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Modelling the solar wind interaction with Mercury by a quasi-neutral hybrid model

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6. Propagate the particle velocities $\mathbf{v}_i^{n+1}$ from

$$m_i \frac{\mathbf{v}_i^{n+1} - \mathbf{v}_i^n}{\Delta t} = q_i \left(\frac{1}{2}(\mathbf{v}_i^n + \mathbf{v}_i^{n+1}) - \mathbf{u}_e^n \right) \times \mathbf{B}^{n+1/2}. \quad (15)$$ *

The electron flow $\mathbf{u}_e^n$ is not time-centred, but that cannot be avoided.

* Note: We assume that **E** = -**U**$_e$ x **B**

The particle mover is split into a position mover and a velocity mover. The positions and velocities are propagated by following a time-reversible second-order accurate Buneman scheme as follows (Hockney and Eastwood, 1988, p. 112). The position mover is,

$$\mathbf{x}_i^{n+1/2} = \mathbf{x}_i^{n-1/2} + \Delta t\, \mathbf{v}_i^n. \quad (16)$$

The velocity update formula

$$m_i \frac{\mathbf{v}_i^{n+1} - \mathbf{v}_i^n}{\Delta t} = q_i \left(\frac{1}{2}(\mathbf{v}_i^n + \mathbf{v}_i^{n+1}) - \mathbf{u}_e^n \right) \times \mathbf{B}^{n+1/2} \quad (17)$$

is solved for $\mathbf{v}_i^{n+1}$:

$$\mathbf{v}_i^{n+1} = \mathbf{v}_i^n + \frac{\left[a(\mathbf{v}_i^n - \mathbf{u}_e^n) + \frac{1}{2}a^2(\mathbf{v}_i^n - \mathbf{u}_e^n) \times \mathbf{B}^{n+1/2}\right] \times \mathbf{B}^{n+1/2}}{1 + (\frac{1}{2}aB^{n+1/2})^2}, \quad (18)$$

where $a = (q_i/m_i)\Delta t$ and $\mathbf{B}^{n+1/2}$ must be evaluated at the particle position $\mathbf{x}_i^{n+1/2}$.

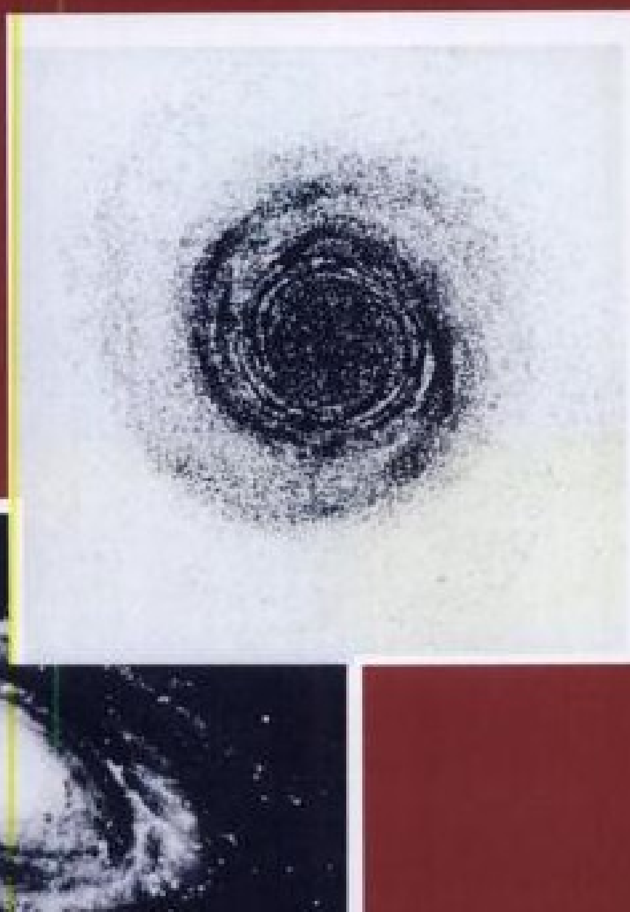
By defining the vector $\boldsymbol{\omega} = (1/2)\ a\ \mathbf{B}^{n+1/2}$, the update operation can be written in a slightly more compact way as

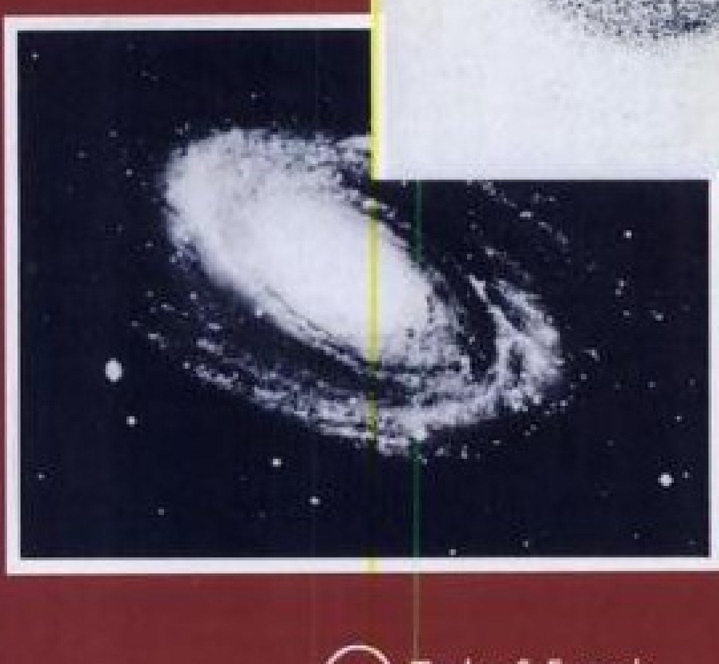
$$\mathbf{v}_i^{n+1} = \mathbf{v}_i^n + \frac{2}{1+w^2}\left[(\mathbf{v}_i^n - \mathbf{u}_e^n) + (\mathbf{v}_i^n - \mathbf{u}_e^n) \times \boldsymbol{\omega}\right] \times \boldsymbol{\omega} \quad (19)$$

Boris-Buneman

COMPUTER SIMULATION USING PARTICLES

R W Hockney
J W Eastwood





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4-7 EXAMPLES OF INTEGRATION SCHEMES

4-7-1 Lorentz Force Integrators

In the presence of a magnetic field **B** the force on a particle of charge q with velocity **v** is given by the Lorentz force:

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B} \tag{4-89}$$

Positions and velocities are obtained by integrating

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \qquad \frac{d\mathbf{v}}{dt} = \mathbf{v} \times \mathbf{\Omega} \tag{4-90}$$

where $\mathbf{\Omega} = q\mathbf{B}/m$ is the cyclotron (or gyro) frequency.

Consider first the case where $\mathbf{\Omega} = \Omega\hat{\mathbf{z}}$, where $\Omega =$ constant. Equation (4-90) describes circular orbits of radius $|\mathbf{v}|$ in the v_x-v_y plane and of radius $|\mathbf{v}|/\Omega$ in the x-y plane, where in both instances the angular frequency is given by Ω. A consistent time-centered finite-difference approximation to Eq. (4-90) is

$$\mathbf{x}^{n+1} - \mathbf{x}^{n} = \mathbf{v}^{n+1/2} DT \tag{4-91}$$

$$\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2} = (\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}) \times \frac{\mathbf{\Omega} DT}{2} \tag{4-92}$$

This scheme was recommended by Buneman (1967) and used by Hockney (1966*a*) in the study of anomalous plasma diffusion (see Chapter 9). The equations, although implicit in velocities, can be readily solved for new values in terms of old by suitably rearranging Eq. (4-92) (cf. below). They are time-reversible and second-order accurate. The energy constants ($=|\mathbf{v}|^2$) are identical for both the differential and difference equations. In addition, Eqs. (4-91) and (4-92) are unconditionally stable: this may be readily established by using the amplification matrix method, yielding the four roots of the characteristic equation

$$\begin{aligned} \lambda_1 &= \lambda_2 = 1 \\ \lambda_3 &= \lambda_4^* = \frac{1 + i\Omega DT/2}{1 - i\Omega DT/2} \end{aligned} \tag{4-93}$$

The first pair of roots (at $\lambda = 1$) correspond to Eq. (4-91), while the second pair of roots, which traverse the unit circle as conjugate pairs moving from $\lambda = +1$ to $\lambda = -1$ as DT increases from zero to infinity, correspond to Eq. (4-92).

The discrete approximation, Eq. (4-92), gives velocities lying on a circle of radius $|\mathbf{v}|$ in the $v_x - v_y$ and positions lying on a circle of radius R' in the x-y plane. The effect of finite timestep is to cause the frequency to be higher than the correct frequency Ω (cf. Sec. 4-6) and the radius R' to differ from the cyclotron radius $R = |\mathbf{v}|/\Omega$. The frequency ω of the orbits described by Eq. (4-92) may be found by setting λ_3 or λ_4 to $\exp(i\omega DT)$ in Eq. (4-93), yielding

$$\tan\frac{\omega DT}{2} = \pm\frac{\Omega DT}{2} \tag{4-94}$$

The radius R' may be found from Eqs. (4-91) and (4-92) using Eq. (4-94) and the result that $|\mathbf{v}| = \text{constant}$:

$$R' = \frac{|\mathbf{v}|}{\Omega}\sec\frac{\omega DT}{2} \tag{4-95}$$

As in the case of the leapfrog harmonic oscillator, the error in the frequency can be eliminated by adjusting the frequency appearing in the difference equations (see Hockney, 1966*a*, pp. 93–98). In this case, Eq. (4-94) tells us that we must replace $\Omega DT/2$ in Eq. (4-92) by $\tan(\Omega DT/2)$.

The results for $\mathbf{\Omega} = \text{constant}$ immediately generalize to a variable $\mathbf{\Omega}$ by replacing $\mathbf{\Omega}$ by $\mathbf{\Omega}^n = \mathbf{\Omega}(\mathbf{x}^n)$ in Eq. (4-92). In addition, if there is an electric field present, then the leapfrog approximation for the electric field force can be combined with the Lorentz force integrator to give the scheme

$$\mathbf{x}^{n+1} - \mathbf{x}^n = \mathbf{v}^{n+1/2}DT \tag{4-96}$$

$$\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2} = \frac{q\mathbf{E}^n}{m}DT + (\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}) \times \frac{\mathbf{\Omega}^n DT}{2} \tag{4-97}$$

The components of Eqs. (4-96) and (4-97) parallel to the magnetic field are simply the leapfrog scheme, and so must satisfy the leapfrog stability criterion. The components perpendicular to the magnetic field are unconditionally stable and have the interesting property that for large timestep they tend towards the adiabatic drift equation:

$$\bar{\mathbf{v}}^n = \frac{(\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2})}{2} = \frac{\mathbf{E}^n \times \mathbf{B}^n}{|B^n|^2} + O(DT^{-1}) \tag{4-98}$$

This property was used by Levy and Hockney (1968) in the study of crossed-field electron beams, and has been extensively exploited by Birdsall and his coworkers (Birdsall and Langdon, 1981).

The electric acceleration terms and the rotational (Lorentz force) terms in Eq. (4-97) can be separated by introducing two intermediate velocities $\mathbf{v}_1^*$ and $\mathbf{v}_2^*$:

$$\mathbf{v}_1^* = \mathbf{v}^{n-1/2} + \frac{q}{m}\mathbf{E}^n\frac{DT}{2} \tag{4-99}$$

$$\mathbf{v}_2^* = \mathbf{v}_1^* + (\mathbf{v}_2^* + \mathbf{v}_1^*) \times \frac{\mathbf{\Omega}^n DT}{2} \tag{4-100}$$

$$\mathbf{v}^{n+1/2} = \mathbf{v}_2^* + \frac{q}{m}\mathbf{E}^n\frac{DT}{2} \tag{4-101}$$

Equation (4-100) may further be factorized by taking its cross product with $\boldsymbol{\Omega} DT/2$ and eliminating the triple cross-product term involving $\mathbf{v}_2^*$ to yield

$$\mathbf{v}_2^* = \mathbf{v}_1^* + \frac{2}{1+\left(\frac{\Omega DT}{2}\right)^2} \mathbf{v}_3^* \times \boldsymbol{\Omega} \tag{4-102}$$

where

$$\mathbf{v}_3^* = \mathbf{v}_1^* + \mathbf{v}_1^* \times \frac{\boldsymbol{\Omega} DT}{2} \tag{4-103}$$

The factorization equations [Eqs. (4-99), (4-103), (4-102), and (4-101)] form the basis of Boris' CYLRAD algorithm (Boris, 1970).

The frequency correction factor introduced for the constant $\boldsymbol{\Omega}$ case can also be incorporated into the more general form [Eq. (4-97)]. If we assume that $\mathbf{E}$ and $\boldsymbol{\Omega}$ are approximately constant over a timestep, then the equation of motion