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ON THE QUESTION OF CONSISTENT BOUNDARY CONDITIONS WHEN
SIMULATING REVERSED FIELD PINCH DYNAMICS

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The issue of proper boundary conditions when performing magnetohydrodynamic simulations of the reversed field pinch is examined. Of particular concern is the choice of constant current, which when combined with other commonly used boundary conditions, may, under careless implementation, lead to an inconsistency. It is shown that this may cause erroneous results. Cases both with and without Hall terms are presented.

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I. INTRODUCTION

The proper choice of boundary conditions is one of the most difficult problems facing the computational physicist. The case of magnetohydrodynamic (MHD) simulations of the reversed field pinch (RFP) is no exception. In a recent study in which this author took part¹, five of the leading three-dimensional MHD codes were used to simulate the identical problem in RFP dynamics, and it was affirmed that compressibility is an important feature of RFP physics. Shortly thereafter, this author participated in a two code comparison involving a very similar test problem, for the purpose of ascertaining the effects of Hall terms². It was at this time that the realization was made that inconsistent boundary conditions were being used in both studies. This led to a further investigation, whose aim was to determine how to properly implement boundary conditions for RFP simulations.

The results of that study are reported on here. Section II contains the basic equations and numerics. Section III discusses the boundary conditions. Results of simulations are presented in Section IV. Section V contains further discussion.

II. BASIC EQUATIONS AND NUMERICS

The basic equations are those of single fluid, compressible, resistive MHD in the low beta limit. In nondimensional form they are as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad (1)$$

$$\frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \nabla \underline{v} = \frac{1}{\rho} \underline{J} \times \underline{B} \quad (2)$$

$$\frac{\partial \underline{B}}{\partial t} = - \nabla \times \underline{E} \quad (3)$$

with the auxiliary conditions

$$\underline{J} = \nabla \times \underline{B} \quad (4)$$

$$\underline{E} = - \underline{v} \times \underline{B} + \frac{\eta}{S} \underline{J} + \underline{E}_{\text{Hall}} \quad (5)$$

$$\underline{E}_{\text{Hall}} = \frac{\nu}{\rho} \underline{J} \times \underline{B}. \quad (6)$$

In Eqs. (1-5), ρ is the mass density, $\underline{v}$ is the velocity, $\underline{B}$ is the magnetic field, $\underline{E}$ is the electric field, $\underline{J}$ is the current density, S is the Lundquist number τ_R/τ_A , the ratio of resistive diffusion time to Alfvén time, η is the resistivity (taken to be 1 everywhere) and ν is the Hall parameter $(\omega_{ci}\tau_A)^{-1}$. Time is measured in Alfvén units.

The above system is integrated numerically using the three-dimensional MHD code TEMCO^{3,4}. A cylindrical coordinate system is used, and a Fourier expansion is performed in the angular (poloidal) variable,

$$w(r, \phi, z) = w_0(r, z) + \sum_{m>0} [w_{mc}(r, z) \cos m\phi + w_{ms}(r, z) \sin m\phi]. \quad (7)$$

Although it is not done in the code other than for mode filtering or diagnostic purposes, it is convenient to further expand in the toroidal (z) direction:

$$w_{\pm}(r, z) = w_{\pm}^0(r) + \sum_{n>0} [w_{\pm}^{nc}(r) \cos nz + w_{\pm}^{ns}(r) \sin nz]. \quad (8)$$

Spatial derivatives are approximated with central differences. Operator splitting is invoked; the resistive terms are advanced using forward time differencing and the main system is advanced using a leapfrog method. The term in the induction equation $-\nabla \times (\nabla \times \underline{B})$ is differenced in the form $\nabla^2 \underline{B}$, leading to an ensuing truncation error in $\nabla \cdot \underline{B}$; hence, an option to eliminate the non-solenoidal part of $\underline{B}$ ("divergence cleaning") is included.

III. BOUNDARY CONDITIONS

Periodic boundary conditions are specified in the z (toroidal) direction, and at $r = 0$ regularity is assumed. The remainder of this section deals with the conditions at the outer wall ($r = a$). A possible choice of boundary conditions is the following:

$$v_r = 0 \quad (9)$$

$$\frac{\partial}{\partial r} (v_T) = 0 \quad (10)$$

$$B_r = 0 \quad (11)$$

$$E_T = 0, \quad (12)$$

where the subscript T refers to the tangential component. Eq. (10), which corresponds to inviscid flow, is used instead of an evolutionary equation for v_T because it is easier to implement and has been found to give essentially equivalent results. Eqs. (11) and (12) state that the outer wall is a perfectly conducting boundary and a flux surface. In

light of Eqs. (9) and (11), Eq. (12) may be replaced by the condition

$$(\underline{E} + \underline{v} \times \underline{B})_T = 0, \quad (13)$$

which in the absence of Hall terms is equivalent to

$$\underline{J}_T = 0. \quad (14)$$

When Hall terms are included, Eq. (13) may be written in the form

$$\underline{J}_T + \frac{\nu S}{\eta \rho} (\underline{J} \times \underline{B})_T = 0, \quad (15)$$

which is a rather complicated system of nonlinear equations coupling the Fourier components of $\underline{B}$ and its derivatives. An expedient, though physically unmotivated, solution technique is to assume that the Hall parameter ν (which goes as $\rho^{-1/2}$) approaches 0 at the wall, in which case Eq. (15) reduces to Eq. (14). The calculations presented here assume a profile of ν of the form

$$\nu = \nu_0 [1 - (r/a)^8]. \quad (16)$$

In modeling a reversed field pinch it is often desirable to assume a constant toroidal current. This is equivalent to stipulating that

$$B_{\phi 0}^0(a) = \text{constant} \quad (17)$$

(see Eqs. (7-8) for notation). This condition, when combined with Eqs.

(9-11, 14) (the latter for $(m,n) \neq (0,0)$), generally leads to an inconsistency. This can be seen by looking at a cylindrically symmetric equilibrium perturbed by a single helical state. Letting superscript 0 denote the $(m,n) = (0,0)$ state and 1 denote the helical perturbation, the radial component of Eq. (2) (when linearized) may be written

$$\frac{\partial v_r^0}{\partial t} = \frac{1}{\rho_0} (J_\phi^0 B_z^0 - J_z^0 B_\phi^0). \quad (18)$$

As r approaches a , J_ϕ^0 approaches 0 but B_ϕ^0 and J_z^0 do not in general approach 0; hence v_r^0 does not approach 0, in violation of Eq. (9). This is a manifestation of the fact that Eq. (18) is an ordinary differential equation for v_r^0 . This discontinuity can be removed by changing the boundary condition on v_r^0 ; however that can lead to other problems (see Sect. V). The fact that v_r^0 is discontinuous at $r=a$ leads to difficulties when solving the induction equation. The perturbed part of Ohm's law (Eq. (5)) states

$$E_\phi^1 = v_r^0 B_z^1 + v_r^1 B_z^0 - v_z^0 B_r^1 - v_z^1 B_r^0 + \frac{\eta}{S} J_\phi^1 + \nu \left[\frac{\mathbf{J} \times \mathbf{B}}{\rho} \right]_\phi^1 \quad (19)$$

$$E_z^1 = v_\phi^0 B_r^1 + v_\phi^1 B_r^0 - v_r^0 B_\phi^1 - v_r^1 B_\phi^0 + \frac{\eta}{S} J_z^1 + \nu \left[\frac{\mathbf{J} \times \mathbf{B}}{\rho} \right]_z^1. \quad (20)$$

As r approaches a , given that v_r^0 has a nonzero limit, all terms approach 0 except $v_r^0 B_z^1$ and $v_r^1 B_z^0$, which means that E_ϕ^1 and E_z^1 do not go to 0; hence Eq. (12) is being violated.

The fact that Eq. (11) is being enforced means that the radial component of Faraday's law does not hold at the boundary. This manifests itself in a nonzero divergence of $\underline{B}$. As noted in Section II, the actual equation solved by the code is

$$\frac{\partial \underline{B}}{\partial t} = - \nabla \times (- \underline{v} \times \underline{B} + \underline{E}_{Hall}) + \eta \nabla^2 \underline{B}, \quad (21)$$

which is equivalent to Eq. (3) if and only if $\nabla \cdot \underline{B}$ is 0. Since Eq. (21) is not in conservation form, $\nabla \cdot \underline{B}$ is not apriori preserved. In fact $\underline{B}$ is guaranteed to remain divergence free if and only if its boundary conditions are consistent with Faraday's law. This can be seen by taking the divergence of Eq. (21). Letting u stand for $\nabla \cdot \underline{B}$, one obtains

$$\frac{\partial u}{\partial t} = \eta \nabla \cdot \nabla^2 \underline{B} = \eta \nabla^2 u, \quad (22)$$

subject to the initial condition $u = 0$. Satisfaction of the radial component of Eq. (3) is equivalent to $\frac{\partial u}{\partial r} = 0$, which is the condition that u be 0 everywhere. It is apparent that the above set of boundary conditions leads to a contradiction.

IV. RESULTS OF USING INCONSISTENT BOUNDARY CONDITIONS.

In a recent study, TEMCO and four other leading three-dimensional MHD codes were used to simulate the identical problem in RFP dynamics¹. The comparison case consisted of a cylindrically symmetric equilibrium having a safety factor

$$q(r) = 0.4 (1.0 - 1.8748r^2 + 0.83232r^4) \quad (23)$$

along with initial $(m,n) = (1,-1)$ and $(1,-2)$ perturbations computed from a linear stability calculation and applied at the 1% level. Combined constant current / conducting wall boundary conditions (i.e. Eqs. (9-11) and (17), and Eq. (15) for $(m,n) \neq (0,0)$) were invoked. The Lundquist number S was chosen to be 1000 and Hall terms were excluded. The principal result of the study was that the three compressible codes predicted field reversal maintenance while the two incompressible codes did not, leading to the conclusion that compressibility is a not-to-be-ignored feature of RFP physics.

In that study, the compressible code TEMCO was run utilizing the option of divergence cleaning. It was decided subsequently to rerun the same case, but without divergence cleaning. A comparison of results is shown in Fig. 1, in which the field reversal parameter F (defined as the average B_z at the wall divided by the volume-averaged B_z) is plotted versus time. It can be seen that although disparate results are obtained, either case predicts a reversed field (except in the initial transient) for at least 100 Alfvén times. It was at first thought that the above disparity was due to poor mesh resolution. Subsequent mesh refinement, however, did not cause a substantial change in the results. This seemed to be in contradiction to the consistency and convergence properties of the difference algorithm, since, according to Eq. (3), $\nabla \cdot \underline{B}$ should be preserved in the analytic limit.

The paradox can now be understood, in light of the discussion of Section III. The constant current boundary condition was causing E_T^1 at the

wall to be nonzero, resulting in the violation of the radial component of Faraday's law. Thus, $\nabla \cdot \underline{B}$ could not be preserved analytically.

The improper implementation of the "constant current / conducting wall" boundary conditions becomes more apparent when Hall terms are included. This is illustrated using the above case but including only the (1,-2) mode initially. The constant part of the Hall parameter, ν_0 (see Eq. (16)), is taken to be 0.1. Figures 2 and 3 show contours of the helical flux function ψ at various times both with and without divergence cleaning, respectively. The function ψ is defined according to

$$B_r = \frac{1}{rh} \frac{\partial \psi}{\partial \mu} \quad (24)$$

and

$$B_z = -\frac{1}{r} \left(\frac{\partial \psi}{\partial r} + h B_\phi \right), \quad (25)$$

where h is the helicity m/nk and $\mu = \phi + h^{-1}z$, k being the inverse aspect ratio. It can be seen that without divergence cleaning the configuration rotates poloidally about 135° within 100 Alfvén times (Fig. 3), but that there is at best a 10° rotation in 310 Alfvén times when $\nabla \cdot \underline{B}$ is constrained to zero. The situation hardly changes when the resolution is increased. It was in fact this discrepancy which led to the discovery of the inconsistency in the boundary conditions.

Figure 4 shows a plot of the (0,0) component of v_r versus r (without divergence cleaning) at $t = 62$. There is a clear discontinuity in v_r^0 at the wall, which is brought on by the fact that v_r^0 does not want to approach 0, in accordance with the discussion of Sect. III. To underscore the importance of the role of v_r^0 , when the case is rerun setting v_r^0 identically equal to 0 (hence E_T^1 approaching 0 at the wall) at the end of each timestep, divergence cleaning has no discernible effect on the results.

It is of further interest to note that for this problem, the constant current boundary condition is vital to sustainment of the dynamo. When conducting wall boundary conditions (Eq. (12)) are used for all modes, field reversal is lost almost immediately.

V. DISCUSSION

It has been demonstrated that the use of Eqs. (9-11) and (17) and Eq. (15) for $(m,n) \neq (0,0)$ can lead to erroneous results. This is especially apparent when Hall terms are included in Ohm's law.

The problem originates from the fact that the radial component of velocity does not naturally approach zero at the wall. This leads to a violation of the radial component of Faraday's law because of an incorrect implementation of Eq. (12) and ultimately results in a nonsolenoidal magnetic field. The fact that Eq. (9) is not meant to hold means that Eq. (12) can not be replaced by Eq. (13). Hence Eq. (15) must be replaced by

$$-(\underline{v} \times \underline{B})_T + \frac{\eta}{S} j_T + \frac{\nu}{\rho} (\underline{j} \times \underline{B})_T = 0, \quad (26)$$

which when combined with Eq. (8) yields the component equations

$$v_r B_z - \frac{\eta}{S} \frac{\partial}{\partial r} (B_z) - \frac{\nu}{\rho} B_z \left[\frac{1}{r} \frac{\partial}{\partial \phi} (B_z) - \frac{\partial}{\partial z} (B_\phi) \right] = 0 \quad (27)$$

$$- v_r B_\phi + \frac{\eta}{S} \frac{\partial}{\partial r} (r B_\phi) + \frac{\nu}{\rho} B_\phi \left[\frac{1}{r} \frac{\partial}{\partial \phi} (B_z) - \frac{\partial}{\partial z} (B_\phi) \right] = 0 \quad (28)$$

Eqs. (27-28) are seen to nonlinearly couple the Fourier components of B_ϕ and B_z . When the Hall parameter vanishes at the wall, Eqs. (27-28) reduce to a coupled linear system. These conditions are not without potential difficulties, however, as small values of resistivity might lead to large wall-gradients of B_ϕ and B_z . Furthermore, the specification of a nonzero wall-value of v_r must be justified in physical terms. Eq. (26) has yet to be implemented in TEMCO.

When a viscosity is included the velocity boundary conditions may be more freely specified. One could choose to invoke Eq. (9) at the risk of having to resolve a fine boundary layer at the wall.

A definitive answer as to the validity of the five-code comparison can be obtained only through proper choice of boundary conditions. Some of the other coauthors of the comparison have been working in this direction; indications are that the principal conclusion of Ref. 1 (namely that compressibility can be important for field reversal maintenance) will stand⁵. This, together with the fact that TEMCO predicts field reversal maintenance both with and without divergence cleaning, is reason to be optimistic.

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FIGURE CAPTIONS

Fig. 1 Field reversal parameter F versus time both (a) with and (b) without divergence cleaning; time is measured in Alfvén units. Hall terms are not included.

Fig. 2 Helical flux contours for Hall term case with divergence cleaning at (a) $t = 65$ and (b) $t = 310$.

Fig. 3 Helical flux contours for Hall term case without divergence cleaning at (a) $t = 0$, (b) $t = 35$, (c) $t = 65$ and (d) $t = 100$.

Fig. 4 Plot of v_r^0 versus r for Hall term case without divergence cleaning at $t = 62$.

Figure 1a

Figure 1b

Figure 2a

Figure 2b

Figure 3a

Figure 3b

Figure 3c

Figure 3d