

## PROBLEMS

4-2a Sketch the locations of  $a$ ,  $v$ , and  $x$  for the alternative integrator,

$$\frac{v_{t+\Delta t} - v_t}{\Delta t} = \frac{1}{2}(3a_t - a_{t-\Delta t}) \quad (11)$$

$$\frac{x_{t+\Delta t} - x_t}{\Delta t} = \frac{1}{2}(v_{t+\Delta t} + v_t) \quad (12)$$

Show that this integrator produces a frequency for the simple harmonic oscillator (1) of

$$\omega \approx \omega_0 \left[ 1 + \frac{1}{6}(\omega_0 \Delta t)^2 + i \frac{(\omega_0 \Delta t)^3}{8} + \dots \right] \quad (13)$$

*Hint:* Use  $x_{t \pm n\Delta t} = z^{\pm n} x_t$ ,  $z \equiv \exp(-i\omega\Delta t)$  and write (11) and (12) as a matrix. Set the determinant of the coefficients equal to zero to produce an equation in  $z$  (cubic) to be solved. The phase error is four times larger than that of the leap-frog scheme, and there is mild growth. Show how (with a sketch, as in Figure 2-4a)  $\Delta t$  can be halved or doubled in one step. This method has the disadvantage of requiring storage of the previous acceleration  $a_{t-\Delta t}$  in addition to previous velocity  $v_t$  and position  $x_t$ .

4-2b Discuss the possible use of *integer arithmetic* (no floating point) in the mover, with some care as to the number of bits needed for reasonable accuracy. Keep in mind that small changes are lost; that is, nothing happens unless  $v\Delta t$  exceeds the least step in  $x$  and  $a\Delta t$  exceeds the least velocity. *Hint:* 17 bits is marginal or fatal in quiet start. This coding was exploited by *Estabrook and Tull* (1980) for very high speed, almost twice as fast on the CDC-7600 (in machine language) as ES1 is on the CRAY-I (in FORTRAN)!

### 4-3 NEWTON-LORENTZ FORCE; THREE-DIMENSIONAL $\mathbf{v} \times \mathbf{B}$ INTEGRATOR

The particle equations of motion to be integrated are

$$m \frac{d\mathbf{v}}{dt} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (1)$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \quad (2)$$

We desire a centered-difference form of the Newton-Lorentz equations of motion. The magnetic term is centered by averaging  $\mathbf{v}_{t-\Delta t/2}$  and  $\mathbf{v}_{t+\Delta t/2}$ , following *Buneman* (1967). The other terms are treated as before. Hence, (1) becomes

$$\frac{\mathbf{v}_{t+\Delta t/2} - \mathbf{v}_{t-\Delta t/2}}{\Delta t} = \frac{q}{m} \left[ \mathbf{E} + \frac{\mathbf{v}_{t+\Delta t/2} + \mathbf{v}_{t-\Delta t/2}}{2} \times \mathbf{B} \right] \quad (3)$$

This vector equation for  $\mathbf{v}_{t+\Delta t/2}$  can be solved as three simultaneous scalar equations, one for each component. Instead, we choose to obtain a simpler solution using several steps.

The first method (*Buneman*, 1967) is to subtract the drift velocity  $\mathbf{E} \times \mathbf{B} / B^2$  from  $\mathbf{v}$ , as

$$\mathbf{v}'_{\text{old}} = \mathbf{v}_{t-\Delta t/2} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}$$

$$\mathbf{v}'_{\text{new}} = \mathbf{v}_{t+\Delta t/2} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}$$

Similar to (1), this leaves just a rotation of  $\mathbf{v}_{\perp}$  and free acceleration

$$\frac{\mathbf{v}'_{\text{new}} - \mathbf{v}'_{\text{old}}}{\Delta t} = \frac{q}{m} \left[ \mathbf{E}_{\parallel} + \frac{\mathbf{v}'_{\text{new}} + \mathbf{v}'_{\text{old}}}{2} \times \mathbf{B} \right]$$

We discuss the rotation in Problem 4-3a and Section 4-4.

Another method separates the electric and magnetic forces (*Boris*, 1970b). Substitute

$$\mathbf{v}_{t-\Delta t/2} = \mathbf{v}^- - \frac{q\mathbf{E}}{m} \frac{\Delta t}{2}$$

$$\mathbf{v}_{t+\Delta t/2} = \mathbf{v}^+ + \frac{q\mathbf{E}}{m} \frac{\Delta t}{2}$$

into (3); then  $\mathbf{E}$  cancels entirely (not just  $\mathbf{E}_{\perp}$ ), which leaves

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2m} (\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}$$

which is a rotation (see Problem 4-3a). The steps to compute are the electric impulse to  $\mathbf{v}_{t-\Delta t/2}$  using (7) to obtain  $\mathbf{v}^-$ ; rotate according to obtain  $\mathbf{v}^+$ , and add the remaining half of the electric impulse (8)  $\mathbf{v}_{t+\Delta t/2}$ . These are the same steps, motivated differently, as in Section 4-4. Separation of parallel and perpendicular components is not needed in *Boris'* method, and the relativistic generalization is straightforward.

Finally, we check the angle of rotation  $\theta$  which we expect to be  $\omega_c \Delta t = qB\Delta t / m$ . By inspection of Figure 4-3a, we see that

$$\left| \tan \frac{\theta}{2} \right| = \frac{|\mathbf{v}_{\perp}^+ - \mathbf{v}_{\perp}^-|}{|\mathbf{v}_{\perp}^+ + \mathbf{v}_{\perp}^-|} = \frac{qB}{m} \frac{\Delta t}{2} = \frac{\omega_c \Delta t}{2}$$

where we have used (9) in the last step. Hence, the difference equation produces a rotation through angle

$$\theta = 2 \arctan \left( \frac{qB}{m} \frac{\Delta t}{2} \right) = \omega_c \Delta t \left[ 1 - \frac{(\omega_c \Delta t)^2}{12} + \dots \right]$$

which has less than one percent error for  $\omega_c \Delta t < 0.35$ .

## PROBLEMS

4-3a Show that (9) is only a *rotation* of  $\mathbf{v}$ . *Hint:* take the scalar product of (9) with  $(\mathbf{v}^+ + \mathbf{v}^-)$ .

4-3b Consider a model with  $\mathbf{B}_0$  uniform and  $\mathbf{E}_{\perp} = 0$ , in which a particle at speed  $v$  moves in the  $x_1$  plane. Let the orbit be followed by (subscripts refer to time steps)

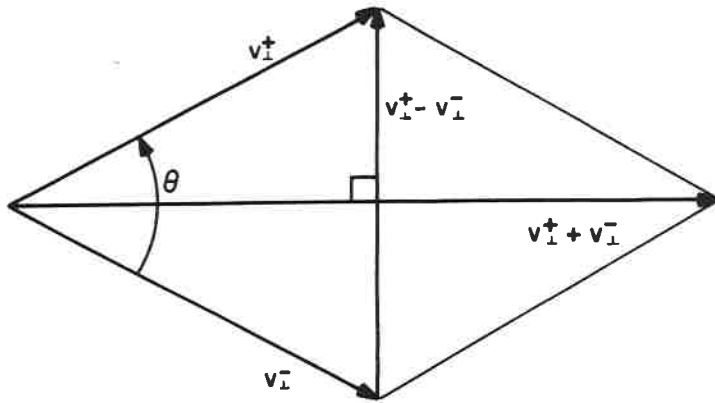


Figure 4-3a Knowing that (9) represents a rotation, we construct this diagram, from which  $\tan(\theta/2)$  is readily obtained.

$$\frac{\mathbf{x}^+ - \mathbf{x}^0}{\Delta t} = \mathbf{v}^+ \quad \frac{\mathbf{x}^0 - \mathbf{x}^-}{\Delta t} = \mathbf{v}^-$$

with  $\mathbf{v}^+$  obtained from

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \lambda \left( \frac{\mathbf{v}^+ + \mathbf{v}^-}{2} \right) \times \left( \frac{q\mathbf{B}}{m} \right)$$

as shown in Figure 4-3b. Using  $\tan \alpha$  from this figure [Hint: see (10)], show that

$$\lambda = \frac{\tan \alpha}{\frac{1}{2}\omega_c \Delta t}$$

which is  $(\tan \alpha)/\alpha$  if we ask that the mover produce the correct gyrophase,  $\alpha = \omega_c \Delta t/2$ . Next, requiring that the gyroradius and period be reproduced correctly, show that

$$|\mathbf{v}^+| = |\mathbf{v}^-| = v \left( \frac{\sin \alpha}{\alpha} \right)$$

Last, show that when  $\mathbf{E}_\perp$  is included, the  $\lambda$  multiplier appears as  $\lambda(\mathbf{E}_\perp + \mathbf{v} \times \mathbf{B})$  in order to produce the correct  $\mathbf{E} \times \mathbf{B}/B^2$  drift. [These ideas came from Hockney (1966), Buneman (1967), and R. H. Gordon (unpublished Berkeley seminar, 1971).]

4-3c (Due to R. H. Gordon). Using any of the  $\mathbf{v} \times \mathbf{B}$  integrators given here, for uniform  $B_0 \hat{z}$ , plot particle orbits in the  $x, y$  plane:

- Without the  $\tan \alpha/\alpha$  correction, supposedly with an integral number of steps per cyclotron period; note where points on the second and succeeding cycles are with respect to those on the first.
- Repeat (a) with  $\tan \alpha/\alpha$  correction; try  $0 < \alpha < \pi$ .
- Like (b), with  $\omega_c \Delta t = 2\pi$ ; compare with true orbit; explain the motion; is this instability?
- Like (b), with  $\omega_c \Delta t = 2\pi - \delta$ ; compare with true orbit; explain the motion.

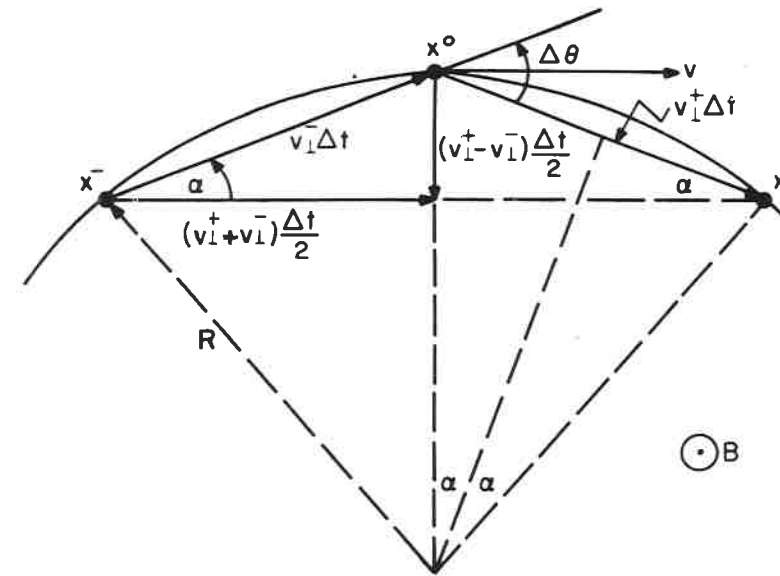


Figure 4-3b Velocities and positions in the plane normal to the uniform magnetic field  $\mathbf{E}_\perp = 0$  in which the particle orbit is a circle (cyclotron motion). The computer difference orbit is made up of straight line segments connecting old and new positions.

#### 4.4 IMPLEMENTATION OF THE $\mathbf{v} \times \mathbf{B}$ ROTATION

First consider the case in which  $\mathbf{B}$  is parallel to the  $z$  axis. In the  $x, y$  plane the rotation is through an angle  $\theta$  where

$$\tan \frac{\theta}{2} = -\frac{qB \Delta t}{m \omega_c}$$

This gives a good approximation to rotation angle  $\theta$  when  $\theta$  is not too large [4-3(11)], and is convenient when  $B$  is not constant. In ES1,  $B$  is constant; we evaluate  $\tan \theta/2 = -\tan(qB \Delta t/2m)$ ; obtaining the correct angle costs nothing more.

Now we use this value of  $\tan \theta/2$  in the half-angle formulas for  $\cos \theta$  and  $\sin \theta$  for the velocity rotation. Letting

$$t = -\tan \frac{\theta}{2}$$

we have

$$s \equiv -\sin \theta = \frac{2t}{1+t^2}$$

$$c \equiv \cos \theta = \frac{1 - t^2}{1 + t^2} \quad (4)$$

The rotation becomes

$$v_x^+ = cv_x^- + sv_y^- \quad (5)$$

$$v_y^+ = -sv_x^- + cv_y^- \quad (6)$$

The mover requires no evaluation of transcendental functions, which is a significant time saving when  $B$  is not constant. Equations (3) to (6) require 7 multiplies, 1 divide, and 5 adds. *Buneman* (1973) reduces this to:

$$v'_x = v_x^- + v_y^- t \quad (7)$$

$$v'_y = v_y^- - v'_x s \quad (8)$$

$$v_x^+ = v'_x + v'_y t \quad (9)$$

with 4 multiplies, 1 divide, and 5 adds. The saving of 3 multiplies per particle per time step is desirable.

When the directions of  $\mathbf{B}$  and  $\mathbf{v}$  are arbitrary, a convenient rotation in vector form is described by *Boris* (1970). First  $\mathbf{v}^-$  is incremented to produce a vector  $\mathbf{v}'$  which is perpendicular to  $(\mathbf{v}^+ - \mathbf{v}^-)$  and  $\mathbf{B}$  (see Figure 4-4a).

$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t} \quad (10)$$

The angle between  $\mathbf{v}^-$  and  $\mathbf{v}'$  is just  $\theta/2$ , therefore the vector  $\mathbf{t}$  is seen from Figure 4-4a to be given by

$$\mathbf{t} \equiv -\hat{\mathbf{b}} \tan \frac{\theta}{2} = \frac{q\mathbf{B}}{m} \frac{\Delta t}{2} \quad (11)$$

Finally,  $\mathbf{v}^+ - \mathbf{v}^-$  is parallel to  $\mathbf{v}' \times \mathbf{B}$ , so

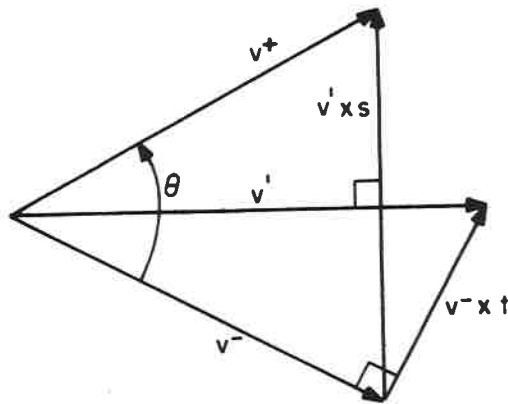


Figure 4-4a Velocity space showing the rotation from  $\mathbf{v}^-$  to  $\mathbf{v}^+$ . The velocities shown are projections of the total velocities onto the plane perpendicular to  $\mathbf{B}$ .

$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$$

where  $\mathbf{s}$  is parallel to  $\mathbf{B}$  and its magnitude is determined by the relation  $|\mathbf{v}^-|^2 = |\mathbf{v}^+|^2$

$$\mathbf{s} = \frac{2\mathbf{t}}{1 + t^2}$$

Boris' algorithm is readily made relativistic; see Chapter 15.

PROBLEMS

4-4a Verify that (7) - (9) has the same result as (5) and (6).

4-4b Using  $|\mathbf{v}^+| = |\mathbf{v}^-|$  (a rotation), obtain  $s$  (13).

4-4c Show that Boris' rotation satisfies the equation of motion 4-3(9), if  $\mathbf{t} = q\mathbf{B}\Delta t/m$ .

4-5 APPLICATION TO ONE-DIMENSIONAL PROGRAMS

In programs with one dimension  $x$  and with *two velocities*,  $v_x$  and  $v_z$ , and allow a magnetic field  $B_z$ , the motion is all perpendicular to  $\mathbf{B}$ . Hence, using the vector equations of the previous sections, we obtain the 1d3v rotate-accel algorithm in Section 2-4.

A program with one dimension and with *three velocities* 1d3v3v is set up as shown in Figure 4-5a. Let  $\mathbf{B}_0$  (constant, uniform) be in the  $z$  direction and make an angle  $\theta$  with the  $x$  axis. The self-consistent  $\mathbf{E}$  and  $\mathbf{B}$  are along  $x$ , normal to the sheets. If we stopped here, then the perpendicular motion in  $z$  could be ignored ( $F_z = 0$ ). However, on occasion we are interested in applying an electric field  $E_{ext}$  along  $y$  which produces a drift. In turn produces an  $F_z = -qv_y B_x$  and a  $z$  drift,  $(v_E)_z = -(E_{ext})_y/B_x$ . A point of the exercise is to include both  $v_{||}$  and  $v_{\perp}$  as well as  $k_{||}$  and  $k_{\perp}$  in the model. It is convenient to have the motion solved for in the perpendicular directions, which leads to the invention of the  $x'$  coordinate system ( $x'$   $\perp$  to  $\mathbf{B}_0$ , at angle  $\theta$  with respect to  $x$ ). Call the field due to the self-consistent fields  $\mathbf{E}_{sc}$ . Then the fields are:

$$\mathbf{E}_{sc} = \hat{\mathbf{x}}E_{sc} = \hat{\mathbf{x}}'E_{sc} \cos \theta + \hat{\mathbf{b}}_0 E_{sc} \sin \theta$$

$$\mathbf{E}_{ext} = \hat{\mathbf{y}}E_{ext}$$

$$\mathbf{B} = \mathbf{B}_0$$

The equations of motion in the  $(x', y, B_0)$  coordinates are integrated using the accel-rot-accel method, as follows

$$v_{x_1} = v_{x'}(t - \Delta t/2) + \frac{q}{m} \frac{\Delta t}{2} E_{sc} \cos \theta$$