".
3. R. P. FEYNMAN and J. A. WHEELER, *Rev. Mod. Phys.* **17**, 157 (1945).
4. F. J. ALDER and T. WAINWRIGHT, as reported in C. Kittel, "Elementary Statistical Physics." Wiley, New York (1958).
5. O. BUNEMAN and D. A. DUNN, *Sci. J.* **1**, 34 (1966).
6. C. K. BIRDSALL and W. B. BRIDGES, *J. Appl. Phys.* **32**, 2611 (1961).
7. R. W. HOCKNEY, *Phys. Fluids* **9**, 1826 (1966).
8. S. P. YU, G. P. KOOYERS, and O. BUNEMAN, *J. Appl. Phys.* **36**, 2550 (1965).
9. P. BURGER, *J. Appl. Phys.* **35**, 3048 (1964).
10. S. R. DEGROOT, "Thermodynamics of Irreversible Processes," Chaps. 1.2 and 2.6. North Holland, Amsterdam (1951).
11. J. D. JACKSON, "Classical Electrodynamics," Chap. 12, Problem 10b. Wiley, New York (1962).

12. L. LANDAU and E. LIFSHITZ, "The Classical Theory of Fields," Chap. 3.9, Problem 2. Addison Wesley, Reading, Massachusetts (1951).
13. R. BURN and O. BUNEMAN, "Computer Experiments on Sheet Pinch Stability," Abstract 5R-7, *Bull. Am. Phys. Soc.* **12**, 787 (1966).
14. E. JAHNKE and F. EMDE, "Tables of Functions," Chap. II. Dover, New York (1945).
15. J. KILLEEN and S. L. ROMPEL, *J. Computational Phys.* **1**, 29 (1966).
16. C. E. LEITH, *Methods Computational Phys.* **4**, 1 (1965).
17. F. H. HARLOW, *Methods Computational Phys.* **3**, 319 (1964).
18. R. D. RICHTMYER, "Difference Methods for Initial Value Problems," Wiley, New York (1957).
19. J. CRANK and P. NICHOLSON, *Proc. Cambridge Phil. Soc.* **43**, 50 (1947).
20. E. C. DUFORT and S. P. FRANKEL, *Math. Tables Aids Computation* **7**, 135 (1953).
21. D. WILLIAMSON, *J. Computational Phys.* **1**, 51 (1966).
22. R. A. GENTRY, R. E. MARTIN, and B. J. DALY, *J. Computational Phys.* **1**, 87 (1966).
23. A. ARAKAWA, *J. Computational Phys.* **1**, 119 (1966).
24. J. FROMM, *Methods Computational Phys.* **3**, 345 (1964).
25. O. BUNEMAN, "Radiation and Waves in Plasmas" (M. Mitchener, Ed.) p. 54. Stanford University Press, Stanford, California (1961).