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Note

Consistent Finite Difference Operators That Satisfy $\nabla \cdot \nabla \times = 0$*

In this note we investigate problems associated with constructing finite difference operators in noncartesian geometry that satisfy $\nabla \cdot \nabla \times = 0$ as an identity. We concern ourselves with cylindrical geometry (r, θ, z) only, where the dependence on poloidal angle θ is represented as a Fourier series $e^{im\theta}$ and the axial dependence z as e^{inz}. (This is useful for resolving helical structures.) The latter is for convenience; we could just as well use a finite difference representation for the z coordinate. We show that a straightforward, formally second-order accurate differencing of operators of the form $(1/r)(\partial/\partial r)\, ru$ is always inconsistent in the first derivative of the function u when $r \sim O(\Delta r)$ for the often important $m = 1$ component. (This corresponds to lateral motion across the line $r = 0$.) If this derivative is then used on the RHS of a time dependent system of equations (as the current $\mathbf{j}$, for example, in the MHD fluid model) this system is inconsistent in that certain spatial terms are nonuniformly convergent as $r \to 0$. We show how this can be remedied and the desirable $\nabla \cdot \nabla \times = 0$ property identically retained. Although the result given is for cylindrical geometry, any interior boundary fitted coordinate system has at least one coordinate singularity where the inverse mapping to cartesian coordinates is not one to one. Thus the problem discussed here has wider applicability.

In cylindrical geometry the regularity conditions for a scalar and a vector represented in the θ, z coordinates by a Fourier series as $r \to 0$ is almost trivially derived by considering solutions to $\nabla^2 \phi = 0$. For scalar components, $\phi_m \sim f(r, z)\, e^{im\theta}$, the regular solutions are given by Bessel functions $J_m(r) \sim r^m g(r^2) \sim \phi_m$ as $r \to 0$, defining the r dependence of ϕ_m in this limit (note that $g(r^2) \sim \sum_{n=0}^{\infty} a_n r^{2n}$). To find the corresponding r dependence of arbitrary vectors $\mathbf{C}$, we simply note that these have the same powers of r as $\nabla \phi_m$. Thus for $\nabla \equiv \hat{r}(\partial/\partial r) + (\hat{\theta}/r)(\partial/\partial \theta) + \hat{z}(\partial/\partial z)$ we see that as $r \to 0$, $C_r(m=0) \sim r g(r^2)$, $C_{r,\theta}(m \geqslant 1) \sim r^{m-1} g_{r,\theta}(r^2)$, $C_z(m \geqslant 0) \sim r^m g_z(r^2)$. Thus, only the $m = 1$ components of C_r, C_θ are finite at $r = 0$. Also, from the requirement that $\nabla \cdot \mathbf{C}$ be finite as $r \to 0$ these components must agree in the constant term of their series expansion. Thus, the equations evolving them in time must preserve this property. So evolutionary equations for the $m = 1$ components of C_r and C_θ become linearly dependent as $r \to 0$ for all physically well-posed problems.

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As our prototype equation we consider Faraday's law

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \tag{1}$$

where $\mathbf{E}$ is given by an Ohm's law at least as complicated as $\mathbf{E} = -\mathbf{V} \times \mathbf{B} + \eta \mathbf{j}$; $\mathbf{V}$ is a time evolved velocity, η is the resistivity, and $\mathbf{j} = \nabla \times \mathbf{B}$ is the current. We consider a simplified equation for $\mathbf{V}$ given as

$$\frac{\partial \mathbf{V}}{\partial t} + V \cdot \nabla \mathbf{V} = \mathbf{j} \times \mathbf{B}. \tag{2}$$

Equation (1) preserves $\nabla \cdot \mathbf{B} = 0$ in time once given as an initial condition. For this to be preserved in difference form, the discretized version of $\nabla \cdot \nabla \times \mathbf{E}$ must be zero. The common way to do this is to use a staggered grid in radius r, where B_r, E_θ, and E_z are defined at the o points and B_θ, B_z, and E_r at the staggered x points as shown in Fig. 1. Differencing the expression for $(\partial/\partial t) \nabla \cdot \mathbf{B} = -\nabla \cdot \nabla \times E$ at the x points j (the only points where $\nabla \cdot \mathbf{B}$ is defined), using second-order accurate differences, yields for the parts of $(\partial/\partial t) \nabla \cdot \mathbf{B}$ the result,

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{1}{r}\frac{\partial}{\partial r} rB_r\right)_j &= \frac{\partial}{\partial t}\frac{1}{r_j \Delta r}\{(rB_r)_{j+1/2} - (rB_r)_{j-1/2}\} \\ &= \frac{1}{r_j \Delta r}\{im(E_{z_{j+1/2}} - E_{z_{j-1/2}}) - in[(rE_\theta)_{j+1/2} - (rE_\theta)_{j-1/2}]\}, \end{aligned} \tag{3a}$$

$$\frac{\partial}{\partial t}\left(\frac{imB_\theta}{r}\right)_j = -mn\left(\frac{E_r}{r}\right)_j - \frac{im}{r_j \Delta r}(E_{z_{j+1/2}} - E_{z_{j-1/2}}), \tag{3b}$$

$$\frac{\partial}{\partial t}(inB_z)_j = \frac{in}{r_j \Delta r}\{(rE_\theta)_{j+1/2} - (rE_\theta)_{j-1/2}\} + nm\left(\frac{E_r}{r}\right)_j. \tag{3c}$$

If we sum Eqs. (3a), (3b), (3c) we see that zero is identically obtained on the RHS so that $\nabla \cdot \mathbf{B} = 0$ is satisfied numerically to round off error. We next examine the accuracy of this type of spatial differencing.

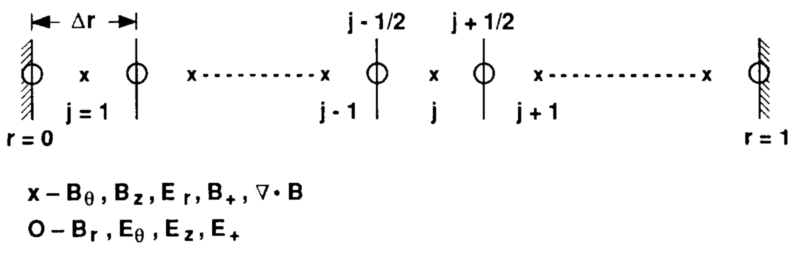

FIG. 1. Staggered radial grid showing placement of variables.

Consider $\nabla \cdot \mathbf{B} = 0$ differenced as in Eq. (3), where we set $m = 1$ and to be specific choose the phase of $\mathbf{B}$ as

$$\begin{aligned} B_r &= b_r \sin(\theta - nz), \\ B_\theta &= b_\theta \cos(\theta - nz), \\ B_z &= b_z \cos(\theta - nz). \end{aligned} \tag{4}$$

Then if we solve this discretized expression for nb_z we have

$$(nb_z)_j = \left(\frac{b_\theta}{r}\right)_j - \frac{1}{r_j \Delta r} \{(rb_r)_{j+1/2} - (rb_r)_{j-1/2}\}. \tag{5}$$

For the $m = 1$ components of b_r and b_θ we choose the test functions $b_r = b_\theta = b_0 + b_2 r^2$. If we use these expressions to evaluate the RHS of Eq. (5) at the point $j = 1$, $r = \Delta r/2$ (cf., Fig. 1) we obtain the result $(nb_z)_{j=1} = -\frac{3}{2} b_2 \Delta r = -3b_2 r_{j=1}$. The analytically calculated answer is $nb_z = -2b_2 r_{j=1} = -(b_2 \Delta r)$. The answer given at $j = 1$, $r = \Delta r/2$ by Eq. (5) is thus off by 50%. If we examine how the relative error $e(r)$, defined as the absolute value of nb_z as given by Eq. (5) minus the analytically obtained result divided by the latter for the given test functions, decreases as r increases, we find that it decays as

$$e(r) = 0.5 \left(\frac{(\Delta r)^2}{4r^2}\right) \tag{6}$$

for $r \geqslant \Delta r/2$, where r has unit domain. Thus for 50 grid cells and a typical truncation error of 5×10^{-3}, $r > 0.1$ to have $e(r)$ less than truncation error. The truncation error and $e(r)$ from Eq. (6) both decay as $(\Delta r)^2$ for centered differencing so that this situation does not change with increasing the number of grid points, although the error does shrink in closer to $r = 0$.

The problem we have found is that the error in B_z/r or the differenced from of $\partial B_z/\partial r$ as calculated by Eq. (5) for the $m = 1$ component is $O(1)$ when $r \sim O(\Delta r)$. This appears as an error $O(1)$ in the $m = 1$ components of both j_r and j_θ (j_z does converge pointwise). For example, B_z/r is in error as given by Eq. (6). $\partial B_z/\partial r$, defined at the o points, is off by $\frac{1}{6}$ at $r = \Delta r$ the first left-hand grid point at which it is defined. (It obeys a slightly different error formula than Eq. (6).) This error enters the RHS of Eq. (2) in the Lorentz force term and makes this type of differencing of Eqs. (1) and (2) inconsistent in that the RHS of Eq. (2) has a finite error near the axis.

The word inconsistent as used here applies to terms involving spatial derivatives that are nonuniformly convergent as $r \to 0$. Thus one or more time derivatives, $\partial \mathbf{V}/\partial t$ for example, are nonuniformly convergent in space. Numerically this will appear as a persistent glitch in $\mathbf{V}$ and $\mathbf{j}$ as $r \to 0$. Even if $\mathbf{B}$ converges uniformly $\mathbf{V}$ will not even for the steady state case, since if $\partial V/\partial t = 0$ in Eq. (2), $V \cdot \nabla \mathbf{V}$ cannot be pointwise convergent unless $\mathbf{j} \times \mathbf{B}$ is also. We thus emphasize the problem of consistency here as opposed to the stability problems that usually dominate the construction of finite difference schemes.

What we have shown is that centered differencing of terms of the form $(1/r)(\partial/\partial r)\, r(\ )$ leads to a fundamental inconsistency in the first derivative of the function when $r \sim O(\Delta r)$; that is, the derivative of the function converges pointwise but nonuniformly as $\Delta r \to 0$. This has been shown easily by use of a staggered grid so that the differenced form of $\nabla \cdot \mathbf{B} = 0$ is an identity. Therefore, in spite of the complicated form that $\nabla \times \mathbf{E}$ in Eq. (1) may have when the Ohm's law is written out in full, the differenced form of this equation (cf., Eq. (3)) preserves the error inherent in Eq. (5) for the $m = 1$ component of the solution since it is an invariant. Note that all $m \neq 1$ components of the solution do not have this difficulty; differencing $(1/r)(\partial/\partial r)\, r(\ )$ as in Eq. (3) gives a consistent algorithm for all of them.

A difference algorithm consistent with the original system, Eqs. (1) and (2), for the $m = 1$ component can be constructed by simply expanding terms of the form $(1/r)(\partial/\partial r)\, r(\ )$ before discretization. Then $\nabla \cdot \mathbf{B} = 0$ becomes

$$\frac{\partial B_r}{\partial r} + \frac{B_r + imB_\theta}{r} + inB_z = 0. \tag{7}$$

If we repeat the previous exercise for Eq. (7) using centered differences, then given the same test data as before for B_r and B_θ, we obtain the correct answer for B_z on an unstaggered grid for the $m = 1$ component. But for the staggered grid given in Fig. 1 we have the same error as before owing to the fact that we must define values of B_r at the x points by second-order accurate averaging. That is, we still lose one order of accuracy as $\Delta r/r \sim O(1)$ and this appears as an inconsistent j_r, j_θ current. Thus, if we are satisfied with $\nabla \cdot \nabla \times \neq 0$ identically then we may use centered, second-order finite differences and an unstaggered grid with curvature terms expanded as in Eq. (7). Alternatively, we may use higher order finite difference or finite element methods so that we retain at least second-order accuracy in the principal variables when $\Delta r/r \sim O(1)$. This may introduce additional complications, particularly since the equations for the r and θ components of $m = 1$ vectors must become equal as $r \to 0$. Also, the errors associated with $\nabla \cdot \nabla \times \neq 0$ may be significant [1]. These can be kept small by means of "divergence cleansing" [1–3].

Since the consistency difficulties arise only for $m = 1$ vector components, it would be desirable to fix the consistency problems with the staggered grid scheme and keep $\nabla \cdot \nabla \times = 0$ as an identity. We now show how to accomplish this.

We define the new dependent variables

$$B_+ = B_r + imB_\theta, \tag{8a}$$

$$E_+ = E_r + imE_\theta, \tag{8b}$$

and eliminate B_θ, E_θ in favor of B_+, E_+ everywhere in our system of equations (cf., Eq. (1)). We define B_+ and E_+ on the same grid points as B_θ and E_θ, respectively. Defining $(\nabla\times E)_+ \equiv (\nabla\times E)_r + im(\nabla\times E)_\theta$ we have

$$(\nabla\times E)_r = -\frac{n}{m}E_+ + \frac{n}{m}E_r + \frac{imE_z}{r}, \tag{9a}$$

$$(\nabla\times E)_+ = \left(\frac{n}{m} - nm\right)E_r - \frac{n}{m}E_+ - imr\frac{\partial}{\partial r}\left(\frac{E_z}{r}\right), \tag{9b}$$

$$(\nabla\times E)_z = -\frac{i}{m}\frac{\partial E_+}{\partial r} + \frac{i}{m}\frac{\partial E_r}{\partial r} - \frac{iE_+}{mr} + \frac{iE_r}{r}\left(\frac{1}{m} - m\right). \tag{9c}$$

Note that in Eq. (9c) we have split the term $(1/r)(\partial/\partial r)\,rE_\theta$ into two terms; also, in Eq. (9b) we have combined

$$-im\left(\frac{\partial E_z}{\partial r} - \frac{E_z}{r}\right) = -imr\frac{\partial}{\partial r}\left(\frac{E_z}{r}\right). \tag{10}$$

(Note that finite differencing of the RHS of Eq. (10) poses no problems as $r\to 0$. Since $E_z(m=1)\sim r$ is defined on the o points we just define E_z/r as $r\to 0$ as $E_z(r=\Delta r)/\Delta r$. For $m=1$, Eqs. (9) greatly simplify. Thus we recommend using the transformation given by Eqs. (8) only for the $m=1$ components. With Eqs. (9) and the form for the divergence of a vector as given by Eq. (7) we show that the $m=1$ component of $\nabla\cdot\nabla\times\mathbf{E}\equiv 0$ in difference form. Thus, for variables staggered as shown in Fig. 1 we have at the x point

$$\begin{aligned} -\frac{\partial}{\partial t}\frac{\partial B_r}{\partial r}\bigg|_j &= \frac{\partial}{\partial r}(\nabla\times E)_r\bigg|_j \\ &= \frac{n}{\Delta r}(E_{r_{j+1/2}} - E_{r_{j-1/2}}) + i\frac{\partial}{\partial r}\left(\frac{E_z}{r}\right)\bigg|_j - n\frac{\partial E_+}{\partial r}\bigg|_j, \end{aligned} \tag{11a}$$

$$\begin{aligned} -\frac{\partial}{\partial t}\frac{B_+}{r}\bigg|_j &= \frac{(\nabla\times E)_+}{r}\bigg|_j \\ &= -n\frac{E_{+j}}{r_j} - i\frac{\partial}{\partial r}\left(\frac{E_z}{r}\right)\bigg|_j \end{aligned} \tag{11b}$$

$$\begin{aligned} -\frac{\partial}{\partial t}inB_z\bigg|_j &= in(\nabla\times E)_z\bigg|_j \\ &= n\frac{\partial E_+}{\partial r}\bigg|_j + n\frac{E_{+j}}{r_j} - \frac{n}{\Delta r}(E_{r_{j+1/2}} - E_{r_{j-1/2}}). \end{aligned} \tag{11c}$$

So from the sum of the RHSs of Eqs. (11a), (11b), (11c) we see that zero is identically obtained. Of course, the terms $(\partial/\partial r)(E_z/r)$ and $(\partial E_+/\partial r)$ at the x points j must be defined everywhere consistently. For the given test data $(B_+=0,$

$B_r = b_0 + b_2 r^2$) this scheme is trivially seen to give the correct values of nb_z and is thus consistent. Thus the difference form given by Eqs. (11) is consistent since it is just Eq. (7) center-differenced. This is unlike Eqs. (3) which as shown from Eq. (5) are inconsistent in the first spatial derivative. By using, for every vector $\mathbf{C}$ in Eq. (1), the transformation $C_+ = C_r + iC_\theta$ in place of C_θ for the $m=1$ component we remove the linear dependence of the evolution equations for C_r and C_θ; the value of $C_+(r=0)$ is, of course, zero. (This can also be done for the velocity equation to remove the linear dependence as $r \to 0$ of V_r and V_θ; for example, $V_\pm = V_r \pm iV_\theta$ as well as V_+ can be defined. Whether or not this is desirable may depend the precise form of Eq. (2). The point is to avoid nonuniformity convergent spatial terms.) Thus we construct for the $m=1$ mode in place of the $\partial B_\theta/\partial t$ component of Eq. (1) an equation for $\partial B_+/\partial t$ using Eqs. (9); this equation is utilized everywhere in radius, and not just near $r=0$. This causes no peculiarities for hyperbolic systems. Physically what happens in the vicinity of $r=0$ for any hyperbolic system of equations in cylindrical coordinates is that the characteristics have the form $r^2 t = \text{const}$ or $r^2/t = \text{const}$ in the $t-r$ plane. Thus, the point $r=0$ is always a characteristic. This is how the equations distinguish physically meaningful $r \geqslant 0$ from unphysical $r < 0$.

For parabolic operators such as ∇^2 the algebraic terms resulting from the Fourier series expansion in θ combine to robustly guarantee that $B_+ \to 0$ as $r \to 0$ giving

$$\frac{\partial B_+}{\partial t} \approx -a(r) B_+, \tag{12}$$

where $a(r) \to +\infty$ as $r \to 0$. Therefore, such terms must always be implicitly time-differenced. This is easy to do. (Parabolic operators are usually implicitly differenced anyway.)

In conclusion, we have shown that the consistency of finite difference schemes in noncartesian coordinate systems must be carefully considered when the coordinate variable becomes the order of the grid spacing. It was demonstrated for the MHD equations in cylindrical geometry with a Fourier series expansion in poloidal angle that the $m=1$ vector component of the current is represented inconsistently by formally second-order accurate finite differencing of operators of the form $(1/r)(\partial/\partial r)\, r(\;)$. This was easy to show because the equations preserved an inconsistent discrete form of $\nabla \cdot \nabla \times \mathbf{E} = 0$. This difficulty could be overcome by a transformation $C_+ = C_r + iC_\theta$ (for the $m=1$ component of every vector $\mathbf{C}$) in the induction equation that everywhere removes C_θ in favor of C_+, and by appropriately rewriting certain terms before spatial differencing. This eliminates the linear dependence of C_r and C_θ as $r \to 0$ and, in addition, preserves $\nabla \cdot \nabla \times \mathbf{C} = 0$ identically on a staggered grid. The expression for $\mathbf{C}$ (the Ohm's law) can be arbitrarily complicated. The $m \neq 1$ components were consistent in their original form and may be radially differenced in the usual manner.

Although we have only considered in detail a cylindrical coordinate system, all interior noncartesian coordinate systems have a coordinate center with problems similar to those considered in this note. Thus, similar difficulties may arise. We expect the type of solution proposed here (a transformation of certain dependent variables and some algebraic rearrangement of terms) to carry over in an appropriately modified form.

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E. J. Caramana
Los Alamos National Laboratory
Los Alamos, New Mexico 87545