JOURNAL OF COMPUTATIONAL PHYSICS 28, 279–286 (1978)

Note

Exact Magnetic Energy Conservation on a Nonuniform Mesh

1. INTRODUCTION

Coupled sets of partial differential equations occurring in classical physics often satisfy exact conservation laws for quantities such as mass, momentum, energy, electric charge and magnetic flux. When these equations are put into difference form for numerical solution on a computer there is some advantage in retaining the differential conservation laws as exact difference identities [1–4]. This improves confidence in the solution, and can be of considerable practical help in showing up minor errors in the difference algebra and the coding which frequently make themselves apparent by a lack of exact conservation, although for this it has proved essential to use double precision on 32-bit machines. Boundary conditions are also often expressed more elegantly and satisfactorily in conservative form.

To establish difference identities is usually straightforward for linear quantities like mass, charge and magnetic flux. Energy may, however, involve quadratic or cubic expressions such as $\rho \mathbf{v}^2$, $\mathbf{B}^2$, ρT, $\mathbf{J}^2$ where as usual ρ is the density, $\mathbf{v}$ the velocity, $\mathbf{B}$ the magnetic field, T the temperature and $\mathbf{J}$ is the current density. Here there appears to be no general guarantee that an exact difference identity can always be found [3].

A general discussion of conservative and nonconservative MHD difference schemes has been given by Lindemuth [2]. Our intention in this Note is to examine in detail one particular example, indicating the complexities that arise in practice and how they can be resolved. The problem chosen is that of ensuring *exact* conservation of energy during magnetic field diffusion so that energy which is lost from the magnetic field reappears as ohmic heating of the plasma. The algorithm to be described forms part of the 1DMHD equilibrium and diffusion code ATHENE 1 [5, 6], which studies the evolution of a plasma in cylindrical geometry using a moving Lagrangian mesh which necessarily becomes spatially nonuniform. This nonuniformity complicates the algebra but an optimum choice of difference formulas can nevertheless be obtained.

2. MHD EQUATION

Cylindrical geometry (r, θ, z) is used with the physical variables depending only on (r, t). The model used in ATHENE 1 assumes a magnetically confined plasma to evolve through a sequence of pressure equilibria satisfying

$$\nabla p = \mathbf{J} \times \mathbf{B}, \tag{1}$$

0021-9991/78/0282–0279$02.00/0

where $p = 2nkT$ is the plasma pressure and n is the number density. (For brevity in this Note we assume equal electron and ion temperatures and set $\mu_0 = 1$.) Diffusion of magnetic fields and thermal energy is described by

$$\frac{\partial B_\theta}{\partial t} = \frac{\partial E_z}{\partial r}, \qquad \frac{\partial B_z}{\partial t} = -\frac{1}{r}\frac{\partial (rE_\theta)}{\partial r}, \tag{2}$$

$$C\frac{\partial T}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(rF) + \mathbf{J}\cdot\mathbf{E}, \tag{3}$$

where $C = 2nk/(\gamma - 1)$ is the specific heat, $\mathbf{E}$ is the electric field and F is the thermal flux.

Each equilibrium satisfying (1) is calculated by a two-stage process [5]. Stage I is an Eulerian timestep in which the computational mesh is temporarily frozen and the diffusion equations are solved; hence the omission of advective terms from (2) and (3). This is followed by Stage II, a Lagrangian timestep in which the variables n, T, B_θ and B_z change adiabatically by relaxation of the mesh until (1) is satisfied. Only Stage I of the calculation will be discussed here, Stage II having been described together with a listing of the FORTRAN code and test results in Ref. [5].

Apart from inessential numerical factors the thermal and magnetic energy contents of a cylinder of radius a are

$$W_T = \int_0^a CTr\, dr, \qquad W_\theta = \int_0^a \tfrac{1}{2}B_\theta^2 r\, dr, \qquad W_z = \int_0^a \tfrac{1}{2}B_z^2 r\, dr. \tag{4}$$

To demonstrate that the differential equations conserve the energy sum $W = W_T + W_\theta + W_z$ the standard method is to multiply Eqs. (2) by B_θ and B_z respectively and add to (3). Integration by parts from $r = 0$ to $r = a$ yields

$$\frac{\partial W}{\partial t} = -a[\mathbf{E}\times\mathbf{B} + F]_{r=a}. \tag{5}$$

When (1)–(3) are solved by finite differences an error ΔW results [2]. Denoting the relative errors $\epsilon = \Delta W/W$ of the two stages by ϵ_{I} and ϵ_{II} respectively we show in the following sections that ϵ_{I} can be eliminated completely provided that the appropriate formulas are used for the ohmic heating term in (3). The proof involves a generalization of the two processes of multiplication by $\mathbf{B}$ and integration by parts to the finite difference case. It is interesting that the elimination of ϵ_{I} is quite independent of the functional form of the electric field $\mathbf{E}$ provided that $\mathbf{E}$ enters in an identical way in the difference equivalents of (2), (3) and (5). The error ϵ_{II} associated with motion has been analysed by Lindemuth [2] and is monitored by the ATHENE 1 code to check the accuracy of the calculation.

3. Finite Difference Equations

A nonuniform mesh

$$0 = r_1 , r_2 ,..., r_N , r_{N+1} = a \tag{6}$$

is used which remains fixed in Stage I, a being the radius at which boundary conditions are to be applied. The finite difference notations used in [2] and [5] are adopted here with minor modifications [6]. The dependent variables T, B_θ, B_z are defined at the half-points (cell centers)

$$r \equiv r_{j+1/2} = \tfrac{1}{2}(r_{j+1} + r_j) \equiv \tfrac{1}{2}(r_+ + r_-), \tag{7}$$

and subscripts $(j - \frac{1}{2}, j + 1, j + \frac{3}{2})$ are denoted respectively by $(--, -, +, ++)$. These variables are to be regarded as cell averages, i.e., the magnetic fluxes and the energies associated with cell $j + \frac{1}{2}$ are defined to be

$$B_\theta \, \Delta r, \qquad B_z \, \Delta A, \tag{8}$$

and

$$CT \, \Delta A, \qquad \tfrac{1}{2}B_\theta^2 \, \Delta A, \qquad \tfrac{1}{2}B_z^2 \, \Delta A, \tag{9}$$

with

$$\Delta r = r_+ - r_- , \qquad \Delta A = r \, \Delta r = \tfrac{1}{2}(r_+^2 - r_-^2). \tag{10}$$

Variables at the new time level $n + 1$ are indicated by an asterisk. Then the difference equivalents of (2) and (3) are

$$\Delta r(B_\theta^* - B_\theta) = \Delta t \, \delta E_z , \tag{11}$$

$$\Delta A(B_z^* - B_z) = -\Delta t \, \delta(rE_\theta), \tag{12}$$

$$C \, \Delta A(T^* - T) = \Delta t(-\delta(rF) + \Delta A \, \mathbf{E} \cdot \mathbf{J}), \tag{13}$$

where δ is the difference operator defined here by

$$\delta f = f_+ - f_- , \qquad \delta f_+ = f_{++} - f, \qquad \delta f_- = f - f_{--} , \tag{14}$$

and the time levels at which the expressions on the right-hand sides of (11)–(13) are to be evaluated are for the moment left unspecified.

Conservation of magnetic flux is exhibited in the usual way by summing (11) and (12) over all mesh intervals:

$$\sum_1^N (B_\theta^* \, \Delta r - B_\theta \, \Delta r) = \Delta t(E_{z,N+1} - E_{z,1}) \tag{15}$$

$$\sum_1^N (B_z^* \, \Delta A - B_z \, \Delta A) = -\Delta t(rE_\theta)_{N+1} . \tag{16}$$

These identities are independent of the expressions used for (E_θ , E_z), provided that

the *same* expressions are used for both of the adjacent cells $j - \frac{1}{2}$, $j + \frac{1}{2}$, but two points should be noticed. First, one frequently wishes to use an implicit scheme [1]

$$\tilde{E} = \theta E^{n+1} + (1 - \theta) E^n \tag{17}$$

in order to allow Δt to take a value limited only by the accuracy of the calculation, and in ATHENE 1 a fully-implicit scheme ($\theta = 1$) is in fact used for both magnetic and thermal energy diffusion. Second, it is desirable to be able to represent the frequently encountered case of a uniform axial current distribution

$$J_z \equiv \frac{1}{r}\frac{\partial}{\partial r}(rB_\theta) = \alpha, \qquad B_\theta = \frac{1}{2}\alpha r \tag{18}$$

exactly on a nonuniform space mesh, which forces the choice of difference formula

$$J_{z,+} = \frac{1}{\bar{r}_+}\{(rB_\theta)_{++} - (rB_\theta)\} \tag{19}$$

with

$$\bar{r}_+ \equiv \tfrac{1}{2}(r_{++} + r). \tag{20}$$

4. Energy Sums

For large Δt the ohmic heating term $\Delta t(\Delta A\, \mathbf{E} \cdot \mathbf{J})$ in (13) can also become large, especially when anomalous or turbulent transport coefficients are used [7]. It is therefore necessary to ensure that there are no truncation errors in the calculation of $\mathbf{E} \cdot \mathbf{J}$. To obtain a finite difference analog of (5) we multiply (11) and (12) by the time averages [2]

$$r\hat{B}_\theta \equiv \tfrac{1}{2}r(B_\theta^* + B_\theta), \qquad \hat{B}_z \equiv \tfrac{1}{2}(B_z^* + B_z) \tag{21}$$

respectively and sum over the cells $j = (1, N)$. Pairing terms on the right-hand sides with the same index j then gives

$$W_\theta^* - W_\theta = \Delta t \left\{ -\sum_2^N \delta(r\hat{B}_\theta)\,\tilde{E}_z - (r\hat{B}_\theta)_{3/2}\,\tilde{E}_{z,1} + (r\hat{B}_\theta)_{N+1/2}\,\tilde{E}_{z,N+1} \right\}, \tag{22}$$

$$W_z^* - W_z = \Delta t \left\{ -\sum_2^N \delta\hat{B}_z(r\tilde{E}_\theta) - \hat{B}_{z,N+1/2}(r\tilde{E}_\theta)_{N+1} \right\}. \tag{23}$$

The Poynting vector at the outer boundary and the ohmic heating associated with the outermost half-cell are simplified by defining $r_{N+3/2} = r_{N+1} = a$. We also define time-average current densities

$$\hat{J}_{z,j} = \frac{\delta(r\hat{B}_\theta)}{\bar{r}_j\,\Delta r_j} \quad (j = 2,\ldots, N+1), \qquad \hat{J}_{z,1} = \frac{2\hat{B}_{\theta,3/2}}{r_{3/2}}, \tag{24}$$

$$\hat{J}_{\theta,j} = -\frac{\delta\hat{B}_z}{\Delta r_j} \quad (j = 2,\ldots, N+1), \qquad \hat{J}_{\theta,1} = 0, \tag{25}$$

with $\Delta r_j = r_{j+1/2} - r_{j-1/2} = \frac{1}{2}(r_{j+1} - r_{j-1})$ from (7), and two separate sequences of area elements

$$\Delta' A_j = \bar{r}_j \, \Delta r_j \quad (j = 2,..., N+1), \qquad \Delta' A_1 = \tfrac{1}{2} r_{1/2}^2 , \tag{26}$$

$$\Delta'' A_j = r_j \, \Delta r_j \quad (j = 2,..., N+1), \qquad \Delta'' A_1 = \tfrac{1}{2} r_{3/2}^2 , \tag{27}$$

with

$$\sum_{j=1}^{N+1} \Delta' A_j = \sum_{j=1}^{N+1} \Delta'' A_j = \sum_{j=1}^{N} \Delta A_{j+1/2} = a^2/2. \tag{28}$$

Then (22) and (23) become respectively

$$W_\theta - W_\theta = \Delta t \left\{ - \sum_{1}^{N+1} (\Delta' A \hat{J}_z \tilde{E}_z)_j + (r\hat{B}_\theta)_{N+3/2} \, \tilde{E}_{z,N+1} \right\}, \tag{29}$$

$$W_z^* - W_z = \Delta t \left\{ - \sum_{1}^{N+1} (\Delta'' A \hat{J}_\theta \tilde{E}_\theta)_j - \hat{B}_{z,N+3/2} (r\tilde{E}_\theta)_{N+1} \right\}, \tag{30}$$

where the summation is over all cell boundaries (although in (30) the central point $j = 1$ does not contribute).

5. Ohmic Heating

Summation of Eq. (13) over all cells gives

$$W_T^* - W_T = \Delta t \left\{ -(rF)_{N+1} + \sum_{j=1}^{N} (J_\theta E_\theta + J_z E_z)_{j+1/2} \, \Delta A_{j+1/2} \right\} \tag{31}$$

so that exact conservation of energy is ensured if $\mathbf{E} = \tilde{\mathbf{E}}$ is defined by (17) with the same value of θ that is used in the diffusion equations ($\theta = 1$ in ATHENE 1), if $\mathbf{J} = \hat{\mathbf{J}} \equiv \frac{1}{2}(J^{n+1} + J^n)$, and if the summation in (31) precisely corresponds to those of (29) and (30). This can be achieved by allocating the ohmic heating associated with each cell boundary j in (29) and (30) in an appropriate way. For $2 \leqslant j \leqslant N$ we have found it best to assign $(\mathbf{J} \cdot \mathbf{E})_j$ to the cells on either side in proportion to the "half-masses" $\rho_{j-1/2}(r_j^2 - r_{j-1/2}^2)/2$ and $\rho_{j+1/2}(r_{j+1/2}^2 - r_j^2)/2$. All the heating associated with the central point $r = 0$ is assigned to cell $j = \frac{3}{2}$, and that associated with the outer boundary $r = a$ is either given to the outermost cell $j = N + \frac{1}{2}$ or, in practice, treated as a direct loss to the wall or liner since this makes the calculation run more stably.

Allocation in proportion to the masses leads to equal temperature increments and therefore to a smooth temperature profile. Allocation in proportion to the areas $\Delta A_{j\pm1/2}$ was also tried, but is not recommended since it may cause trouble when density gradients are present and in one instance led to an "explosion" of the central cell which by expanding could take almost all the heating associated with point $j = 2$ (instead of its "ration" of $\frac{1}{4}$) as well as that associated with point $j = 1$.

To calculate the ohmic heating it is necessary to know $\hat{J}$ and therefore $\hat{B}$, so that Eqs. (11) and (12) must be solved for $B^* = B^{n+1}$ before solving the temperature Eq. (13).

The prescription given in this Note ensures exact conservation of magnetic energy, both locally and globally, for any form of electric field $\tilde{E}$, e.g., for any value of θ in Eq. (17), and for any value of the timestep Δt. There are no nonphysical heating or cooling terms of the type that appear in [2, Eqs. (37), (47)]. Nevertheless there may be circumstances in which the local value of $\tilde{\mathbf{E}} \cdot \hat{\mathbf{J}}$ could conceivably become negative leading to a nonphysical transfer of energy from the plasma to the magnetic field, and the timestep Δt should in principle be monitored to prevent this. To simplify the discussion we assume the resistivity η (which is in general a tensor) to be a scalar quantity so that $\mathbf{E} = \eta \mathbf{J}$ and

$$\tilde{\mathbf{E}} \cdot \hat{\mathbf{J}} = \eta(\theta \mathbf{J}^* + (1 - \theta)\mathbf{J}) \cdot \tfrac{1}{2}(\mathbf{J}^* + \mathbf{J}). \tag{32}$$

For the Crank–Nicholson scheme $\theta = \frac{1}{2}$ so that (32) is positive definite. Other schemes could only give trouble if $\mathbf{J} \cdot \mathbf{J}^* < 0$, i.e., if the direction of the total current changed by more than 90° during one timestep. This should be prevented on accuracy grounds if $|\mathbf{J}|$ is large, while if $\mathbf{J}$ changes sign by passing through zero the term (32) is quadratically small. No significant restriction on Δt should therefore arise in practice.

6. Numerical Tests

Numerical tests have been carried out using the ATHENE 1 code to solve equations equivalent to (11)–(13) for the ohmic heating phase of a reversed-field pinch plasma. The initial conditions corresponded to a plasma of negligible thermal energy contained by a Bessel-function magnetic field distribution, and further details of the physical parameters are given in Ref. [7]. The diffusion equations are solved by the fully implicit method ($\theta = 1$) and during the development of the code three runs were performed in which the ohmic heating rate took the forms:

$$\begin{aligned} &\text{(A)} \quad \tilde{\mathbf{E}} \cdot \hat{\mathbf{J}} \qquad \text{(recommended in this Note)}, \\ &\text{(B)} \quad \tilde{\mathbf{E}} \cdot \mathbf{J} \qquad \text{(current at time } n\text{)}, \\ &\text{(C)} \quad \tilde{\mathbf{E}} \cdot \mathbf{J}^* \qquad \text{(current at time } n{+}{+}\text{)}, \end{aligned} \tag{33}$$

with $\tilde{\mathbf{E}} = \mathbf{E}^*$. Each run was carried forward 500 steps in double precision (64 bits) on an ICL 4/70 computer using a constant $\Delta t = 50\,\mu$sec, and at each step (consisting of two Stages I and II) the following were calculated: W the energy content at the beginning of the step, W_{I}^* the content after Stage I (diffusion), W_{II}^* the content after Stage II (relaxation to pressure equilibrium), and ΔW_{in} the net energy input at the wall resulting from the thermal flux and the Poynting vector. The boundary conditions at the wall maintained the temperature T constant, and the electric field was programmed to sustain the reversed-field configuration [7]. For each run the formula

used for the Poynting vector was compatible with the corresponding ohmic heating term (33).

Table I shows the relative errors defined as

$$\textit{Stage I:} \qquad \epsilon_{\mathrm{I}} = \frac{1}{W_F} \sum_{n=1}^{500} (W_{\mathrm{I}}^* - W - \Delta W_{\mathrm{in}}), \tag{34}$$

$$\textit{Stage II:} \qquad \epsilon_{\mathrm{II}} = \frac{1}{W_F} \sum_{n=1}^{500} (W_{\mathrm{II}}^* - W_{\mathrm{I}}^*), \tag{35}$$

TABLE I

Relative Energy Errors

	A	B	C
ϵ_{I}	-8.3×10^{-13}	0.0286	0.0269
ϵ_{II}	-8.0×10^{-4}	-9.2×10^{-4}	-8.1×10^{-4}
ϵ'_{I}	-4.6×10^{-12}	0.152	0.144
ϵ'_{II}	-4.4×10^{-3}	-4.9×10^{-3}	-4.8×10^{-3}

where W_F is the total energy at the final step $n = 500$. For convenience we have also normalized the errors to the total thermal energy $W_{T,F}$ at the final step and these are shown as

$$\epsilon'_{\mathrm{I,II}} = \epsilon_{\mathrm{I,II}} W_F / W_{T,F}\,. \tag{36}$$

It can be seen that a substantial error ϵ_{I} has occurred in runs B and C, and that this is considerably greater than the error ϵ_{II} of Stage II which is acceptably small (0.1 %). The error ϵ_{I} arising from the recommended prescription A is entirely negligible and results only from double-precision round-off errors. The difference between the three cases is illustrated in Figure 1 which shows the time variation of the axial temperature,

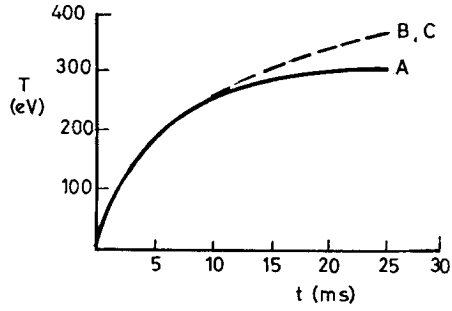

FIG. 1. Variation with time of axial temperature in an ohmically heated reversed field pinch. The ohmic heating term used in the three calculations is given by Eq. (33).

indicating that an incorrect choice of the ohmic heating term can seriously disturb the results of the calculation.

Finally, it should be mentioned that a straightforward and therefore perhaps "natural" choice for the ohmic heat developed in time Δt might be the fully explicit formula $\eta \mathbf{J}^2 \Delta t$, since this depends only on known quantities at time n. This was actually tried in an early version of the program and proved catastrophic, the reason being that the heat production is then proportional to $\eta \Delta t$ and bears little relation to the available magnetic energy $\mathbf{B}^2/2$. A warning may therefore be appropriate in case this formula has been used in other codes.

REFERENCES

1. R. D. RICHTMEYER AND K. W. MORTON, "Difference Methods for Initial Value Problems," Interscience, New York, 1967.
2. I. R. LINDEMUTH, *J. Computational Phys.* **18** (1975), 119; Erratum, **19** (1975), 338.
3. K. W. MORTON, *SIAM–AMS* **2** (1970), 1.
4. P. D. LAX, *Bull. Amer. Math. Soc.* **66** (1960), 32.
5. K. V. ROBERTS, J. P. CHRISTIANSEN, AND J. W. LONG, *Comput. Phys. Commun.* **10** (1975), 264.
6. J. P. CHRISTIANSEN, K. V. ROBERTS, AND J. W. LONG, ATHENE 1, A one-dimensional equilibrium-diffusion code, to appear.
7. J. P. CHRISTIANSEN AND K. V. ROBERTS, *Nucl. Fusion* **18** (1978), 181.

RECEIVED: December 9, 1976; REVISED: November 11, 1977

J. P. CHRISTIANSEN
K. V. ROBERTS

Culham Laboratory, Euratom/UKAEA Fusion Association, Abingdon, Oxon., OX14 3DB, U.K.