The alternating-direction implicit numerical solution of the time-dependent, three-dimensional, single fluid, resistive magnetohydrodynamic equations

Charles H. Finan !!!
(Ph.D. Thesis)

December 1980

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The Alternating Direction Implicit Numerical Solution of the
Time-Dependent, Three-Dimensional, Resistive, Single Fluid
Magnetohydrodynamic Equations

By

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DAVIS

Approved:

Three handwritten signatures are written over a horizontal dotted line. The top signature appears to be 'John Killen', the middle one 'Stanley', and the bottom one 'W. G. DeLoach'.

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THE ALTERNATING-DIRECTION IMPLICIT NUMERICAL SOLUTION
OF THE TIME-DEPENDENT, THREE-DIMENSIONAL, SINGLE FLUID,
RESISTIVE MAGNETOHYDRODYNAMIC EQUATIONS

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ABSTRACT

Resistive magnetohydrodynamics (MHD) is described by a set of eight coupled, nonlinear, three-dimensional, time-dependent, partial differential equations. A computer code, IMP (Implicit MHD Program), has been developed to solve these equations numerically by the method of finite differences on an Eulerian mesh. In this model, the equations are expressed in orthogonal curvilinear coordinates, making the code applicable to a variety of coordinate systems. The Douglas-Gunn algorithm for Alternating-Direction Implicit (ADI) temporal advancement is used to avoid the limitations in timestep size imposed by explicit methods. The equations are solved simultaneously to avoid synchronization errors. While the continuity and magnetic flux equations are expressed as conservation laws, the momentum and energy equations are nonconservative. This is to: (1) provide enhanced numerical stability by eliminating errors introduced by the nonvanishing of $\nabla \cdot \mathbf{B}$ on the finite difference mesh; and, (2) allow the simulation of low β

plasmas. To allow for general simulations, the boundary conditions may be Dirichlet, Neumann, or periodic. A conservation boundary condition based on the physical properties of the wall is presented. The resulting finite difference equations are a coupled system of nonlinear algebraic equations which are solved by the Newton-Raphson iteration technique.

We apply our model to a number of problems of importance in magnetic fusion research. Ideal and resistive internal kink instabilities are simulated in a Cartesian geometry. Growth rates and nonlinear saturation amplitudes are found to be in agreement with previous analytic and numerical predictions. We also simulate these instabilities in a square cross section torus. This demonstrates the versatility of the orthogonal curvilinear coordinate representation employed by our model. In both geometries, long time simulations in resistive plasmas display final states with finite flow fields. Finally, we perform a simulation of the spontaneous field reversal in a high current pinch. In this case, relaxation to a field reversed geometry is demonstrated both for a plasma that initially has a high pinch ratio ($\mu_0/B_z > 1.6$), and for one that initially has a low pinch ratio and is subjected to an external electric field to increase the internal current. In these final Reversed Field Pinch (RFP) cases, we find that the resistive internal kink is the mechanism which causes the field reversal.

To my sons

Chris

and

Mike

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CHAPTER I

· INTRODUCTION

I.1 Motivation

The world's need for reliable, long term sources of energy has become more obvious as the supply of fossil fuels has decreased. In order to provide these energy sources, research has begun in a number of areas. Old energy sources are being re-examined in the light of modern technology, including such diverse areas as the use of wind power for electrical generation and coupling MHD (magnetohydrodynamic) generators to coal-fired electrical generators to raise their efficiency. In addition, new energy sources such as solar, geothermal and controlled nuclear fusion are being explored.

Of these new sources, controlled fusion energy has a number of attractive features. First, the fuel for fusion plants, deuterium, is found in ordinary water (.0153% of the hydrogen in sea water is deuterium¹), making it a viable source of energy which could supply the world's energy needs for millions of years. Secondly, fuel costs would be a negligible part of the total plant construction and operating budgets. Finally, compared to the present day nuclear fission power plants, the fusion power plant poses few significant environmental or safety hazards.

In order to achieve a working thermonuclear fusion reactor, the deuterium fuel must be ionized and contained by magnetic fields at a high kinetic temperature (hotter than the sun's core) for a sufficient amount of time to allow the thermonuclear reactions to produce more power than was expended in the confinement and heating process. The greatest obstacle to

the production of these confined, high temperature plasmas (an ionized gas) is the onset of large-scale instabilities. These instabilities are described by the magnetohydrodynamic (MHD) equations which model the plasma as a conducting fluid immersed in a magnetic field.

The first approach to understanding these large scale instabilities was accomplished by studying the effect of small perturbations in the linearized MHD equations. If the small perturbations grew in time in a given magnetic field configuration, then that magnetic field configuration was declared unstable. While only the most idealized situations could be treated analytically, the gross MHD instabilities became better understood and, consequently, more avoidable.

More recently, researchers have come to realize that some instabilities can be tolerated, and in fact can be beneficial, provided they do not disrupt the plasma before a sufficient amount of power has been produced. Consequently, there is great interest in the nonlinear development of MHD instabilities and the final state of plasmas influenced by these instabilities. The analytical solution of the MHD equations (a system of 8 coupled, nonlinear partial differential equations) is, in general, impossible. Thus, numerical calculations are required for the investigations.

The power of modern computers has barely kept pace with requirements of the fusion community. In the late 1950's and early 1960's, computations were limited to one-dimensional models. In the middle and late 1960's and early 1970's, two-dimensional effects were being studied. Two-dimensional

MHD codes, both linear and nonlinear, are now commonplace at all major fusion research facilities. Currently, models are being developed to study nonlinear effects in three dimensions. These codes tax the capabilities of even the fastest computers, the so-called Class VI machines, which can perform up to 250 million floating point operations per second. Consequently, it is of the utmost importance to design a solution algorithm that efficiently utilizes the available resources.

This thesis details the development of a computer code IMP (Implicit MHD Program). In IMP, the full set of resistive MHD equations, without any ordering of terms, are solved in three dimensions by the method of finite differences. The equations are expressed in orthogonal curvilinear coordinates to allow simulations in varying geometries. Implicit time advancement techniques are used to avoid numerical limitations on the timestep size. The code has been developed on a CDC-7600 computer, which is approximately four times slower than the aforementioned Class VI machine, and has typical running times of 1 to 25 hours, depending on the problem.

I.2 Fusion Energy Sources

As in any other power plant, for the fusion reactor to be feasible, it must produce more power than is necessary to initiate and sustain its reaction. This may be expressed as the ratio

$$Q \equiv \frac{\text{fusion power out}}{\text{total power in}}$$

where Q is called the efficiency of the reactor and must be greater than unity. This requirement can be calculated based on a deuterium-tritium

(D-T) gas heated to a kinetic temperature of 10 keV ($= 1.1605 \times 10^8$ °K). At this temperature, the gas is completely ionized and is called a plasma. The fusion power out can be determined from the known cross sections for fusion and the energy released per fusion event. The total power in includes the energy needed to heat the D-T gas and to confine it long enough to react. Based on these considerations, the requirement $Q > 1$ becomes (the Lawson criterion²):

$$n\tau > 10^{14} \text{ sec/cm}^3 \quad (\text{I.2.1})$$

where n is the particle number density and τ is the confinement time.

There are currently two approaches being taken to satisfy the Lawson criterion. The first method is to implode a deuterium pellet using powerful laser or ion beams, thereby producing a dense plasma ($n \sim 10^{25} \text{ cm}^{-3}$). In this case, the confinement time is extremely short ($\tau \sim 10^{-11} \text{ sec}$). The second method involves confining a lower density plasma ($n \sim 10^{15} \text{ cm}^{-3}$) for a sustained period of time ($\tau \sim .1 \text{ sec}$). The plasma cannot be confined by material walls, as they would provide too great an energy loss mechanism. At thermonuclear densities and temperatures, the mean free path for collisions between particles of the plasma is many times any reasonably-sized containment vessel. Therefore, the collisions of hot particles with the wall would result in a transfer of energy to the wall. The cooled particle would then return to the reacting region and further lower the temperature of the remaining particles. The collisions could also cause sputtering of wall materials into the plasma. These contaminants would

require energy to reach the plasma temperature and would then increase energy losses due to bremsstrahlung radiation.³

Material walls do not solve the confinement problem. However, since the D-T gas is fully ionized, magnetic fields can be substituted. One basic effect can be found in many of the magnetic field geometries that have been tried to date. A current in the plasma produces a magnetic field which "pinches" the plasma. Consider the cylinder of plasma shown in Fig. I.1. If a current is driven along the length of the plasma (in the z direction), a magnetic field will be induced in the θ direction. The B_θ field exerts a pressure $B_\theta^2/8\pi$ (in cgs units) which compresses or pinches the plasma column. As the column contracts the magnetic pressure increases ($p \propto B_\theta^2 \propto 1/r^2$). Thus, the pinching continues until the internal pressure of the constructed plasma column has risen to equal the magnetic pressure.

I.3 Plasma Instabilities

The major problem with pinched discharges and, for that matter, with any system in which charged particles are confined by magnetic fields, is the existence of large scale instabilities. The major instabilities are known as the sausage or necking-off mode, the kink or wriggling mode and the flute modes. All of these instabilities will grow rapidly enough to destroy the plasma confinement well before the Lawson criterion can be satisfied. The driving mechanism for these instabilities can be seen from simple physical arguments. It is assumed in the following discussion that there is no magnetic field in the plasma; that the current flows only on the surface of the plasma; and that the plasma cylinder is of infinite length.

The sausage mode occurs when there is an azimuthally symmetric localized constriction of the plasma (see Fig. I.2). Since the current is a constant along the discharge, the local magnetic pressure is increased at the constriction ($P_M \propto 1/r^2$). Hence, this region then tends to become more and more constricted thereby forcing the plasma into the nonconstricted areas causing them to expand. Eventually, the plasma breaks up into individual "links", destroying the current path and the discharge.

The kink or wriggling instability (Fig. I.3) occurs when a bend forms in the plasma column. In this case, the magnetic pressure is increased on the concave side of the plasma and decreased on the convex side. Thus, the magnetic forces are acting to increase the original perturbation. In this case, the plasma continues to kink or wriggle until it collides with the walls of the containment vessel.

The flute instability (Fig. I.4) is analogous to the class of interchange instabilities found in normal hydrodynamics. In this case, the plasma is able to slip through the magnetic field lines without distorting them--and interchange with them--much as in the case of a heavy fluid supported by a light one (the Rayleigh-Taylor instability).

The sausage mode can be stabilized by including an embedded longitudinal magnetic field (B_z). Unlike the plasma, this field cannot be forced out of the constricted region. When the plasma cross section is decreased, the internal magnetic pressure ($\propto B_z^2$) increases, offsetting the increased external magnetic pressure. The embedded field also acts to stabilize short wavelength kink modes since the field lines exhibit a tension which is

similar to that of a rubber band being stretched. The magnetic tension along the plasma column opposes the magnetic pressure pushing the column, thus inhibiting growth of the mode. The tension is not, however, very effective in opposing long wavelength modes. These modes are controlled by surrounding the plasma with a conducting shell. Image currents in the shell form magnetic fields (via a Lenz's Law effect) which oppose the kinking of the plasma. The flute modes are stabilized by magnetic shear, that is, by having the field lines change their pitch ($\propto B_z/B_\theta$) as a function of position. In general, the magnetic fields in the cylindrical pinch have shear since the magnetic field is a function of radius. The magnetic shear makes the interchange modes energetically unfavorable as they now must do work to deform the magnetic field.

Pinch experiments do not, of course, have infinite length. Most pinch experiments are now being performed in toroidal devices. The straight cylinder can be used to analytically approximate a torus. The major radius R of the torus now fixes the length of the cylinder to be $2\pi R$. The cylinder also must have periodic boundary conditions. These conditions limit the range of wavelengths of modes that can exist in the system. Only integral numbers n can exist in the z or toroidal direction. The same argument holds for the poloidal direction (the short way around the torus). Since the poloidal coordinate θ is periodic, only modes of integral number m can exist. A wave number $\underline{k}$, $\underline{k} \equiv k_\theta \hat{\theta} + k_z \hat{z}$ where $\hat{\theta}$ and $\hat{z}$ are in the θ and z directions can be written such that

$$k_\theta = 1/\lambda_\theta = 2\pi/\lambda_\theta \quad (I.3.1)$$

and

$$k_z = 2\pi/\lambda_z, \quad (I.3.2)$$

where λ_θ and λ_z are the wavelengths in the θ and z directions. At a given minor radius r

$$\lambda_\theta = 2\pi r/m \quad (I.3.3)$$

and for major radius R

$$\lambda_z = 2\pi R/n \quad (I.3.4)$$

where m and n are the poloidal and toroidal mode numbers. This yields

$$\underline{k} = m/r \hat{\theta} + n/R \hat{z}. \quad (I.3.5)$$

The plasma tends to be unstable when the perturbation aligns itself with the magnetic field since in this configuration the instability is required to do a minimum of work on the field. This condition can be stated as $\underline{k} \cdot \underline{B} = 0$ (the wavefronts are perpendicular to the wavevector). For a given magnetic field, $\underline{B} = B_\theta \hat{\theta} + B_z \hat{z}$, we have

$$\frac{rB_z}{RB_\theta} = -\frac{m}{n}. \quad (I.3.6)$$

At any point where the ratio of the magnetic fields reduces to a rational

number, an instability can exist. The ratio $\frac{r_B}{R_B} \frac{z}{\theta}$ is called the safety factor q and surfaces where q is rational are called mode-rational or singular surfaces.

The modes described in this section are also named for their poloidal mode number. The sausage mode results from an $m = 0$ perturbation, the kink from an $m = 1$ and the flute modes from $m \geq 2$. The $m = 1$ kink mode is the only mode in which there is a gross motion of the plasma column. The ratio of the poloidal to toroidal mode numbers describes the helical pitch of mode.

1.4 Computational Concepts

In order to represent continuous functions to the computer, the function values are defined on a discrete set of points in space called a mesh. The functions are also evaluated at discrete points in time called levels. The differential equation is then replaced by a finite difference equation which must have the properties of consistency, accuracy, stability and efficiency. A finite difference approximation is consistent if, in the limit of small time and space steps, the difference equation becomes the differential equation. The accuracy of the finite difference approximation is degraded by truncation errors and by round-off errors (caused by finite precision arithmetic on the computer). A numerical method is stable if a small error at any stage in the calculation produces a smaller total error. The efficiency of the finite difference algorithm can be determined by its use of the available resources weighted by the difficulty of the problem to be solved (efficiency tends to be a highly subjective topic). A finite difference mesh is called Lagrangian when it moves with the fluid. It is

called Eulerian when it is stationary in the laboratory frame. If the mesh has some arbitrary velocity in the laboratory frame, it is called a generalized mesh. The equations are advanced in time via either explicit or implicit techniques. An explicit method uses only information known at preceding time levels to advance to the new time level. An implicit method couples information at the new time level in the advancement algorithm. The explicit techniques, while very fast per timestep, have a limitation as to the size of the timestep that can be used. This limit, which is called the Courant condition, is based on information transmittal rates in the finite difference mesh. Information rates in the MHD equations scale with the Alfven velocity which is proportional to the magnetic field intensity and inversely proportional to the square root of the plasma density. This ratio leads to very large velocities in areas of little plasma because where the magnetic field is strongest, the plasma density is smallest. The implicit techniques have the timestep size limitation relaxed (totally removed for linear finite difference equations with constant coefficients), but are considerably more complex to formulate and are more costly to calculate per timestep as the solution of a system of coupled equations must be solved (1 for each mesh point). For multidimensional problems, the coupled system of equations becomes intractable. In order to avoid this limitation, a technique known as the Alternating Direction Implicit (ADI) method has been devised.⁴ In two dimensions this algorithm breaks the time advancement into two steps. In the first step, variables are advanced implicitly in one dimension and explicitly in the other dimension to a half time level. In the second step, the procedure is reversed and the direction

that was advanced implicitly is advanced explicitly and vice versa. The obvious generalization of this procedure to three dimensions by using three advances of one-third time level each is not numerically unconditionally stable. A stable generalization is given in a paper by Douglas and Gunn.⁵

The details of the various schemes to be named in the next section may be found in such works as Richtmyer and Morton⁶ or Potter.⁷

I.5 Previous Work

The numerical study of MHD stability has followed two paths. In the first, the linearized MHD equations are treated as an initial value problem.^{8,9} The equilibrium state of the system is specified and is given a perturbation. The MHD equations are integrated forward in time to trace the evolution of the plasma. The fastest growing instability eventually dominates over all other motions. The second approach which has been used very successfully is to utilize the energy principle¹⁰⁻¹⁵ to gain information on the full spectrum of ideal MHD instabilities. After the linear modes have been determined by either of the above methods, the resultant eigenmodes may be used to start a nonlinear calculation which can then follow their growth to some final state.^{16,17}

The nonlinear codes are not limited to stability studies. They are also used to simulate total experiments. By incorporating time dependent boundary conditions, such as circuit equations, a simulation can start with a neutral gas, and trace its ionization (via a Saha equation of state¹⁸), and pinching. In this section, the development of two- and three-dimensional initial value codes will be reviewed.

I.5.1 Two-Dimensional Codes

Most two-dimensional codes employ an Eulerian mesh as in the codes of Roberts et al.,¹⁹ Roberts and Weiss,²⁰ Weiss,²¹ Duchs,²² Freeman and Lane,²³ and Peacock et al.^{24,25} All the aforementioned codes use explicit finite difference techniques. One of the difficulties encountered when using a Eulerian mesh is the accurate treatment of advective derivatives (term of the form $\underline{v} \cdot \nabla$). Roberts and Weiss use a fourth order finite difference approximation of the advection terms. Freeman and Lane use an explicit, Lax-Wendroff algorithm with a Lapidus²⁶ artificial diffusion term added to each equation to give added stability. The Peacock code uses a two fluid model with a Lax-Wendroff scheme. The Roberts, Roberts and Weiss, Freeman and Lane, and Peacock codes all examine the (r,z) plane. Duchs has considered the (r,θ) plane.

Explicit linearized codes have been written by Sykes and Wesson,²⁷ and Bateman et al.⁹ These have been used to study stability in rectangular and toroidal geometries. The Sykes and Wesson code uses the Lax-Wendroff scheme while Bateman et al. employ a leapfrog algorithm. These codes produce linear eigenmodes that can be used as initial perturbations in the nonlinear codes.

The only recent Lagrangian MHD calculation in two dimensions is the code of White et al.²⁸ In this code, the set of equations are reduced by applying the so-called Tokamak ordering ($B_z \gg B_\theta$). The torus is approximated as a cylinder and helical symmetry is imposed on

the system. Thus, the (r, ϕ) plane is examined where

$$\phi \equiv m\theta + kz \quad . \quad (I.5.1.1)$$

The plasma is considered to be incompressible. With these constraints, the magnetic field and velocity are computed from potential functions. White et al.²⁹ have also developed an Eulerian code based on the reduced equation that has been used to study the growth of magnetic islands in a resistive plasma.

Morse³⁰ has used the Particle-in-Cell (PIC) method to perform fluid simulations of plasma guns. The fluid PIC model divides the computational region into a set of regular Eulerian zones for computing field variable (i.e., pressure or fluid velocity). Material is transported from cell to cell by using discrete particles. Thus mass is moved in a Lagrangian manner.

Hertwech and Schneider,³¹ Anderson,³² and Jardin³³ use generalized mesh techniques. In these codes, flux coordinates are used which allow for better computation of thermal conduction. Hertwech, Schneider, and Jardin use a nonorthogonal mesh while Anderson keeps an orthogonal mesh and rezones after each timestep. Jardin's code employs a mixed explicit-implicit time advancement algorithm, while Anderson uses a timestep splitting implicit method. The Hertwech-Schneider code is explicit.

Lindemuth and Killeen³⁴ introduced the first ADI code in 1970 in which all terms in the two fluid MHD equations, including transport terms, are differenced implicitly. Lindemuth has since specialized the code to include only one component of the magnetic field and two velocity components.³⁵ This new code has successfully simulated z-pinch implosions. Lui and Chu^{36,37} use implicit methods to simulate screw and belt pinches; however, in their code, the transport coefficients are calculated by using an explicit predictor step. Schnack^{16,17,38} introduced an ADI code to solve the full set of single fluid resistive MHD equations. This code has been used to extensively study resistive tearing instabilities in a variety of coordinate systems. Reviews of other one- and two-dimensional work may be found in Roberts and Potter,²⁵ Killeen,³⁹ and Brackbill.⁴⁰

1.5.2 Three-Dimensional Codes

Currently, three-dimensional calculations are the subject of active research. Wooten et al.⁴¹ have generalized the two-dimensional linear code of Bateman to solve the nonlinear ideal MHD equations in three-dimensions. This code uses an Eulerian mesh with the same explicit, leapfrog time advancement algorithm as is found in the two-dimensional code and has been applied to the simulation of nonlinear ideal MHD internal kink instabilities. Cochran⁴² and Pritchett⁴³ have developed explicit, Eulerian codes which include constant diffusion coefficients and also utilize leapfrog algorithm. They too are applied to study the nonlinear development of internal kink instabilities. Pritchett has also demonstrated spontaneous field reversal caused by an internal kink mode in a highly pinched plasma.

Sykes and Wesson^{44,45} have extended their two-dimensional code to three dimensions. They include tensor resistivity, thermal conductivity, and a radiation loss mechanism. This code uses a generalized Lax-Wendroff difference approximation on an Eulerian mesh and has successfully simulated the "sawtooth"⁴⁶ instability observed in Tokamaks. This instability is characterized by a "sawtooth" or relaxation oscillation in the soft x-ray emission. It has also simulated the spontaneous field reversal caused by $m = 1$ kink instabilities that has been observed in the Culham Reversed Field Pinch⁴⁷ experiment.

Brackbill⁴⁰ has developed an ideal MHD code which utilized a generalized (semi-Lagrangian) mesh based on the ICED-ALE technique of Hirt, Cook, and Amsden.⁴⁸ The code uses an implicit Lagrangian time advance followed by a rezone phase designed to reduce distortion of the mesh and has been applied to the study of the ϕ pinch and the internal kink instability. Currently, Brackbill⁴⁹ is reporting on a refinement to his code based on the work of Jardin which identifies the fast time-scale terms. Only these terms have been differenced fully implicitly. This selective or semi-implicit technique is twice as fast as the older code.

Strauss⁵⁰ has extended the reduced model of White et al.²⁸ to three-dimensions. He uses an Eulerian mesh with a leapfrog time advancement algorithm. As in many of the leapfrog based codes, diffusion terms were differenced via the Dufort-Frankel method. Strauss has applied his code to the nonlinear evolution of the internal

kink mode in the low β (β is the ratio of plasma energy to confining magnetic field energy), large aspect ratio (ratio of length to cross section), incompressible limit in a rectangular pipe.

Jardin and Johnson⁵¹ have extended Jardin's "dynamical grid method" to three dimensions. In this work, the "Tokamak ordering" is used to reduce three three-dimensional implicit algorithm to a series of two-dimensional implicit (ADI) solutions coupled by an explicit solution in the third direction and has been applied to nonlinear studies of internal instabilities in Tokamaks.

Hicks et al.,⁵² have reported on a series of codes which investigate the nonlinear resistive evolution of plasmas in Tokamaks. Once again, the assumptions of Tokamak ordering and low β are made. The code uses an Eulerian grid and a mixed implicit (ADI) and explicit time advancement algorithm. Another code based on a Fourier transform technique has also been reported by Hicks in this paper.

I.6 Scope of Present Work

The three-dimensional calculations discussed in the previous section have limited applications. A number of them treat only the ideal MHD approximation or, if they have included non-ideal effects such as finite resistivity, are limited in achievable timestep by the use of explicit finite difference algorithms. A number of the codes use Tokamak ordering to remove fast timescales from the problem. These codes are limited to low β devices.

In this work, a computer program, IMP (Implicit MHD Program), which does not suffer these limitations is described. In IMP, the full set of resistive MHD equations is solved by implicit techniques on a variable Eulerian mesh. The equations are finite differenced in orthogonal curvilinear coordinates to allow the specification of arbitrary coordinate representations. The evolution of the pressure, rather than the total energy density, is followed in time to allow the simulation of both high and low β plasmas. The model used in IMP is given in Chapter II. The use of the Douglas-Gunn algorithm (DGA) for alternating direction implicit time-steps allows the use of a timestep that is many times larger than ones that an explicit code can use. All variables are advanced simultaneously to avoid any synchronization errors that may occur in a staggered timestep scheme.

The large timestep sizes allowed by the DGA pose problems of their own. Since the MHD equations are nonlinear, we arrive, after spatial and temporal discretization, at a system of nonlinear algebraic equations that must be solved. This system is solved via a Newton-Raphson iteration procedure. The iterations continue until a convergence criterion is met. This process involves the calculation and inversion of the Jacobian of the system. The Jacobian calculation requires the analytic evaluation of a number of functional derivatives of the finite difference equations at all the mesh points. This calculation is carried out on the REDUCE⁵³ algebraic processor. The REDUCE program is given the finite difference equations and is programmed to generate the Jacobian matrix elements. The resultant matrix elements are then output as a FORTRAN subroutine for use in the main

code. This procedure has proven to be extremely useful as it has allowed the testing of a number of different finite difference representations. Without the REDUCE generated Jacobian subroutine the evaluation of these coefficients would have required many weeks of work to correctly derive and enter into the computer. A discussion of the iteration techniques can be found in Section III.5 while Appendix B contains a listing of the REDUCE program used to generate the Jacobian matrix.

A second problem posed by the large timestep allowed by the implicit algorithm is that of selecting the correct timestep size to use. Clearly, if one uses too large a timestep, the results will be incorrect. Also, since the problem is nonlinear, there is no guarantee that the timestep chosen will lead to a stable time advancement algorithm. Yet, if one uses a very conservative timestep, the efficiency of the implicit algorithm is lowered--perhaps to the point where an explicit scheme is more efficient. The dynamic nature of the problems being run is such that, during their early stages the problems are nearly linear and, therefore, the linear stability analysis should prove to be correct. However, in their latter stages, the problems are highly nonlinear and the results of linear stability analysis do not apply. In order to prevent the early timesteps from being limited by the latter conditions and to allow the physics occurring in the problem to dictate the timestep size chosen, a set of dynamic timestep controls are incorporated in IMP. These are described in Section III.7.

The boundary conditions implemented in the code are quite general. Any type of Neumann or Dirichlet or mixed boundary condition is allowed.

The conservation boundary condition outlined by Lindemuth,⁵⁴ which is based on the wall being a flux surface of the plasma, and a pseudo-circuit equation boundary condition are also implemented.

Current versions of IMP do not allow for a concentration point in the coordinates (e.g., $r = 0$ in cylindrical coordinates). For this reason simulations are carried out in rectangular cross section pipes and tori. This aspect of IMP is not a serious shortcoming and parallels the work of Wooten et al. and Sykes and Wesson.

The code is applied to the study of internal kink modes in varying geometries. These are the most dangerous modes to plasma stability as they cause a gross motion of the plasma column. Recently, theories have been put forth which relate the internal kink to the "sawtooth-oscillations" or internal disruptions that are observed in the soft x-ray emissions from Tokamak discharges.⁴⁶

In Chapter IV, a torus is approximated in Cartesian coordinates with a straight rectangular pipe. A great deal of work has been done in this geometry and provides a basis for comparison. Agreement is found with the linear growth rates calculated by the Bateman ideal MHD linear instability code. These linear eigenmodes are then allowed to evolve until they eventually saturate. The saturation amplitudes of the ideal modes agree with the nonlinear calculations of Hicks et al.⁵⁵ In IMP, the linear eigenmodes generated by the Bateman code are used as the initial perturbations and display an immediate exponential growth. This growth implies that the

eigenmodes found by using small perturbations in IMP are in close agreement with the eigenmodes determined by the linear code. Next, a finite resistivity is added to the problem. The modification of growth rates as a function of the magnetic Reynolds number for a particular wavelength instability is shown.

In Chapter V, we consider a square cross section torus which is represented in a cylindrical coordinate system. Agreement is found in the form and growth rates of the linear, ideal eigenfunctions. Finite resistivity is once again added. A $m = 1/n = 1$ mode is allowed to evolve in an $S = 10^5$ plasma for over 1000 Alfvén transit times. The 1/1 mode is observed to grow initially, followed by saturation. The system then relaxes to an axisymmetric equilibrium with a $m = 1$ flow field appearing near the outer edge of the torus.

In Chapter VI, another plasma regime, the reversed field pinch (RFP), is investigated. A Cartesian grid is used for these simulations. A high pinch ratio, χ ($\chi \equiv 2I/aB_z$), equilibrium is perturbed in velocity by a $m = 1/n = 1$ mode. This mode is shown to grow and to cause a spontaneous reversal of the B_z field in the outer regions of the plasma. This field reversal increases the shear and stabilizes the kink.

Next, a low pinch ratio equilibrium (the same one used in Chapter IV) is raised to the high pinch regime by imposing an external electric field along the walls of the pipe. The external field causes the current to increase in the plasma, which then pinches itself to the higher χ regime. A von Neumann⁵⁶ artificial viscosity is added to stabilize numeric problems

caused by the compression of the plasma. Once again, an internal kink mode causes the spontaneous field reversal.

Appendix A details a two-dimensional calculation of the resistive sheet pinch. This calculation, which has been performed by Schnack, leads to a strictly resistive instability--the resistive tearing mode (e.g., Furth, Killeen, and Rosenbluth).⁵⁷ The problem is run in all three possible planes and has verified the correct inclusion of the resistive terms in IMP. The power of the Newton-Raphson iterations, coupled with the dynamic timestep controls, has allowed IMP to perform the calculation at timesteps one hundred times larger than those used by Schnack.

In all the aforementioned problems, IMP was able to use timesteps ranging from 5 to 150 times larger than the linear Courant limit--the largest possible timestep an explicit calculation can utilize.

Figure I.1 A magnetic field line that is wound on a cylindrical flux surface.

Figure 1.2 The $m = 0$ sausage mode.

Figure I.3 The $m = 1$ kink mode.

Figure 1.4 The $m = 2$ flute mode.

CHAPTER II

MATHEMATICAL MODEL

II.1 Introduction

The single fluid, resistive MHD equations implemented in the IMP code will be presented in this chapter. A heuristic derivation will be given to point out the approximations that are being made. Next, we will show how to cast the equations in conservation form. Then we explain why we chose not to use this computational technique. Finally, we will normalize the vector equations and expand them in orthogonal curvilinear coordinates to obtain the set of equations that we use to follow plasma behavior in IMP.

II.2 Resistive Single Fluid MHD Equations

The MHD equations describe the behavior of an electrically neutral conducting fluid in the presence of electromagnetic fields and also describe self-consistently the effect that the fluid has on the fields. The macroscopic variables that describe the fluid are a density $\rho(\underline{x},t)$, a velocity $\underline{v}(\underline{x},t)$, and an internal energy $\epsilon(\underline{x},t)$. We also require the associated electromagnetic quantities: the electric field $\underline{E}(\underline{x},t)$; the magnetic flux density $\underline{B}(\underline{x},t)$; the charge density $q(\underline{x},t)$; and the current density $\underline{j}(\underline{x},t)$. The equations of a nonconducting inviscid, compressible fluid must be modified to add in electromagnetic effects.

The first fluid equation expresses conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad (\text{II.2.1})$$

and is correct in the absence of sources of mass.

The equation of motion

$$\rho \frac{d\mathbf{v}}{dt} \equiv \rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla P + \frac{1}{c} \mathbf{j} \times \mathbf{B} \quad (\text{II.2.2})$$

requires an additional force term, the Lorentz force, to account for the electromagnetic forces of the field on the conducting fluid. Notice the absence of the $q\mathbf{E}$ term in the Lorentz force. This is dropped by the assumption of charge neutrality ($q = 0$). In Eulerian (fixed reference frame) form (after expansion of the convective derivative and substitution of Eq. II.2.1 for $\frac{\partial \rho}{\partial t}$), Eq. II.2.2 becomes

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) + \nabla P - \frac{1}{c} \mathbf{j} \times \mathbf{B} = 0 \quad (\text{II.2.3})$$

The internal energy equation requires the inclusion of an additional term due to ohmic heating, i.e., the heating of the resistive fluid due to the current flowing in it and becomes

$$\frac{\partial \rho \epsilon}{\partial t} + \nabla \cdot (\rho \epsilon \mathbf{v}) + P \nabla \cdot \mathbf{v} - \eta j^2 = 0 \quad (\text{II.2.4})$$

We also need equations expressing the effects of the fluid on the electromagnetic fields. The fields are described by Maxwell's equations:

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \quad (\text{II.2.5.a})$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \quad (\text{II.2.5.b})$$

In the MHD approximation, we assume that the displacement current in Ampere's law is of order v^2/c^2 and, since our flows are to be non-relativistic, may be ignored. The requirement that $\nabla \cdot \underline{B} = 0$ follows from (II.2.5.b) if we impose $\nabla \cdot \underline{B} = 0$ initially. In order to determine the electric field $\underline{E}$, we use Ohm's law in the form

$$\underline{\eta j} = \underline{E} + \frac{1}{c} \underline{v} \times \underline{B} . \quad (\text{II.2.6})$$

We now have a set of 14 equations in 15 unknowns: $\underline{j}$, $\underline{E}$, $\underline{v}$, ρ , $\underline{B}$, ϵ , P . The system is closed by the provision of an equation of state which relates the pressure, P , to the internal energy, ϵ , and density, ρ . The plasma is considered an ideal monatomic gas which gives us

$$P(\epsilon, \rho) = (\gamma - 1) \rho \epsilon , \quad (\text{II.2.7})$$

where $\gamma = c_p/c_v$ is the ratio of the specific heats of the plasma. We have now a complete, though unwieldy, system of 15 equations in 15 unknowns.

This system is reduced in the following manner. The current density $\underline{j}$ is eliminated from Ohm's law (II.2.6) by the use of Eq. II.2.5.a. The resulting relationship for the electric field $\underline{E}$ is then substituted into Eq. II.2.5.b yielding

$$\frac{\partial \underline{B}}{\partial t} + \nabla \times \left\{ (\underline{v} \times \underline{B}) - \frac{c^2 \eta}{4\pi} \nabla \times \underline{B} \right\} = 0 . \quad (\text{II.2.8.a})$$

The momentum equation (II.2.3) also has $\underline{j}$ eliminated via Eq. II.2.5.a. This gives

$$\frac{\partial \rho \underline{v}}{\partial t} + \nabla \cdot (\rho \underline{v} \underline{v}) + \nabla P + \frac{1}{4\pi} \underline{B} \times (\nabla \times \underline{B}) = 0 \quad . \quad (\text{II.2.8.b})$$

The continuity equation (II.2.1) remains

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad . \quad (\text{II.2.8.c})$$

Finally, the internal energy ε in Eq. II.2.4 is replaced with the pressure by using the equation of state (II.2.7) and the current density $\underline{j}$ is once again replaced via Eq. II.2.5.a, yielding

$$\frac{\partial P}{\partial t} + \nabla \cdot (P \underline{v}) + (\gamma - 1) \left(P \nabla \cdot \underline{v} - \frac{c^2 \eta}{(4\pi)^2} (\nabla \times \underline{B})^2 \right) = 0$$

After using the vector identity $\nabla \cdot \underline{A} \underline{B} = \underline{A} \cdot \nabla \underline{B} + \underline{B} \cdot \nabla \underline{A}$, this becomes

$$\frac{\partial P}{\partial t} + \nabla \cdot (P \underline{v}) - (\gamma - 1) \left\{ \underline{v} \cdot \nabla P - \frac{c^2 \eta}{(4\pi)^2} (\nabla \times \underline{B})^2 \right\} = 0 \quad . \quad (\text{II.2.8.d})$$

Equations (II.2.8) are a system of 8 equations in 8 unknowns.

II.3 Normalization

Our next step is to normalize the equations. We introduce a set of nondimensional variables where the 0 subscripted quantities are character-

istic values for our system,

$$\underline{x} \rightarrow \underline{x}' x_0, \quad \underline{B} \rightarrow \underline{B}' B_0, \quad \rho \rightarrow \rho' \rho_0,$$

$$\underline{v} \rightarrow \underline{v}' v_0, \quad P \rightarrow P' P_0, \quad t \rightarrow t' t_0, \quad \eta \rightarrow \eta' \eta_0$$

We then rewrite (II.2.9.a) as

$$\frac{B_0}{t_0} \frac{\partial \underline{B}'}{\partial t'} + \frac{v_0 B_0}{x_0} \nabla' \times (\underline{v}' \times \underline{B}') - \frac{c^2 \eta_0}{4\pi x_0^2} \nabla \times \eta' (\nabla \times \underline{B}') = 0 \quad (\text{II.3.1})$$

By letting $x_0 = v_0 t_0$, (II.3.1) simplifies to

$$\frac{\partial \underline{B}'}{\partial t} + \nabla' \times (\underline{v}' \times \underline{B}') - \frac{1}{S} \nabla \times \eta' (\nabla \times \underline{B}') = 0 \quad (\text{II.3.2})$$

where $S \equiv \frac{4\pi v_0 x_0}{c^2 \eta_0}$. By choosing $v_0 = v_A$ (the Alfvén velocity)
 $\equiv B_0 / \sqrt{4\pi \rho_0}$ and $P_0 = B_0^2 / 8\pi = \frac{1}{2} \rho_0 v_A^2$, we may define the Alfvén transit time $\tau_A = v_A / x_0$ and the resistive diffusion time $\tau_R = 4\pi x_0^2 / c^2 \eta$. Thus S is the magnetic Reynolds number τ_R / τ_A . This gives us a measure of the ratio of the resistive timescale to the Alfvén timescale. Next, we define t_0 such that an Alfvén wave travels a distance x_0 in 1 unit of time, where x_0 is generally dictated by the dimensions of the problem. When we apply the above procedure to the rest of the equations in (II.2.8), we arrive at the set of normalized MHD equations that are modeled in the IMP code:

$$\frac{\partial \underline{B}}{\partial t} - \nabla \times (\underline{v} \times \underline{B} - \frac{\eta}{S} \nabla \times \underline{B}) = 0 \quad (\text{II.3.3.a})$$

$$\frac{\partial \rho \underline{v}}{\partial t} + \nabla \cdot (\rho \underline{v} \underline{v}) + \frac{1}{2} \nabla P + \underline{B} \times (\nabla \times \underline{B}) = 0 \quad (\text{II.3.3.b})$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad (\text{II.3.3.c})$$

$$\frac{\partial P}{\partial t} + \nabla \cdot (\gamma P \underline{v}) - (\gamma - 1) \left\{ \underline{v} \cdot \nabla P + \frac{2\eta}{S} (\nabla \times \underline{B})^2 \right\} = 0 \quad (\text{II.3.3.d})$$

II.4 An Alternate Model

The above set of equations are not all in conservation form. An equation is said to be in conservation form when it has one of the following forms:

- a) a scalar conservation law

$$\frac{\partial \rho}{\partial t} = - \nabla \cdot \underline{F} \quad (\text{II.4.1})$$

- b) a vector conservation law

$$\frac{\partial \underline{v}}{\partial t} = - \nabla \cdot \underline{T} \quad (\text{II.4.2})$$

or

- c) a pseudovector conservation law

$$\frac{\partial \underline{w}}{\partial t} = \nabla \times \underline{G} \quad (\text{II.4.3})$$

where ρ is a scalar; $\underline{F}$, $\underline{v}$ and $\underline{G}$ are vectors; $\underline{w}$ is a pseudovector; and $\underline{T}$ symmetric second rank tensor (a dyad). $\underline{F}$ is the flux of ρ into the volume

element and $\underline{T}$ is the flux of $\underline{v}$ into it. In the case of Eq. II.4.3, $\underline{w}$ is termed a flux density in the volume element and its variation is driven by the circulation of the vector $\underline{G}$ around the element rather than the amount of $\underline{G}$ flowing into or out of it. The use of conservation form is common in computer codes because the calculation of the conservation sums,

$$M = \int_V \rho d\tau \quad (\text{II.4.4})$$

$$V = \int_V V d\tau \quad (\text{II.4.5})$$

and

$$\phi = \int_S \underline{w} \cdot d\underline{a} \quad , \quad (\text{II.4.6})$$

gives a convenient test of the consistency of one's coding. It also ensures that no nonphysical sources or sinks of mass, momentum or energy exist. The continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad (\text{II.3.3.c})$$

is in strict conservation form. The magnetic flux equation

$$\frac{\partial \underline{B}}{\partial t} - \nabla \times (\underline{v} \times \underline{B} - \frac{\eta}{S} \nabla \times \underline{B}) = 0 \quad (\text{II.3.3.a})$$

is also in conservation form, although here we have a pseudovector conservation rather than the normal scalar or vector conservation (see Schnack³⁸

for further details). Equation (II.3.3.b), the momentum equation, could be converted to conservation form by adding $\underline{B}(\nabla \cdot \underline{B}) = 0$ yielding

$$\frac{\partial \rho \underline{v}}{\partial t} + \nabla \cdot \left(\rho \underline{v} \underline{v} - \underline{B} \underline{B} + \frac{1}{2} (P + B^2) \underline{I} \right) = 0 \quad (\text{II.4.7})$$

This addition has not been done because, on a finite difference mesh, $\nabla \cdot \underline{B}$ is not necessarily zero--even if the analytic $\underline{B}$ field does correctly display this property. This error arises from the fact that the numeric derivatives are only accurate to order Δx^2 . We are thus adding this extra error into our equations for advancing the state variables ($\underline{B}$, ρ , $\underline{v}$, P), giving us a feedback of error--the $\nabla \cdot \underline{B}$ error induces extra errors in $\underline{v}$ and the extra errors in $\underline{v}$ induce errors in $\underline{B}$ which, in turn, magnify the errors in $\nabla \cdot \underline{B}$ --a vicious cycle. Runs have been made comparing the two forms of the momentum equation and they show much better numerical results for the nonconservation form of the equation. We achieved much larger time steps with greatly reduced noise. The recognition of this source of error has been independently arrived at by Brackbill and Barnes.^{58,59}

The pressure equation (II.3.3.d) is also not in conservation form. If we define in our normalized variables a total energy density w as

$$w \equiv \frac{1}{2} \rho v^2 + B^2 + P/(\gamma - 1) \quad (\text{II.4.8})$$

and combine the set of MHD equations as

$$\underline{B} \cdot \frac{\partial \underline{B}}{\partial t} - \frac{1}{2} |\underline{v}|^2 \frac{\partial \rho}{\partial t} + \frac{\partial (\rho \epsilon)}{\partial t} + \underline{v} \cdot \frac{\partial \rho \underline{v}}{\partial t} = 0, \quad (\text{II.4.9})$$

we obtain

$$\frac{\partial w}{\partial t} + \nabla \cdot \left[(w + P) \underline{v} + (B^2 \underline{I} - 2 \underline{B} \underline{B}) \cdot \underline{v} + \frac{2\eta}{S} (\underline{B} \cdot \nabla \underline{B} - \nabla \underline{B} \cdot \underline{B}) \right] = 0 \quad (\text{II.4.10})$$

This form of the equation is not used because now the pressure becomes a subsidiary variable,

$$P = (\gamma - 1) (w - B^2 - \rho v^2) \quad . \quad (\text{II.4.11})$$

When the plasma β ($= P/B^2$) is small, the error in the pressure calculation becomes equal to or greater than the calculated pressure. In this form, then, low β plasmas cannot be simulated. Total energy conservation is used, instead, as a check on the accuracy of, rather than as a requirement of, the solution.

II.5 Orthogonal Curvilinear Coordinates

As we stated in Chapter I, we wish to apply our MHD model to problems in varying coordinate systems. Rather than having to generate the equations for each coordinate system of interest, we adopt the procedure of Schnack³⁸ and expand the equations (II.3.3) in orthogonal curvilinear coordinates. In this thesis, we extend the work of Schnack to allow variations in all three coordinate directions. The "h" factors are then calculated in a FUNCTION subroutine so that we may simply vary the subroutine to run in different coordinate systems.

In orthogonal curvilinear coordinates, we take the differential arc length to be

$$ds^2 = h_1^2 dx_1^2 + h_2^2 dx_2^2 + h_3^2 dx_3^2 \quad (\text{II.5.1})$$

where the terms $h_i dx_i$ measure the differential arc length in the $\hat{e}_i$ direction. In this system, the metric g is given by

$$g = (h_1 h_2 h_3)^2, \quad (\text{II.5.2})$$

and the volume element by $d\tau = h_1 h_2 h_3 dx_1 dx_2 dx_3$. We also have the relations for the unit vectors $\hat{e}$

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} \quad (\text{II.5.3})$$

where δ_{ij} is the Kronecker delta and

$$\hat{e}_i \times \hat{e}_j = \epsilon_{ijk} \hat{e}_k$$

where ϵ_{ijk} is the Levi-Civita permutation symbol which is defined as

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (ijk) = (123), (312), (231) \text{ (i.e., even permutations of } (ijk)) \\ -1 & \text{if } (ijk) = \text{odd permutations of } (ijk) \\ 0 & \text{otherwise} \end{cases}$$

In this system the gradient operator becomes

$$\nabla \equiv \frac{\hat{e}_1}{h_1} \frac{\partial}{\partial x_1} + \frac{\hat{e}_2}{h_2} \frac{\partial}{\partial x_2} + \frac{\hat{e}_3}{h_3} \frac{\partial}{\partial x_3} = \sum_i \frac{\hat{e}_i}{h_i} \frac{\partial}{\partial x_i} \quad (\text{II.5.5})$$

where the summation runs from 1 to 3. In these terms, we may now define the gradient of a scalar and the divergence and curl of a vector.

The gradient of a scalar ψ is

$$\nabla \psi = \sum_i \frac{1}{h_i} \frac{\partial \psi}{\partial x_i} \hat{e}_i \quad . \quad (\text{II.5.6})$$

The divergence of a vector $\underline{v}$ is

$$\nabla \cdot \underline{v} = \sum_i \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_i} \left(\sqrt{g} \frac{v_i}{h_i} \right). \quad (\text{II.5.7})$$

The curl of a vector $\underline{v}$ is

$$\nabla \times \underline{v} = \sum_i \frac{\hat{e}_i}{\sqrt{g}} \sum_{\ell, m} \epsilon_{i\ell m} \frac{\partial h_m v_m}{\partial x_\ell} \quad . \quad (\text{II.5.8})$$

This is expanded for clarity to give

$$\begin{aligned} (\nabla \times \underline{v}) &= \frac{\hat{e}_1}{h_2 h_3} \left[\frac{\partial}{\partial x_2} (h_3 v_3) - \frac{\partial}{\partial x_3} (h_2 v_2) \right] \\ &+ \frac{\hat{e}_2}{h_1 h_3} \left[\frac{\partial}{\partial x_3} (h_1 v_1) - \frac{\partial}{\partial x_1} (h_3 v_3) \right] \\ &+ \frac{\hat{e}_3}{h_1 h_2} \left[\frac{\partial}{\partial x_1} (h_2 v_2) - \frac{\partial}{\partial x_2} (h_1 v_1) \right] \quad . \end{aligned} \quad (\text{II.5.9})$$

The final relation we need is the divergence of a tensor $\underline{T}$. This is given by⁶⁰

$$(\nabla \cdot \underline{T})_j = \sum_i h_j \hat{e}_j t_{,i}^{ij} = \sum_i \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_i} (\sqrt{g} t^{ij}) + \sum_k t^{ik} \left\{ \begin{matrix} j \\ ki \end{matrix} \right\} \quad (\text{II.5.10})$$

where $t^{ij} = T_{ij}/h_i h_j$ is the contravariant form of the tensor T_{ij} and $t_{,j}^{ij}$ is the covariant derivative of t . $\left\{ \begin{matrix} j \\ ik \end{matrix} \right\}$ is a Christoffel symbol whose properties are

$$\left\{ \begin{matrix} i \\ ii \end{matrix} \right\} = \frac{1}{h_i} \frac{\partial h_i}{\partial x_i} ; \left\{ \begin{matrix} i \\ ij \end{matrix} \right\} = \left\{ \begin{matrix} i \\ ji \end{matrix} \right\} = \frac{1}{h_i} \frac{\partial h_i}{\partial x_j} ;$$

$$\left\{ \begin{matrix} j \\ ii \end{matrix} \right\} = - \frac{h_i}{(h_j)^2} \frac{\partial h_i}{\partial x_j} ; \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} = 0 \quad \text{for } i, j, k \text{ all different.} \quad (\text{II.5.11})$$

The Christoffel symbols give the change in directions of the unit vectors as one moves in space, and vanish for Cartesian coordinates. We will expand, for clarity, the first component of $\nabla \cdot \underline{T}$ to show the actual form of these terms

$$(\nabla \cdot \underline{T})_1 = \frac{1}{h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 T_{11}) + \frac{\partial}{\partial x_2} (h_1 h_3 T_{21}) \right.$$

$$+ \frac{\partial}{\partial x_3} (h_1 h_2 T_{31}) + h_3 \frac{\partial h_1}{\partial x_2} T_{12} + h_2 \frac{\partial h_1}{\partial x_3} T_{13}$$

$$\left. - \left[h_3 \frac{\partial h_2}{\partial x_1} T_{22} + h_2 \frac{\partial h_3}{\partial x_1} T_{33} \right] \right\} \quad (\text{II.5.12})$$

Equation (II.5.10) contains terms which look like the normal vector divergence terms plus a set of extra terms that arise due to the change in

direction of the unit vectors with changes in position. These are called the Coriolis terms.

We may now write down the equations (II.3.3) in component form.

$$\begin{aligned} \frac{\partial B_1}{\partial t} + \frac{1}{h_2 h_3} \left[\frac{\partial}{\partial x_2} \left(h_3 \left\{ B_1 v_2 - B_2 v_1 - \frac{\eta}{S} \frac{1}{h_1 h_2} \left\{ \frac{\partial}{\partial x_2} (h_1 B_1) \right. \right. \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_1} (h_2 B_2) \right\} \right) \right) + \frac{\partial}{\partial x_3} \left(h_2 \left\{ B_1 v_3 - B_3 v_1 \right. \right. \right. \\ \left. \left. \left. - \frac{\eta}{S} \frac{1}{h_1 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right\} \right) \right) \right] = 0 \end{aligned} \quad (\text{II.5.13.a})$$

$$\begin{aligned} \frac{\partial B_2}{\partial t} + \frac{1}{h_1 h_3} \left[\frac{\partial}{\partial x_1} \left(h_3 \left\{ B_2 v_1 - B_1 v_2 - \frac{\eta}{S} \frac{1}{h_1 h_2} \left\{ \frac{\partial}{\partial x_1} (h_2 B_2) \right. \right. \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_2} (h_1 B_1) \right\} \right) \right) + \frac{\partial}{\partial x_3} \left(h_1 \left\{ B_2 v_3 - B_3 v_2 \right. \right. \right. \\ \left. \left. \left. - \frac{\eta}{S} \frac{1}{h_2 h_3} \left\{ \frac{\partial}{\partial x_3} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_3 B_3) \right\} \right) \right) \right] = 0 \end{aligned} \quad (\text{II.5.13.b})$$

$$\begin{aligned} \frac{\partial B_3}{\partial t} + \frac{1}{h_1 h_2} \left[\frac{\partial}{\partial x_1} \left(h_2 \left\{ B_3 v_1 - B_1 v_3 - \frac{\eta}{S} \frac{1}{h_1 h_3} \left\{ \frac{\partial}{\partial x_1} (h_3 B_3) \right. \right. \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_3} (h_1 B_1) \right\} \right) \right) + \frac{\partial}{\partial x_2} \left(h_1 \left\{ B_3 v_2 - B_2 v_3 \right. \right. \right. \\ \left. \left. \left. - \frac{\eta}{S} \frac{1}{h_2 h_3} \left\{ \frac{\partial}{\partial x_2} (h_3 B_3) - \frac{\partial}{\partial x_3} (h_2 B_2) \right\} \right) \right) \right] = 0 \end{aligned} \quad (\text{II.5.13.c})$$

$$\begin{aligned}
 & \frac{\partial \rho v_1}{\partial t} + \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1^2) + \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_1 v_2) \right. \\
 & \quad + \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_1 v_3) + h_3 \rho v_1 v_2 \frac{\partial h_1}{\partial x_2} + h_2 \rho v_1 v_3 \frac{\partial h_1}{\partial x_3} \\
 & \quad - \left[h_3 \rho v_2^2 \frac{\partial h_2}{\partial x_1} + h_2 \rho v_3^2 \frac{\partial h_3}{\partial x_1} \right] \left. \right\} + \frac{1}{2h_1} \frac{\partial P}{\partial x_1} \\
 & \quad + \left[\frac{B_2}{h_1 h_2} \left\{ \frac{\partial}{\partial x_1} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_1 B_1) \right\} \right. \\
 & \quad \left. + \frac{B_3}{h_1 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right\} \right] = 0 \quad (II.5.13.d)
 \end{aligned}$$

$$\begin{aligned}
 & \frac{\partial \rho v_2}{\partial t} + \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1 v_2) + \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2^2) \right. \\
 & \quad + \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_2 v_3) + h_3 \rho v_1 v_2 \frac{\partial h_2}{\partial x_1} + h_1 \rho v_2 v_3 \frac{\partial h_2}{\partial x_3} \\
 & \quad - \left[h_3 \rho v_1^2 \frac{\partial h_1}{\partial x_2} + h_1 \rho v_3^2 \frac{\partial h_3}{\partial x_2} \right] \left. \right\} + \frac{1}{2h_2} \frac{\partial P}{\partial x_2} \\
 & \quad + \left[\frac{B_3}{h_2 h_3} \left\{ \frac{\partial}{\partial x_2} (h_3 B_3) - \frac{\partial}{\partial x_3} (h_2 B_2) \right\} \right. \\
 & \quad \left. + \frac{B_1}{h_1 h_2} \left\{ \frac{\partial}{\partial x_1} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_1 B_1) \right\} \right] = 0 \quad (II.5.13.e)
 \end{aligned}$$

$$\begin{aligned}
 & \frac{\partial \rho v_3}{\partial t} + \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1 v_3) + \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2 v_3) \right. \\
 & \quad + \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_3^2) + h_2 \rho v_1 v_3 \frac{\partial h_3}{\partial x_1} + h_1 \rho v_2 v_3 \frac{\partial h_3}{\partial x_2} \\
 & \quad \left. - \left[h_2 \rho v_1^2 \frac{\partial h_1}{\partial x_3} + h_1 \rho v_2^2 \frac{\partial h_2}{\partial x_3} \right] \right\} + \frac{1}{2h_3} \frac{\partial P}{\partial x_3} \\
 & \quad + \left[\frac{B_1}{h_1 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right\} \right. \\
 & \quad \left. + \frac{B_2}{h_2 h_3} \left\{ \frac{\partial}{\partial x_3} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_3 B_3) \right\} \right] = 0 \quad (\text{II.5.13.f})
 \end{aligned}$$

$$\begin{aligned}
 & \frac{\partial \rho}{\partial t} + \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1) + \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2) \right. \\
 & \quad \left. + \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_3) \right\} = 0 \quad (\text{II.5.13.g})
 \end{aligned}$$

$$\begin{aligned}
 & \frac{\partial P}{\partial t} + \frac{\gamma}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 P v_1) + \frac{\partial}{\partial x_2} (h_1 h_3 P v_2) \right. \\
 & \quad + \frac{\partial}{\partial x_3} (h_1 h_2 P v_3) \left. \right\} - (\gamma - 1) \left[\left\{ \frac{v_1}{h_1} \frac{\partial P}{\partial x_1} + \frac{v_2}{h_2} \frac{\partial P}{\partial x_2} \right. \right. \\
 & \quad \left. \left. + \frac{v_3}{h_3} \frac{\partial P}{\partial x_3} \right\} + \frac{2\eta}{S} \left\{ \frac{1}{(h_2 h_3)^2} \left[\frac{\partial}{\partial x_2} (h_3 B_3) - \frac{\partial}{\partial x_3} (h_2 B_2) \right]^2 \right. \right. \\
 & \quad \left. \left. + \frac{1}{(h_1 h_3)^2} \left[\frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right]^2 \right. \right. \\
 & \quad \left. \left. + \frac{1}{(h_1 h_2)^2} \left[\frac{\partial}{\partial x_1} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_1 B_1) \right]^2 \right\} \right] = 0 \quad (\text{II.5.13.h})
 \end{aligned}$$

These are the equations that IMP uses to simulate plasma behavior. The next chapter will discuss how they are solved.

CHAPTER III

COMPUTATIONAL TECHNIQUES

III.1 Introduction

The nonlinear, time dependent, three-dimensional coupled set of MHD equations that were presented in Chapter II are solved via alternating direction implicit (ADI) finite difference techniques on a nonuniform Eulerian mesh. In this chapter, the implementation of these techniques in the IMP (Implicit MHD Program) code is discussed, including descriptions of the computational mesh, the ADI algorithm, and the spatial finite differencing. An improved technique for the linearization of the resulting nonlinear algebraic equations is also presented. The solution algorithm for the block tridiagonal matrices that arise from the implicit equations is derived for both periodic and nonperiodic boundary conditions. The boundary conditions that are implemented in IMP are described. Finally, the timestep size controls that have been implemented are presented.

The MHD equations (II.3.3) are expressed as

$$\frac{\partial \underline{U}(\underline{u})}{\partial t} + \underline{F}(\underline{u}) + \underline{G}(\underline{u}) + \underline{H}(\underline{u}) = 0 \quad (\text{III.1.1})$$

where $\underline{u} \equiv \{ \underline{B}, \underline{v}, \rho, P \}$ is the state variable of the system and $\underline{U}(\underline{u}) \equiv \{ \underline{B}, \rho \underline{v}, \rho, P \}$ are the quantities advanced in time. Notice that even the vector $\underline{U}$ is nonlinear and requires an eventual linearization. The advantage of using $\underline{u}$ as our state vector rather than using $\underline{U}$ as has been done previously³⁸ is that the velocity no longer needs to lag the solution in either time or iteration space.

We now define the three functions F, G, and H. The function F(u) contains all terms in Eqs. II.5.13 that have leading derivatives with respect to x_1 . By leading derivatives, we mean any of the following forms: (1) $\propto \frac{\partial \phi}{\partial x_1}$; (2) $\frac{\partial \alpha \phi}{\partial x_1}$; (3) $\propto \frac{\partial \phi}{\partial x_1} \frac{\partial \psi}{\partial x_2}$; (4) $\frac{\partial}{\partial x_1} \left(\propto \frac{\partial \phi}{\partial x_1} \right)$; or (5) $\frac{\partial}{\partial x_1} \left(\propto \frac{\partial \phi}{\partial x_2} \right)$ (note: all $\frac{\partial}{\partial x_2}$'s may be replaced by $\frac{\partial}{\partial x_3}$'s). Similarly, the functions G(u) and H(u) contain all the terms in Eqs. (II.3.12) that have leading derivatives with respect to x_2 and x_3 respectively. In the case of form 3 above, the term is split between both F and G by setting $\frac{\partial \phi}{\partial x_1} \frac{\partial \psi}{\partial x_2} = 1/2 \left(\frac{\partial \phi}{\partial x_1} \frac{\partial \psi}{\partial x_2} + \frac{\partial \psi}{\partial x_2} \frac{\partial \phi}{\partial x_1} \right)$. The functions, then, are:

(III.1.2)

$$F_1(u) = 0$$

$$F_2(u) = \frac{1}{h_1 h_3} \frac{\partial}{\partial x_1} \left\{ h_3 \left(B_2 v_1 - B_1 v_2 - \frac{\eta}{S} \frac{1}{h_1 h_2} \right. \right. \\ \left. \left. \times \left[\frac{\partial}{\partial x_1} (h_2 B_2') - \frac{\partial}{\partial x_2} (h_1 B_2') \right] \right) \right\}$$

$$F_3(u) = \frac{1}{h_1 h_2} \frac{\partial}{\partial x_1} \left\{ h_2 \left(B_3 v_1 - B_1 v_3 - \frac{\eta}{S} \frac{1}{h_1 h_3} \right. \right. \\ \left. \left. \times \left[\frac{\partial}{\partial x_1} (h_3 B_3') - \frac{\partial}{\partial x_3} (h_1 B_1') \right] \right) \right\}$$

$$F_4(u) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} \left(h_2 h_3 v_1^2 \right) - \left[h_3 v_2^2 \frac{\partial h_2}{\partial x_1} \right. \right. \\ \left. \left. + h_2 v_3^2 \frac{\partial h_3}{\partial x_1} \right] \right\} + \frac{1}{2 h_1} \frac{\partial P}{\partial x_1} + \frac{B_2}{h_1 h_2} \frac{\partial}{\partial x_1} (h_2 B_2) \\ + \frac{B_3}{h_1 h_3} \frac{\partial}{\partial x_1} (h_3 B_3)$$

$$F_5(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1 v_2) + h_3 \rho v_1 v_2 \frac{\partial h_2}{\partial x_1} \right\} \\ - \frac{B_1}{h_1 h_2} \frac{\partial}{\partial x_1} (h_2 B_2)$$

$$F_6(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1 v_3) + h_2 \rho v_1 v_3 \frac{\partial h_3}{\partial x_1} \right\} \\ - \frac{B_1}{h_1 h_3} \frac{\partial}{\partial x_1} (h_3 B_3)$$

$$F_7(\underline{u}) = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1)$$

$$F_8(\underline{u}) = \frac{\gamma}{h_1 h_2 h_3} \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1) - (\gamma - 1) \left[\frac{v_1}{h_1} \frac{\partial p}{\partial x_1} \right. \\ + \frac{2\eta}{S} \left\{ \frac{1}{(h_1 h_3)^2} \frac{\partial (h_1 B_3)}{\partial x_1} \left(\frac{\partial (h_3 B_3)}{\partial x_1} - \frac{\partial (h_1 B_1)}{\partial x_3} \right) \right. \\ \left. \left. + \frac{1}{(h_1 h_2)^2} \frac{\partial (h_2 B_2)}{\partial x_1} \left(\frac{\partial h_2 B_2}{\partial x_1} - \frac{\partial (h_1 B_1)}{\partial x_2} \right) \right\} \right]$$

and

(III.1.3)

$$G_1(\underline{u}) = \frac{1}{h_2 h_3} \frac{\partial}{\partial x_2} \left\{ h_3 \left(\rho v_1 v_2 - B_2 v_1 - \frac{\eta}{S} \frac{1}{h_1 h_2} \left[\frac{\partial}{\partial x_2} (h_1 B_1) \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_1} (h_2 B_2) \right) \right] \right\}$$

$$G_2(\underline{u}) = 0$$

$$G_3(\underline{u}) = \frac{1}{h_1 h_2} \frac{\partial}{\partial x_2} \left\{ h_1 \left(B_3 v_2 - B_2 v_3 - \frac{n}{s} \frac{1}{h_2 h_3} \left[\frac{\partial}{\partial x_2} (h_3 B_3) \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_3} (h_2 B_2) \right] \right) \right\}$$

$$G_4(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_1 v_2) + h_3 \rho v_1 v_2 \frac{\partial h_1}{\partial x_2} \right\} \\ - \frac{B_2}{h_1 h_2} \frac{\partial}{\partial x_2} (h_1 B_1)$$

$$G_5(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2^2) - \left[h_3 \rho v_1^2 \frac{\partial h_1}{\partial x_2} \right. \right. \\ \left. \left. + h_1 \rho v_3^2 \frac{\partial h_3}{\partial x_2} \right] \right\} + \frac{1}{2h_2} \frac{\partial p}{\partial x_2} + \frac{B_1}{h_1 h_2} \frac{\partial}{\partial x_2} (h_1 B_1) \\ + \frac{B_3}{h_2 h_3} \frac{\partial}{\partial x_2} (h_3 B_3)$$

$$G_6(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2 v_3) + h_1 \rho v_2 v_3 \frac{\partial h_3}{\partial x_2} \right\} \\ - \frac{B_2}{h_2 h_3} \frac{\partial}{\partial x_2} (h_3 B_3)$$

$$G_7(\underline{u}) = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_2)$$

$$G_8(\underline{u}) = \frac{\gamma}{h_1 h_2 h_3} \frac{\partial}{\partial x_2} (h_1 h_3 P v_2) - (\gamma - 1) \left[\frac{v_2}{h_2} \frac{\partial P}{\partial x_2} \right. \\ \left. + \frac{2\eta}{S} \left\{ \frac{1}{(h_1 h_3)^2} \frac{\partial (h_3 B_3)}{\partial x_2} \left(\frac{\partial (h_3 B_3)}{\partial x_2} - \frac{\partial (h_2 B_2)}{\partial x_3} \right) \right. \right. \\ \left. \left. + \frac{1}{(h_1 h_2)^2} \frac{\partial (h_1 B_1)}{\partial x_2} \left(\frac{\partial (h_1 B_1)}{\partial x_2} - \frac{\partial (h_2 B_2)}{\partial x_1} \right) \right\} \right]$$

and, finally,

(III.1.4)

$$H_1(\underline{u}) = \frac{1}{h_2 h_3} \frac{\partial}{\partial x_3} \left\{ h_2 \left(B_1 v_3 - B_3 v_1 - \frac{\eta}{S} \frac{1}{h_1 h_3} \left[\frac{\partial}{\partial x_3} (h_1 B_1) \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_1} (h_3 B_3) \right] \right) \right\}$$

$$H_2(\underline{u}) = \frac{1}{h_1 h_3} \frac{\partial}{\partial x_3} \left\{ h_1 \left(B_2 v_3 - B_3 v_2 - \frac{\eta}{S} \frac{1}{h_2 h_3} \left[\frac{\partial}{\partial x_3} (h_2 B_2) \right. \right. \right. \\ \left. \left. \left. - \frac{\partial}{\partial x_2} (h_3 B_3) \right] \right) \right\}$$

$$H_3(\underline{u}) = 0$$

$$H_4(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_1 v_3) + h_2 \rho v_1 v_3 \frac{\partial h_1}{\partial x_3} \right\} \\ - \frac{B_3}{h_1 h_3} \frac{\partial}{\partial x_3} (h_1 B_1)$$

$$H_5(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_2 v_3) + h_1 \rho v_2 v_3 \frac{\partial h_2}{\partial x_3} \right\} \\ - \frac{B_3}{h_2 h_3} \frac{\partial}{\partial x_3} (h_2 B_2)$$

$$H_6(\underline{u}) = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_3} h_1 h_2 \rho v_3^2 - \left[h_2 \rho v_1^2 \frac{\partial h_1}{\partial x_3} \right. \right. \\ \left. \left. + h_1 \rho v_2^2 \frac{\partial h_2}{\partial x_3} \right] \right\} + \frac{1}{2h_3} \frac{\partial P}{\partial x_3} + \frac{B_1}{h_1 h_3} \frac{\partial}{\partial x_3} (h_1 B_1) \\ + \frac{B_2}{h_2 h_3} \frac{\partial}{\partial x_3} (h_2 B_2)$$

$$H_7(\underline{u}) = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_3)$$

$$H_8(\underline{u}) = \frac{\gamma}{h_1 h_2 h_3} \frac{\partial}{\partial x_3} (h_1 h_2 P v_3) - (\gamma - 1) \left[\frac{v_3}{h_3} \frac{\partial P}{\partial x_3} \right. \\ \left. + \frac{2\eta}{S} \left\{ \frac{1}{(h_2 h_3)^2} \frac{\partial}{\partial x_3} (h_2 B_2) \left(\frac{\partial}{\partial x_3} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_3 B_3) \right) \right. \right. \\ \left. \left. + \frac{1}{(h_1 h_3)^2} \frac{\partial}{\partial x_3} (h_1 B_1) \left(\frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right) \right\} \right]$$

Careful examination of F, G, and H reveals an extremely useful symmetry. If all 1 subscripts in F are interchanged with all 2 subscripts, F becomes identical to G. In a similar fashion, a 1,3 interchange on F yields H. We utilize this feature of the equations to greatly simplify our

coding in IMP. Finally, one component of the magnetic field equation is zero in each of the functions, $\underline{F}$, $\underline{G}$, and $\underline{H}$. This reduces the number of equations that need to be solved simultaneously at each mesh point from 8 to 7, a savings of 20% on the work required per mesh point (work scales as n^2).

III.1.1.1 Basic Numerical Analysis

We now introduce some concepts from numerical analysis that will be referred to throughout the remainder of this thesis. For ease of notation, this section will deal with representations in only one spatial dimension. The extension of these concepts to two and three spatial dimensions is relatively straightforward and will be deferred to later.

We begin with a continuous set of functions $\underline{U}(x,t)$ which are defined on the domain (X_1, X_2) . The domain is represented as a set of discrete points x_i , $1 \leq i \leq I$, such that

$$x_i = X_1 + \sum_{j=1}^{i-1} \Delta x_j \quad (\text{III.1.1.1})$$

where

$$\Delta x_j \equiv x_j - x_{j-1} \quad (\text{III.1.1.2})$$

The points x_i form a mesh or a grid. The mesh points themselves may move with some velocity v_G with respect to an observer who is stationary in the laboratory frame. If this velocity is zero, the

mesh is called Eulerian. If the velocity v_G equals the velocity of the fluid at all points on the mesh, the mesh is called Lagrangian. Since the velocity v_G may, in general, vary from the two above limits, a mesh that explicitly contains the grid velocity in its definition is called a generalized mesh.

Time is also discretized so that

$$t^n = t^\phi + \sum_{j=0}^{n-1} \Delta t^j \quad (\text{III.1.1.3})$$

where t^ϕ is some initial time (usually 0) and

$$\Delta t^j \equiv t^j - t^{j-1} \quad (\text{III.1.1.4})$$

The continuous functions $\underline{U}(x,t)$ are now expressed as the discrete functions $\underline{U}_i^n \equiv \underline{U}(x_i, t^n)$.

We are interested in solving the initial value problem in which we are given $\underline{U}_i^n$ for all i and want to know $\underline{U}_i^{n+1}$. In order to advance from time $t = t^n$ and $t = t^{n+1}$ we must solve the system of m coupled partial differential equations

$$\frac{\partial \underline{U}(x,t)}{\partial t} = \underline{N}(\underline{U}(x,t), x, t) \quad (\text{III.1.1.5})$$

where $\underline{N}$ is some set of m (possibly nonlinear) spatial differential operators. This system is replaced by a set of $m \times I$ (possibly

coupled) algebraic equations via finite difference techniques. These may be represented by

$$\begin{aligned} \underline{u}_i^{n+1} = & \underline{u}_i^n + \Delta t \left((1 - \theta) \left(N \underline{u}_{i+1}^n, \underline{u}_i^n, \underline{u}_{i-1}^n, x_i, t^n \right) \right. \\ & \left. + \theta \left(N \underline{u}_{i+1}^{n+1}, \underline{u}_i^{n+1}, \underline{u}_{i-1}^{n+1}, x_i, t^{n+1} \right) \right) \end{aligned} \quad (\text{III.1.1.6})$$

where $0 \leq \theta \leq 1$.

If θ equals zero, then the $\underline{u}_i^{n+1}$ are not coupled with any other $\underline{u}^{n+1}$ values and is an explicit time advance algorithm. In this case, the advance to the new time level requires only the solution of $m \times I$ uncoupled algebraic equations. Since the value of $\underline{u}_i^{n+1}$ is a function of only $\underline{u}_{i+1}^n$, $\underline{u}_i^n$, $\underline{u}_{i-1}^n$, we see that information can only propagate one spatial zone per time advance (timestep). We, then, can expect this to put an upper limit on the size of an explicit timestep. This limit is called a Courant-Fredricks-Lewy (CFL) condition and it must be met in every zone of the problem otherwise numeric instabilities will ensue.

If we consider Eq. (III.1.1.5) to be simple advection equation

$$\frac{\partial \underline{u}}{\partial t} = -v \frac{\partial \underline{u}}{\partial x}, \quad (\text{III.1.1.7})$$

where v is a constant velocity of the advection, the CFL condition is

$$\Delta t \leq \frac{\Delta x}{|v|} \quad (\text{III.1.1.8})$$

This condition ensures that the velocity of the physical process (the advection) is less than the velocity of information transmittal on the mesh. In the case of the MHD equations, the characteristic physical velocity is the Alfven velocity (v_A) which is proportional to the magnetic flux (B) and inversely proportional to the square root of the density (ρ) ($v_A \propto B/\sqrt{\rho}$). In general, areas of high magnetic flux tend to have low densities--thus leading to very large Alfven velocities. These high flux-low density zones generally are not where the interesting physics is occurring but they can severely limit the allowable explicit timestep.

Similarly, if Eq. (III.1.1.5) is the diffusion equation

$$\frac{\partial U}{\partial t} = D \frac{\partial^2 U}{\partial x^2} , \quad (\text{III.1.1.9})$$

where D is a constant coefficient of diffusion, the CFL condition is

$$\Delta t \leq \frac{(\Delta x)^2}{2D} . \quad (\text{III.1.1.10})$$

In this case, we see that the mesh spacing Δx can be a significant limit on the allowable timestep. If we halve the mesh spacing (double the number of mesh points), we cut the maximum allowable timestep by a factor of four. Thus, we must perform eight times as much work to follow the equation for the same amount of simulation time.

In order to bypass these strict limitations on timestep size, we may let θ in Eq. (III.1.1.6) be greater than or equal to one half ($\theta \geq 1/2$). In this case, the values of $\underline{u}_i^{n+1}$ are fully coupled together and the velocity of information transmittal on the mesh is infinite⁷ and is termed an implicit time advancement algorithm. In the case of (III.1.1.5) being a set of linear equations, any time step size will be stable; and even when $\underline{N}$ in (III.1.1.5) is a nonlinear operator, we may expect an improvement in the maximum allowable timestep size. The price paid here is that the $m \times I$ system of equations are coupled which necessitates the inversion of a $(m \times I) \times (m \times I)$ matrix (i.e., $\underline{A} \underline{u}^{n+1} = \underline{B}$). This inversion requires of order $(m \times I)^3$ arithmetic operations.⁶¹ For the MHD equations, m is equal to eight (see Chapter II). If we consider a 100 point mesh, this is 5.12×10^8 operations. A CDC-7600 computer can perform 3×10^6 operations per second which says that we may invert this matrix in a little under 2-1/2 minutes. While this rate seems to be expensive, yet feasible, consider a three-dimensional mesh with $20 \times 20 \times 20$ points. Here we would have a 64000×64000 matrix ($m \times I \times J \times K$) to invert-- 10^{14} operations or over 7200 hours per inversion.

These times can be decreased by many orders of magnitude by examining the structure of the matrix $\underline{A}$ to be inverted. In the one-dimensional case, we see that $\underline{u}_i^{n+1}$ is directly coupled only to $\underline{u}_{i+1}^{n+1}$, $\underline{u}_i^{n+1}$ and $\underline{u}_{i-1}^{n+1}$. Thus, the matrix $\underline{A}$ to be inverted has a block tri-diagonal structure (see Fig. III.1), where each block element is a $m \times m$ submatrix.

$$\underline{A} = \begin{pmatrix} \underline{a}_{11} & \underline{a}_{12} & & & \\ \underline{a}_{21} & \underline{a}_{22} & \underline{a}_{23} & & \\ & \underline{a}_{32} & \underline{a}_{33} & \underline{a}_{34} & \\ & & \underline{a}_{n-1,n-2} & \underline{a}_{n-1,n-1} & \underline{a}_{n-1,n} \\ & & & \underline{a}_{n,n-1} & \underline{a}_{n,n} \end{pmatrix}$$

$$\underline{a}_{i,j} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \dots & \alpha_{1,m} \\ \vdots & \vdots & & \vdots \\ \alpha_{21} & & & \\ \vdots & & & \\ \alpha_{m,1} & & & \alpha_{m,m} \end{pmatrix}$$

Figure III.1

The block tridiagonal matrix structure found in the one-dimensional, three point finite difference equations.

In Section III.4, we develop the algorithm used which takes advantage of the tridiagonal structure to reduce the operations needed for inversion by a factor of I^2 to an $I \times m^3$ dependence. This reduction is accomplished by the need to do full matrix inversions on only one submatrix-sized structure per mesh point. Thus, our 2 minute one-dimensional timestep will now take only 17 seconds. For three-dimensions, this reduction will not work, as we do not have a block tridiagonal matrix with which to work. The best reduction we can achieve is to treat the matrix $\underline{A}$ as a banded matrix. Here the operation count will go as $(m \times I \times J \times K)^2$, ⁶² 68 hours of computer time.

We may, however, use alternating direction implicit techniques (ADI) to achieve a reasonable running time. In this case, we express the three-dimensional problem as three problems in which we advance only one dimension at a time implicitly (see Section III.4 for further details). This technique takes our 64000 x 64000 matrix and reduces it to $3 \times 20^3 \times (8 \times 8)$ matrices yielding a running time of 41 seconds on a CDC-7600 computer. We have assumed here that the problem is linear. Since the MHD equations are nonlinear, we will have to iterate our solutions to assure that we correctly solve the equations. Thus, we may expect running times of 1 to 3 (or more) minutes of 7600 time per timestep.

In the previous discussion, we have not given any criterion for the accuracy of our solution. While it is necessary to have a stable algorithm, it is also necessary to have an accurate one. If we define some factor e , which represents the truncation error of our finite difference equation, as⁶³

$$e = [\text{differential equation}]_{ij}^n - [\text{difference equation}]_{ij}^n \quad (\text{III.1.1.11})$$

then we wish the error to be expressed as some power of the spatial and temporal mesh sizes.

$$e = O(\Delta t^A) + O(\Delta x^B) + O(\Delta y^C) + O(\Delta z^D) \quad (\text{III.1.1.12})$$

The exponents A, B, C, and D are integers greater than zero. We arrive at this accuracy ordering by using Taylor series expansions for our finite difference equations and then subtracting off the original partial differential equation. It is shown in Richtmyer and Morton⁶ that, for the normal centered spatial finite difference approximations on a uniform mesh, the spatial error is of order (Δx^2) . If we allow θ in Eq. (III.1.1.6) to be one-half, we get the so-called Crank-Nickolson time weighting which is also of order (Δt^2) accurate. Thus, we will have the total error as

$$e = O(\Delta t^2) + O(\Delta x^2) + O(\Delta y^2) + O(\Delta z^2) \quad . \quad (\text{III.1.1.13})$$

Our accuracy is only limited by the number of mesh points and by the maximum timestep size we are willing to use. In the limit $\Delta x, \Delta t \rightarrow 0$, the finite difference equation reduces to the partial differential equation.

III.2 The Computational Mesh

As was stated previously, IMP uses an Eulerian mesh. The values of the state variable $\underline{u}$, where $\underline{u} = \{B, v, \rho, P\}$, are kept on a set of points in space called mesh points. The values of $\underline{u}$ are to be cell centered quantities. By cell centered we mean that the value of $\underline{u}_{i,j,k}$ is the average value of u in the three-dimensional cell centered at $(x_{1_i}, x_{2_j}, x_{3_k})$. The mesh is shown in Fig. III.2 and is examined on a single plane in Fig. III.3. In Fig. III.2, the dots represent the points at which the values of $\underline{u}$ are stored and the triangles represent the interface points at

Figure III.2

Figure III.3

which fluxes and forces are to be evaluated. We define here some quantities and operators that are to be used in the rest of this chapter. We adopt the convention that all unvaried subscripts are deleted ($u_{i+1,j,k} \rightarrow u_{i+1}$).

First, we define $\Delta_{n\pm}$ as the distance between points x_{n_i} and $x_{n_{i\pm 1}}$, where $x_n = (x_1, x_2, x_3)$ are some orthogonal curvilinear coordinates,

$$\left. \begin{aligned} \Delta_{1+} &= x_{1_{i+1}} - x_{1_i} , \\ \Delta_{1-} &= x_{1_i} - x_{1_{i-1}} , \\ \Delta_{2+} &= x_{2_{j+1}} - x_{2_j} , \\ \Delta_{2-} &= x_{2_j} - x_{2_{j-1}} , \\ \Delta_{3+} &= x_{3_{k+1}} - x_{3_k} , \\ \Delta_{3-} &= x_{3_k} - x_{3_{k-1}} . \end{aligned} \right\} \quad (\text{III.2.1})$$

These variable Δ 's allow us to specify a nonuniform mesh. Next, the distance between interfaces which is called Δ_n are given as

$$\left. \begin{aligned} 1\Delta &= \frac{1}{2} (\Delta_{1+} + \Delta_{1-}) = x_{1_{i+1/2}} - x_{1_{i-1/2}} \\ 2\Delta &= \frac{1}{2} (\Delta_{2+} + \Delta_{2-}) = x_{2_{j+1/2}} - x_{2_{j-1/2}} \\ 3\Delta &= \frac{1}{2} (\Delta_{3+} + \Delta_{3-}) = x_{3_{k+1/2}} - x_{3_{k-1/2}} \end{aligned} \right\} \quad (\text{III.2.2})$$

The value of a variable at the interface is expressed by a bar (-) operator, such that

$$\left. \begin{aligned} \bar{Q}_{1+} &= \frac{1}{2} (Q_{1+1} + Q_1) \\ \bar{Q}_{2+} &= \frac{1}{2} (Q_{j+1} + Q_j) \\ \bar{Q}_{3+} &= \frac{1}{2} (Q_{k+1} + Q_k) \end{aligned} \right\} \text{(III.2.3)}$$

The + operator gives the difference across an interface:

$$\left. \begin{aligned} \bar{F}_{1+}(F) &= \frac{1}{\Delta_{1+}} (F_{i+1} - F_i) \\ \bar{F}_{1-}(F) &= \frac{1}{\Delta_{1-}} (F_i - F_{i-1}) \\ \bar{F}_{2+}(F) &= \frac{1}{\Delta_{2+}} (F_{j+1} - F_j) \\ \bar{F}_{2-}(F) &= \frac{1}{\Delta_{2-}} (F_j - F_{j-1}) \\ \bar{F}_{3+}(F) &= \frac{1}{\Delta_{3+}} (F_{k+1} - F_k) \\ \bar{F}_{3-}(F) &= \frac{1}{\Delta_{3-}} (F_k - F_{k-1}) \end{aligned} \right\} \text{(III.2.4)}$$

III.3. Spatial Finite Differencing

The MHD Eqs. (II.5.13) contain two basic types of terms. The first type are terms that arise from the divergence of fluxes in the conservation law equations. This includes the pseudovector conservation law of the magnetic flux equation. In the expanded equations, all terms of the form $\frac{\partial}{\partial x_1} (\alpha \phi)$, where ϕ is any general factor, all called FLUX terms. For example, ϕ may be $\frac{\partial \psi}{\partial x_2}$. Thus both plane second derivatives and mixed second derivatives are subsets of the FLUX terms. The second type of term that appears in the (II.5.13) has the form $\alpha \frac{\partial u}{\partial x_1}$ where α is some function of $\underline{u}$. For example, in the momentum equation, we see terms of the form $B \frac{\partial B}{\partial x_1}$ and $\frac{\partial P}{\partial x_1}$ which arise from the $\underline{J} \times \underline{B}$ forces and the pressure gradient forces. Terms of this form also appear in the energy equation (i.e., $v \frac{\partial P}{\partial x_1}$ and $\frac{u}{S} \frac{\partial B}{\partial x_1} \frac{\partial B}{\partial x_2}$). These are categorized as FORCE terms. It is to be stressed that the titles FLUX and FORCE are used to categorize the form of the terms to be differenced and not to label their physical significance.

When we set up our spatial finite differencing, we are representing a system of equations that describe changes to our cell-centered quantities due to fluxes into and out of the cells and forces applied to the cells. Both these fluxes and forces must be calculated at the cell interfaces (see Fig. III.3, triangles). Based on this scheme, we use the following techniques for generating the finite approximations.

III.3.1 Flux Term Differencing

The FLUX terms measure flow into or out of the computational cell. Therefore, these terms must be evaluated at the cell boundaries. Thus,

the finite difference form is

$$\frac{\partial}{\partial x_1} (\alpha F) \rightarrow \frac{\bar{\alpha}_+ \bar{F}_+ - \bar{\alpha}_- \bar{F}_-}{1\Delta} \quad (\text{III.3.1.1})$$

where we use the definitions of Section III.2 for 1Δ and the $\bar{}$ (bar) operator.

When F represents a derivative $\left(F = \frac{\partial G}{\partial x_1}\right)$, we use

$$\frac{\partial}{\partial x_1} \left(\alpha \frac{\partial G}{\partial x_1} \right) = \frac{\bar{\alpha}_+ \delta_{1+}(G) - \bar{\alpha}_- \delta_{1-}(G)}{1\Delta} \quad (\text{III.3.1.2})$$

The δ operator (Section III.2) is the difference across the interface, evaluated at the interface, so we have a consistent approximation. If we assume that we are on a uniform mesh and α is a constant, the definitions given in Eqs. III.3.1.1 and III.3.1.2 reduce to the normal first and second derivative finite difference approximations:

$$\frac{\partial}{\partial x_1} (\alpha F) = \alpha \frac{F_{i+1} - F_{i-1}}{2\Delta x} \quad (\text{III.3.1.3.a})$$

and

$$\frac{\partial}{\partial x_1} \left(\alpha \frac{\partial G}{\partial x_1} \right) = \alpha \frac{G_{i+1} - 2G_i + G_{i-1}}{(\Delta x)^2} \quad (\text{III.3.1.3.b})$$

In the case of mixed derivatives,

$$F = \frac{\partial G}{\partial x_2}, \quad (\text{III.3.1.4})$$

we take the derivative in the x_2 direction at points A_+ , A_- , B_+ and B_- in Fig. III.4 and average them to arrive at a value of $\bar{F}$ at a cell face (x). This gives

$$\frac{\partial}{\partial x_1} \left(\alpha \frac{\partial G}{\partial x_2} \right) = \frac{\bar{\alpha}_+ \left(\frac{\partial G}{\partial x_2} \right)_+ - \bar{\alpha}_- \left(\frac{\partial G}{\partial x_2} \right)_-}{\Delta_1}, \quad (\text{III.3.1.5})$$

i-1, j+1 ○	i, j+1 ○ A_+	i+1, j+1 ○ B_+
i-1, j ○	i, j ○ A_-	i+1, j ○ B_-
i-1, j-1 ○	i, j-1 ○	i+1, j-1 ○
○	○	○

Figure III.4. Mixed Derivative Calculation

where

$$\begin{aligned} \left(\frac{\partial G}{\partial x_2} \right)_+ &= \frac{1}{4} \left([G_{i+1,j+1} - G_{i+1,j} + G_{i,j+1} - G_{i,j}] / \Delta_{2+} \right. \\ &\quad \left. + [G_{i+1,j} - G_{i+1,j-1} + G_{i,j} - G_{i,j-1}] / \Delta_{2-} \right) \end{aligned} \quad (\text{III.3.1.6})$$

Notice that terms are evaluated at the center of the interfaces in all cases.

From the preceding, it can be seen that the FLUX terms are anti-symmetric. That is, the flux $\underline{F}_+$ at the i th grid point becomes minus the flux $\underline{F}_-$ in the $i+1$'s grid point. Therefore, the flux $\underline{F}_+$ is calculated when we are at the i th grid point and is reused as $-\underline{F}_-$ at the next grid point. This double use of $\underline{F}$ allows us to avoid extra calculations and also the extra FORTRAN required for the calculations. This is one less chance for errors to come into the code.

III.3.2 Force Term Differencing

The FORCE terms measure the forces applied on the edges of the computational cell. As such, we define them as the average of the forces applied on each cell face. The finite difference form is

$$\alpha \frac{\partial F}{\partial x_1} = \frac{1}{2} \left(\bar{\alpha}_+ \delta_{1+}(F) + \bar{\alpha}_- \delta_{1-}(F) \right) \quad (\text{III.3.2.1})$$

where the δ_{1+} operator has been defined in Section III.2.

Products of derivatives arise from the η_j^2 terms in the internal energy equation. This product can be put in the form of

$$\alpha \frac{\partial F}{\partial x_1} \rightarrow \frac{\partial G}{\partial x_2} \frac{\partial F}{\partial x_1} = \frac{1}{2} \left[\left(\frac{\partial G}{\partial x_2} \right)_{i+1/2} \delta_{1+}(F) + \left(\frac{\partial G}{\partial x_2} \right)_{i-1/2} \delta_{1-}(F) \right] \quad (\text{III.3.2.2})$$

The term $\left(\frac{\partial G}{\partial x_2} \right)_{i+1/2}$ is evaluated in an identical fashion to $\left(\frac{\partial G}{\partial x_2} \right)_{i+1/2}$ in the FLUX terms (see Eq. III.3.6.3).

The main problem with the mixed derivative and product of derivative terms comes in attempting to correctly time-center them. This will be addressed in the next section.

As the FLUX terms are antisymmetric, the FORCE terms are symmetric. In this case $\underline{F}_+$ at the i th grid point is equal to $\underline{F}_-$ at the $i + 1$ 'st grid point. Once again, this property is taken advantage of in the IMP code.

III.4 Temporal Finite Differencing

As was noted in Chapter I, IMP uses the Douglas-Gunn⁵ algorithm (DGA) for controlling its time advance. The DGA is an extension of normal alternating direction implicit (ADI) techniques to three dimensions. These ADI techniques allow for the solution of the large 3-D matrix problem in reasonable amounts of computer time.

We express the set of MHD equations as the vector equation

$$\frac{\partial \underline{U}(\underline{u})}{\partial t} + \underline{F}(\underline{u}) + \underline{G}(\underline{u}) + \underline{H}(\underline{u}) = 0 \quad (\text{III.4.1})$$

where $\underline{U}$ is the set $\left\{ \underline{B}, \rho \underline{v}, \rho, P \right\}$, $\underline{u}$ is the set $\left\{ \underline{B}, \underline{v}, \rho, P \right\}$ and $\underline{F}(\underline{u})$, $\underline{G}(\underline{u})$ and $\underline{H}(\underline{u})$ are given in Eqs. III.1.2, III.1.3, and III.1.4 respectively. Then the time centering DGA technique yields the three step approach:

$$\frac{\underline{U}^{n*} - \underline{U}^n}{\Delta t} + \frac{1}{2} [\underline{F}(\underline{u}^{n*}) + \underline{F}(\underline{u}^n)] + \underline{G}(\underline{u}^n) + \underline{H}(\underline{u}^n) = 0 \quad (\text{III.4.2})$$

$$\left. \begin{aligned}
 & \frac{\underline{u}^{n**} - \underline{u}^n}{\Delta t} + \frac{1}{2} [\underline{F}(\underline{u}^{n*}) + \underline{F}(\underline{u}^n) + \underline{G}(\underline{u}^{n**}) + \underline{G}(\underline{u}^n)] \\
 & + \underline{H}(\underline{u}^n) = 0 \\
 & \frac{\underline{u}^{n+1} - \underline{u}^n}{\Delta t} + \frac{1}{2} [\underline{F}(\underline{u}^{n*}) + \underline{F}(\underline{u}^n) + \underline{G}(\underline{u}^{n**}) + \underline{G}(\underline{u}^n) \\
 & + \underline{H}(\underline{u}^{n+1}) + \underline{H}(\underline{u}^n)] = 0
 \end{aligned} \right\} \begin{array}{l} \text{(III.4.2)} \\ \text{(continued)} \end{array}$$

Equations III.4.2 are combined to yield the final set

$$\frac{\underline{u}^{n*} - \underline{u}^n}{\Delta t} + \frac{1}{2} (\underline{F}(\underline{u}^{n*}) + \underline{F}(\underline{u}^n)) + \underline{G}(\underline{u}^n) + \underline{H}(\underline{u}^n) = 0 \quad \text{(III.4.3.a)}$$

$$\frac{\underline{u}^{n**} - \underline{u}^{n*}}{\Delta t} + \frac{1}{2} (\underline{G}(\underline{u}^{n**}) - \underline{G}(\underline{u}^n)) = 0 \quad \text{(III.4.3.b)}$$

$$\frac{\underline{u}^{n+1} - \underline{u}^{n**}}{\Delta t} + \frac{1}{2} (\underline{H}(\underline{u}^{n+1}) - \underline{H}(\underline{u}^n)) = 0 \quad \text{(III.4.3.c)}$$

The set of equations III.4.3 describe the time advancement scheme employed in IMP. Equation III.4.3.a may be thought of as a predictor step while III.4.3.b and III.4.3.c are corrector steps. By assuming particular forms for the $\underline{F}$, $\underline{G}$ and $\underline{H}$ in III.4.2, we can arrive at linear stability criterion for DGA. If we let $\underline{F}$, $\underline{G}$ and $\underline{H}$ be diffusion or advection terms, then DGA is linearly unconditionally stable.⁶ The linear unconditional stability is the reason for choosing an implicit time advancement scheme. We are able to let the relevant physics determine our timestep rather than being limited by numeric considerations.

The (1,2) and (1,3) symmetry pointed out in Section III.1 allows us to use identical paths to calculate the F function in III.4.3.a, the G function in III.4.3.b and the H function in III.4.3.c. Therefore, except for the sign change in the explicit function evaluation in the second and third equations and the cross line and cross plane G and H functions in the first equation, we can use identical code for all three subtrimesteps.

The accuracy of the algorithm is found by eliminating $\underline{u}^{n*}$ and $\underline{u}^{n**}$ from the third equation of III.4.2. By defining the following relationships,

$$\Delta \underline{u} = \underline{u}^{n+1} - \underline{u}^n \quad (\text{III.4.4})$$

$$\underline{u}^{n+1/2} \equiv \frac{1}{2} (\underline{u}^{n+1} + \underline{u}^n) \quad (\text{III.4.5})$$

we express $\underline{u}^{n*}$ and $\underline{u}^{n**}$ as

$$\underline{u}^{n*} = \underline{u}^{n+1} + \frac{\Delta t}{2} \left\{ (\underline{G}(\Delta \underline{u}) + \underline{H}(\Delta \underline{u})) + \frac{\Delta t}{2} \underline{G}(\underline{H}(\Delta \underline{u})) \right\} \quad (\text{III.4.6})$$

and

$$\underline{u}^{n**} = \underline{u}^{n+1} + \frac{\Delta t}{2} \underline{H}(\Delta \underline{u}) \quad (\text{III.4.7})$$

Then we have

$$\begin{aligned} & \frac{\underline{u}^{n+1} - \underline{u}^n}{\Delta t} + \underline{F}(\underline{u}^{n+1/2}) + \underline{G}(\underline{u}^{n+1/2}) + \underline{H}(\underline{u}^{n+1/2}) \\ & + \frac{\Delta t}{4} \left\{ \underline{F}(\underline{G}(\Delta \underline{u}) + \underline{H}(\Delta \underline{u})) + \underline{G}(\underline{H}(\Delta \underline{u})) \right\} \\ & + \frac{\Delta t^2}{8} \underline{F}(\underline{G}(\underline{H}(\Delta \underline{u}))) = 0 \quad . \end{aligned} \quad (\text{III.4.8})$$

The first term is the finite difference of $\underline{u}$ time centered at $\underline{u}^{n+1/2}$. The second term is a Crank-Nicholson weighted term which is correct to order Δt^2 . The third term is of order Δt^2 and the fourth of order Δt^3 . Hence the overall time advance algorithm's accuracy is of order Δt^2 . Since the spatial finite differences that make up $\underline{F}$, $\underline{G}$, and $\underline{H}$ are of order Δx_1^2 , Δx_2^2 and Δx_3^2 on a uniform mesh, the overall accuracy for our FDE's (neglecting the mixed derivative and product of derivative terms) is

$$\begin{aligned} e = & O(\Delta t^2) + O(\Delta x_1^2) + O(\Delta x_2^2) + O(\Delta x_3^2) + \\ & O(\Delta x_1 \Delta x_2) + O(\Delta x_1 \Delta x_3) + O(\Delta x_2 \Delta x_3) \end{aligned} \quad (\text{III.4.9})$$

The forms of $\underline{F}$, $\underline{G}$ and $\underline{H}$ in Eq. (III.1.1) are well defined for all but the mixed and product derivatives. Here, we are faced with trying to get advanced time values on rows of the mesh not yet computed. Killeen and Marx⁶⁴ split the time dependence of the cross-line (e.g., x_2 derivatives on an x_1 sweep) derivatives to take the δ_{2-} terms, assuming the calculation was proceeding up the plane, implicitly and the δ_{2+} terms explicitly. One would

then sweep downward on the next sweep to obtain time centering on these terms. One drawback of this method is that the mixed derivative terms are not being calculated in a conservative manner. This may be seen by looking at the term across two rows of the mesh. We will take $\frac{\partial}{\partial x_1} \left(a \frac{\partial F}{\partial x_2} \right)$ on lines j and $j+1$. On line j we have, looking at the $i+1/2$ interface only,

$$\begin{aligned} \frac{\partial}{\partial x_1} \left(a \frac{\partial F}{\partial x_2} \right)^{n*} \Big|_{x_1=x_{1,i+1/2}, x_2=x_2} = \\ \bar{a}_{1+,2+} \left[\delta_{2+,i} (F^n) + \delta_{2+,i+1} (F^n) \right] \\ + \bar{a}_{1+,2-} \left[\delta_{2-,i} (F^{n*}) + \delta_{2-,i+1} (F^{n*}) \right] \end{aligned} \quad (III.4.10)$$

and

$$\begin{aligned} \frac{\partial}{\partial x_1} \left(a \frac{\partial F}{\partial x_2} \right)^{n*} \Big|_{x_1=x_{1,i+1/2}, x_2=x_{2,j+1}} = \\ \bar{a}_{1+,2+} \left[\delta_{2++,i} (F^n) + \delta_{2++,i+1} (F^n) \right] \\ + \bar{a}_{1-,2-} \left[\delta_{2+,i-} (F^{n*}) + \delta_{2+,i+1} (F^{n*}) \right] \end{aligned} \quad (III.4.11)$$

Here, we can see that the δ_{2+} terms are not evaluated at the same time level on successive rows and so, like terms cannot cancel. The lack of cancellation of interior terms means that the equations have not been conservatively differenced (see, e.g., Potter⁷ pp 61-63).

Since we will be required to iterate due to the nonlinearity of the equations (see Section III.7.2), another approach is to evaluate these terms at the last iteration level. That is, we approximate the terms as

$$\begin{aligned} \frac{\partial}{\partial x_i} \left(a \frac{\partial F}{\partial x_2} \right)^{n*} \bigg|_{x_1=x_{1,i+1/2}, x_2=x_{2,i}} = \\ \bar{a}_{1+,2+} \left[\delta_{2+,i}^{(\ell-1)F^{n*}} + \delta_{2+,i+1}^{(\ell-1)F^{n*}} \right] \\ + \bar{a}_{1+,-} \left[\delta_{2-,i}^{(\ell-1)F^{n*}} + \delta_{2-,i+1}^{(\ell-1)F^{n*}} \right] \end{aligned} \quad (\text{III.4.12})$$

where the left superscript ℓ refers to the iteration number (see Section III.5 for a description of the iteration procedure). In this case, the derivative is calculated in a conservative manner since there is no time mixing of terms. The problem that arises here is that we are required to iterate the mesh as a whole to keep everything at the same iteration level. This is wasteful since, in general, the number of iterations required differs from row to row and we are forced to use the maximum number for the whole mesh.

Finally, we can treat the mixed and product terms fully explicitly. This lowers the accuracy to order Δt for these terms and introduces a Courant limit on the time step size. A variation on this explicit method for the product terms that gives some time centering is

$$\left(\frac{\partial F}{\partial x_1} \frac{\partial G}{\partial x_2} \right)^{n*} = \frac{1}{2} \left(\frac{\partial F^n}{\partial x_1} \frac{\partial G^{n*}}{\partial x_2} + \frac{\partial F^{n*}}{\partial x_1} \frac{\partial G^n}{\partial x_2} \right) \quad (\text{III.4.13})$$

All of the above methods can be implemented in IMP but in general we use fully explicit mixed derivatives and use Eq. (III.4.13) for time centering the product of derivative terms. This choice, coupled with time step controls (see Section III.8), has run at hundreds of times the Courant limit for some problems with no ill effects.

III.5 Linearization of the Finite Difference Equations

Applying the results of the preceding sections to the MHD equations yields a set of nonlinear algebraic equations of the form

$$\begin{aligned} \underline{T}(\underline{u}^{n*}) - \underline{T}(\underline{u}^n) + \frac{\Delta t}{2} [\underline{F}(\underline{u}^{n*}) + \underline{F}(\underline{u}^n)] \\ + \Delta t [G(\underline{u}^n) + H(\underline{u}^n)] = 0 \end{aligned} \quad (\text{III.5.1})$$

where $\underline{u} = \{B, v, \rho, P\}$ and $\underline{T}(\underline{u}) = \{B, \rho v, \rho, P\}$. The term ρv in $\underline{T}$ is an example of a nonlinear term. Since, neglecting mixed derivative terms, our differencing is of order $(\Delta x^2, \Delta t^2)$ we would like to linearize the equations to the same accuracy in Δt . We can use a Taylor series expansion in time to yield as a linearization formula for any nonlinear term $\underline{f}$,

$$\underline{f}(t=n*) = \underline{f}(t=n) + \underline{J} \cdot \frac{\partial \underline{u}}{\partial t} \Delta t \quad (\text{III.5.2})$$

where

$$\underline{J} = \frac{\partial \underline{f}}{\partial \underline{u}^{n*}} \quad (\text{III.5.3})$$

which is the Jacobian of the term. This procedure is carried one step further by recognizing that this can be expressed as the first step of a generalized Newton-Raphson iteration. By letting the set of nonlinear algebraic equations (III.5.1) be written

$$\underline{F} = 0 \quad , \quad (\text{III.5.4})$$

we can use III.5.2 and let $\underline{f}(t = n^*) = \underline{F} = 0$. We then have

$$\Delta = {}^{i-1}\underline{F} + {}^{i-1}\underline{J}^{n^*} \cdot \frac{\partial \underline{u}^{n^*}}{\partial t} \Delta t \quad \left. \vphantom{\frac{\partial \underline{u}^{n^*}}{\partial t}} \right\} (\text{III.5.5})$$

or

$$\frac{\partial \underline{u}^{n^*}}{\partial t} = ({}^{i-1}\underline{J}^{n^*})^{-1} \cdot ({}^{i-1}\underline{F}^{n^*})$$

where i is the iteration index. Letting $\underline{u}^{0, n^*}$ take on the value of $\underline{u}^n$ gives us the first step which corresponds to equation III.5.2. To see the form of Eq. (III.5.5) that is actually to be iterated, we multiply through by ${}^{i-1}\underline{J}$ yielding (where n^* superscripts has been suppressed)

$${}^{i-1}\underline{J} \cdot \frac{\partial \underline{u}}{\partial t} = ({}^{i-1}\underline{J}) \cdot ({}^{i-1}\underline{u} - {}^{i-1}\underline{F}) \quad , \quad (\text{III.5.6})$$

When the finite difference approximations are substituted into Eq. III.5.6 for $\underline{F}$, the matrix takes on a block tridiagonal form. This form is

represented by

$$- \underline{A}_j \cdot \underline{u}_{j+1} + \underline{B}_j \cdot \underline{u}_j - \underline{C}_j \cdot \underline{u}_{j-1} = \underline{D}_j \quad (III.5.7)$$

In order to obtain the values of $\underline{A}$, $\underline{B}$, $\underline{C}$, and $\underline{D}$, we must consider the form of the MHD equations $\underline{F}(\underline{u}) = 0$. We express $\underline{F}$ in two parts, the explicit terms $\underline{F}_e$ which depend only on $\underline{u}^n$ and the implicit terms $\underline{F}_i$ which depend on $\underline{u}^{n*}$ and possibly on $\underline{u}^n$. Thus, we have

$$\underline{F}(\underline{u}) = \underline{F}_e(\underline{u}^n) + \underline{F}_i(\underline{u}^{n*}, \underline{u}^n) \quad (III.5.8)$$

Since the Jacobian $\underline{J}$ measures only the $\underline{u}^{n*}$ dependence, we can immediately group all the explicit terms in the right hand side $\underline{D}$ vector of Eq. (III.5.7). Next we look at some point j on the mesh. At this point, the equation to be solved is

$$\begin{aligned} \epsilon_{j+1}^{-1} J_{j+1}^j \cdot \underline{u}_{j+1} + \epsilon_j^{-1} J_j^j \cdot \underline{u}_j + \epsilon_{j-1}^{-1} J_{j-1}^j \cdot \underline{u}_{j-1} = \\ \epsilon_{j+1}^{-1} J_{j+1}^j \cdot \epsilon_{j+1}^{-1} \underline{u}_{j+1} + \epsilon_j^{-1} J_j^j \cdot \epsilon_j^{-1} \underline{u}_j \\ + \epsilon_{j-1}^{-1} J_{j-1}^j \cdot \epsilon_{j-1}^{-1} \underline{u}_{j-1} - \underline{F}_{e_j} \end{aligned} \quad (III.5.9)$$

where

$$\epsilon_{j+1}^{-1} J_{j+1}^j = \frac{\partial \epsilon_{j+1}^{-1} \underline{F}_{i,j}}{\partial \underline{u}_{j+1}^{n*}}, \quad (III.5.10.a)$$

$$F_{i,j}^{n+1} = \frac{F_{i,j}^{n+1} - F_{i,j}^n}{\Delta t} = \frac{F_{i,j}^{n+1} - F_{i,j}^n}{\Delta t} \quad (III.5.10.b)$$

$$F_{i,j}^{n+1} = \frac{F_{i,j}^{n+1} - F_{i,j}^n}{\Delta t} \quad (III.5.10.c)$$

and $F_{i,j}^{n+1}$ is the implicit part of F at the j -th grid point. This equation may be further broken down by using the properties of the spatial finite difference forms. We let $\underline{A}$ be the antisymmetric terms arising from the implicit FORN terms and $\underline{S}$ be the symmetric terms arising from the implicit FORCL terms. We then let

$$F_{i,j}^{n+1} = \underline{A}_{j+1/2}^{n+1} - \underline{A}_{j-1/2}^{n+1} + \underline{S}_{j+1/2}^{n+1} + \underline{S}_{j-1/2}^{n+1} \quad (III.5.11)$$

We redefine the Jacobians (Eq. III.5.10) to be

$$F_{i,j-1}^{n+1} = \frac{F_{i,j-1}^{n+1} - F_{i,j-1}^n}{\Delta t} = (\underline{S}_{j-1/2}^{n+1} - \underline{A}_{j-1/2}^{n+1}) \quad (III.5.12.a)$$

$$F_{i,j+1}^{n+1} = \frac{F_{i,j+1}^{n+1} - F_{i,j+1}^n}{\Delta t} = (\underline{S}_{j+1/2}^{n+1} + \underline{A}_{j+1/2}^{n+1}) \quad (III.5.12.b)$$

$$F_{i,j}^{n+1} = \frac{F_{i,j}^{n+1} - F_{i,j}^n}{\Delta t} = (\underline{S}_{j+1/2}^{n+1} + \underline{S}_{j-1/2}^{n+1} + \underline{A}_{j+1/2}^{n+1} - \underline{A}_{j-1/2}^{n+1} + \underline{T}_j^{n+1}) \quad (III.5.12.c)$$

where $\underline{T}_j^{n+1}$ are the terms arising from the time derivatives in F (e.g., $\frac{\partial}{\partial t}$, $\frac{\partial^2}{\partial t^2}$, etc). Next, we define the functions $\underline{S}$, $\underline{A}$, and $\underline{T}$ such that

$$\underline{S}_j^{n+1} = \frac{\underline{S}_{j+1/2}^{n+1}}{\Delta t} \quad ; \quad (III.5.13)$$

$$\left. \begin{aligned} \underline{S}_j &= - \frac{\partial \underline{S}_{j+1/2}^-}{\partial \underline{u}_j^{n*}} ; \\ \underline{A}_j^+ &= \frac{\partial \underline{A}_{j+1/2}^-}{\partial \underline{u}_{j+1/2}^{n*}} ; \\ \underline{A}_j &= \frac{\partial \underline{A}_{j+1/2}^-}{\partial \underline{u}_j^{n*}} ; \\ \underline{T}_j &= \frac{\partial \underline{T}_j}{\partial \underline{u}_j^{n*}} . \end{aligned} \right\} \quad (\text{III.5.13})$$

Given the above functions, we can now write down the forms of $\underline{A}$, $\underline{B}$, $\underline{C}$, and $\underline{D}$ of equation (III.5.7) that are actually used in IMP. We have

$$\underline{A}_j = - (\underline{S}_j^+ + \underline{A}_j^+) \quad (\text{III.5.14.a})$$

$$\underline{C}_j = - (\underline{S}_{j-1} - \underline{A}_{j-1}) \quad (\text{III.5.14.b})$$

$$\underline{B}_j = \underline{T}_j + \underline{S}_j + \underline{S}_{j-1}^+ + \underline{A}_j - \underline{A}_{j-1}^+ \quad (\text{III.5.14.c})$$

and

$$\underline{D}_j = - \underline{A}_j \cdot \partial^{-1} \underline{u}_{j+1} + \underline{B}_j \cdot \partial^{-1} \underline{u}_j - \underline{C}_j \cdot \partial^{-1} \underline{u}_{j-1} - \underline{F}_e \quad (\text{III.5.14.d})$$

Using the form given in equations III.5.14 allows us to only calculate the Jacobians on the forward cell interface and then reuse the values from the previous cell for the backward interface.

The $\underline{A}^+$, $\underline{A}$, $\underline{S}^+$ and $\underline{S}$ matrix elements must now be generated. They are determined by the analytic derivatives given in Eq. III.5.13 and are 8×8 matrices. We, therefore, must evaluate 5×64 matrix elements, many of which have complicated functional dependences on $\underline{u}^{n*}$, (e.g., we generally use the Spitzer⁶⁵ resistivity $\eta \propto T^{-3/2} \propto \left(\frac{p}{\rho}\right)^{-3/2}$). Any time we wish to try a different difference technique, we must regenerate the elements of the Jacobian matrix. To simplify this procedure, the FDE's were programmed on REDUCE,⁴⁶ an algebraic processor running on the MFE-PDP10. After defining the set of MHD equations and various finite difference techniques to REDUCE, and then programming it to take a Jacobian, the pain of producing the elements of the Jacobian is mostly alleviated. REDUCE can write the matrix elements in the form of a FORTRAN subroutine to further ease the process. The use of the REDUCE processor has allowed us the trial of many different finite difference techniques without spending weeks deriving the various matrix elements and then attempting to enter them into the computer correctly. A listing of the REDUCE generator code is given in Appendix B. Once again we point out that, due to the (1,2) and (1,3) symmetry of the $\underline{F}$, $\underline{G}$ and $\underline{H}$ functions, the Jacobians need only be generated for the first sub-timestep. They are then reused for the second and third sub-timestep.

Having calculated the Jacobian matrix elements, we now have a simple formula (Eq. III.5.6) to follow by which we iterate our mesh to some convergence criterion ($\underline{\epsilon} \leq (\underline{\ell} \underline{u} - \underline{\ell}^{-1} \underline{u}) / \underline{\ell}^{-1} \underline{u}$). The reason we do the iterations and not just stop at one pass as do Brilly and McDonald,⁶⁶ which is formally correct to $O(\Delta t)^2$, is that, when we simplified Eq. (III.4.2) to get the set Eq. (III.4.3), we assumed that previously calculated functions cancelled. For example, we have assumed that $\underline{F}(\underline{u}^{n*})$ in Eq. (III.4.2.a) was equal to $\underline{F}(\underline{u}^{n*})$ in Eq. (III.4.2.b). This cancellation will only be true if we actually iterate the equations to convergence.

III.6 Solution of Difference Equations

As was previously stated, we want to solve a system of I equations whose form is block-tridiagonal. This system can be represented by

$$-\underline{A}_i \cdot \underline{u}_{i+1} + \underline{B}_i \cdot \underline{u}_i - \underline{C}_i \cdot \underline{u}_{i-1} = \underline{D}_i, \quad i = 2, 3, \dots, I-1 \quad (\text{III.6.1})$$

We will assume that the boundary conditions can be expressed in the form

$$\underline{G}_1 \cdot \underline{u}_1 = \underline{H}_1 \cdot \underline{u}_2 + \underline{J}_1 \quad (\text{III.6.2.a})$$

and

$$\underline{G}_I \cdot \underline{u}_I = \underline{H}_I \cdot \underline{u}_{I-1} + \underline{J}_I \quad (\text{III.6.2.b})$$

Taking the relation

$$\underline{u}_i = \underline{E}_i \cdot \underline{u}_{i+1} + \underline{F}_i, \quad i = 1, 2, \dots, I-1 \quad (\text{III.6.3})$$

and substituting for $\underline{u}_{i-1}$ in Eq. (III.6.1), we get the recurrence relations for $\underline{E}_i$ and $\underline{F}_i$ as

$$\underline{E}_i = (\underline{B}_i - \underline{C}_i \cdot \underline{E}_{i-1})^{-1} \cdot \underline{A}_i \quad (\text{III.6.4.a})$$

and

$$\underline{F}_i = (\underline{B}_i - \underline{C}_i \cdot \underline{E}_{i-1})^{-1} \cdot (\underline{D}_i + \underline{C}_i \cdot \underline{F}_{i-1}) \quad (\text{III.6.4.b})$$

for $i = 2, 3, \dots, I-1$. We have, then, a straightforward algorithm for the solution of Eq. (III.6.1), provided we can use the boundary conditions III.6.2 to give us values for $\underline{E}_1$, $\underline{F}_1$ and $\underline{u}_I$.

By writing Eq. (III.6.2.b) in the form of Eq. (III.6.3), we see by inspection that

$$\underline{E}_1 = \underline{G}_1^{-1} \cdot \underline{H}_1 \quad (\text{III.6.5.a})$$

and

$$\underline{F}_1 = \underline{G}_1^{-1} \cdot \underline{J}_1 \quad (\text{III.6.5.b})$$

Next, we use Eq. (III.6.3) to substitute for $\underline{u}_{I-1}$ in Eq. (III.6.2.b). This yields

$$\underline{u}_I = (\underline{G}_I - \underline{H}_I \cdot \underline{E}_{I-1})^{-1} \cdot (\underline{J}_I + \underline{H}_I \cdot \underline{F}_{I-1}) \quad (\text{III.6.6})$$

Our solution method is now clear. We use Eq. (III.6.5) to get $\underline{E}_1$ and $\underline{F}_1$; sweep from $i = 2, 3, \dots, I-1$ solving Eq. (III.6.4) for $\underline{E}_i$ and $\underline{F}_i$; use

Eq. (III.6.6) to get $\underline{u}_I$ and then backsubstitute using Eq. (III.6.3). The most costly part of the algorithm is inverting the matrix $(\underline{B} - \underline{C} \cdot \underline{E})$ at each mesh point. For the MHD equations used in IMP, this is an 8×8 matrix which requires 450 microseconds (or 345 microseconds for the reduced 7×7 set) to produce the inverse on a CDC-7600 using fully optimized machine language LU decomposition subroutines.⁶⁷

The above solution algorithm will work for any boundary conditions that can be cast in the form of Eq. (III.6.2). Periodic boundary conditions, on the other hand, have the relations that $\underline{u}$ and $\frac{\partial \underline{u}}{\partial n}$ (where n is the direction of the line) are equal at the ends of periodic meshes. This is implemented by assuming that

$$\begin{aligned}\underline{u}_1 &= \underline{u}_{I+1} \\ \underline{u}_2 &= \underline{u}_{I+2}\end{aligned}\tag{III.6.7}$$

and that the point $i = 3/2$ is where the periodic boundary occurs. The points $I + 1$ and $I + 2$ do not actually exist as they are redundant. Here, we first assume a recurrence relation

$$\underline{u}_i = \underline{E}_i \cdot \underline{u}_{i+1} + \underline{F}_i + \underline{S}_i \cdot \underline{u}_1\tag{III.6.8}$$

$i = 2, 3, \dots, I-1$. The inclusion of the $\underline{S}_i \cdot \underline{u}_1$ term takes into account the fact that now the matrix has the tridiagonal form plus elements in the upper right and lower left corners (see Fig. III.5). Eliminating $\underline{u}_{i-1}$ from Eq. (III.6.1) now gives us the relations

$$\underline{\underline{A}} = \begin{pmatrix} \underline{\underline{a}}_{11} & \underline{\underline{a}}_{12} & & & \text{O} & \underline{\underline{a}}_{1,n} \\ \underline{\underline{a}}_{21} & \underline{\underline{a}}_{22} & \underline{\underline{a}}_{23} & & & \\ & \underline{\underline{a}}_{32} & \underline{\underline{a}}_{33} & \underline{\underline{a}}_{34} & & \\ & & & & \text{O} & \\ \text{O} & & \underline{\underline{a}}_{n-1,n-2} & \underline{\underline{a}}_{n-1,n-1} & \underline{\underline{a}}_{n-1,n} & \\ \underline{\underline{a}}_{n,1} & & & \underline{\underline{a}}_{n,n-1} & \underline{\underline{a}}_{n,n} & \end{pmatrix}$$

$$\underline{\underline{a}}_{i,j} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{1,m} \\ \alpha_{21} & & \\ \vdots & & \\ \alpha_{m,1} & & \alpha_{m,m} \end{pmatrix}$$

Figure III.5

The block tridiagonal matrix structure found in the one-dimensional, three point finite difference equations with periodic boundary conditions.

$$\underline{\underline{E}}_i = (\underline{\underline{B}}_i - \underline{\underline{C}}_i \cdot \underline{\underline{E}}_{i-1})^{-1} \cdot \underline{\underline{A}}_i \quad (\text{III.6.9.a})$$

$$\underline{\underline{F}}_i = (\underline{\underline{B}}_i - \underline{\underline{C}}_i \cdot \underline{\underline{E}}_{i-1})^{-1} \cdot (\underline{\underline{D}}_i + \underline{\underline{C}}_i \cdot \underline{\underline{F}}_{i-1}) \quad (\text{III.6.9.b})$$

$$\underline{\underline{S}}_i = (\underline{\underline{B}}_i - \underline{\underline{C}}_i \cdot \underline{\underline{E}}_{i-1})^{-1} \cdot (\underline{\underline{C}}_i \cdot \underline{\underline{S}}_{i-1}) \quad (\text{III.6.9.c})$$

for $i = 2, 3, \dots, I$. Once again, we use the boundary conditions to fix the values of $\underline{\underline{E}}_1$, $\underline{\underline{F}}_1$ and $\underline{\underline{S}}_1$. From Eq. (III.6.7) and substituting $i = 1$ into

Eq. (III.6.8), we get

$$\left. \begin{aligned} \underline{E}_1 &= \underline{0} \quad , \\ \underline{F}_1 &= \underline{0} \quad , \\ \underline{S}_1 &= \underline{I} \quad , \end{aligned} \right\} \quad (\text{III.6.10})$$

where $\underline{I}$ is the identity matrix. Next, we need to fix the value of $\underline{u}_i$.

Before we can do this, we must introduce the following relation

$$\underline{u}_i = \underline{T}_i \cdot \underline{u}_1 + \underline{V}_i \quad , \quad i = 1, \dots, 3, 2 \quad (\text{III.6.11})$$

This is substituted into Eq. (III.6.8) for $\underline{u}_{i+1}$ yielding the relations

$$\underline{T}_i = \underline{E}_i \cdot \underline{T}_{i+1} + \underline{S}_i \quad (\text{III.6.12.a})$$

and

$$\underline{V}_i = \underline{E}_i \cdot \underline{V}_{i+1} + \underline{F}_i \quad , \quad i = 1, \dots, 3, 2 \quad (\text{III.6.12.b})$$

Next, the values of $\underline{T}_{I+1}$ and $\underline{V}_{I+1}$ are fixed by evaluating Eq. (III.6.11)

at $i = I+1$ and using Eq. (III.6.7) yielding

$$\underline{T}_{I+1} = \underline{I} \quad (\text{III.6.13.a})$$

and

$$\underline{V}_{I+1} = \underline{0} \quad . \quad (\text{III.6.13.b})$$

Finally, we substitute $i = 1$ into Eq. (III.6.1) and use Eq. (III.6.11) to eliminate $\underline{u}_2$ and the periodicity to eliminate $\underline{u}_1$. The value of $\underline{u}_1$ thus fixes as

$$\underline{u}_1 = (\underline{B}_1 - \underline{A}_1 \cdot \underline{T}_2 - \underline{C}_1 \cdot \underline{T}_1)^{-1} \cdot (\underline{D}_1 + \underline{A}_1 \cdot \underline{V}_2 + \underline{C}_1 \cdot \underline{V}_1) \quad (\text{III.6.14})$$

Thus, our algorithm for periodic boundaries consists of three sweeps through the mesh. Pass one sweeps from $i = 2, 3, \dots, I$ solving Eq. (III.6.9) for $\underline{E}$, $\underline{F}$ and $\underline{S}$, using Eq. (III.6.10) as starting values. Pass two sweeps from $i = 1, I-1, \dots, 2$ solving Eq. (III.6.12) for $\underline{T}$ and $\underline{V}$ using Eq. (III.6.13) as starting points. Finally, we use Eq. (III.6.14) to fix $\underline{u}_1$ and then solve Eq. (III.6.11) for $\underline{u}_i$ across the mesh. Once again, the most time consuming part of the operation is the inversion of the $(\underline{B} - \underline{C} \cdot \underline{E})$ matrix at every grid point.

III.7 Boundary Conditions

This section will describe the types of boundary conditions implemented in IMP. As was mentioned in Section III.6, the block tridiagonal solver requires a boundary condition of the form

$$\underline{G} \cdot \underline{u}_{B.P.} = \underline{H} \cdot \underline{u}_{INT} + \underline{N} \cdot \underline{J} \quad (\text{III.7.1})$$

where $\underline{u}_{B.P.}$ is the boundary point and $\underline{u}_{INT}$ is the next interior point. All forms of Neumann, Dirichlet and mixed boundary conditions can be represented

by the equation

$$\underline{a} \cdot \frac{\partial \underline{u}}{\partial n} + \underline{b} \cdot \underline{u} = \underline{y} \quad , \quad (\text{III.7.2})$$

where $\frac{\partial}{\partial n}$ is the derivative normal to the boundary. If we finite difference Eq. (III.7.2) via the rules of Section III.4, we obtain

$$\left(\frac{\underline{a}}{\underline{a}_+} + \frac{1}{2} \frac{\underline{b}}{\underline{b}_+} \right) \cdot \underline{u}_{\text{B.P.}} = \left(\frac{\underline{a}}{\underline{a}_-} - \frac{1}{2} \frac{\underline{b}}{\underline{b}_-} \right) \cdot \underline{u}_{\text{INT}} + \underline{y} \quad (\text{III.7.3})$$

where the top sign is taken at the $i = 1$ boundary and the bottom sign is taken at the $i = I$ boundary. We see then that Eq. (III.7.1) allows a very general class of boundary conditions to be implemented.

III.7.1 GHOST Point Boundary Conditions

One consideration is the accuracy of the boundary conditions. If the boundary point is picked so that the wall lies on the last mesh point, the differences given in Eq. (III.7.3) are one-sided. This leads to first order accurate boundary values. If we choose the last mesh point so that the wall lies halfway between it and the next interior point, we get second order accurate difference approximations to the derivatives. IMP uses the second method of placing "ghost" points outside the wall as one form of its boundary conditions.

To assign values for $\underline{G}$, $\underline{H}$ and $\underline{J}$, we will assume that the plasma is surrounded by a perfectly conducting, adiabatic wall. The electro-

magnetic field equations give us, for a perfectly conducting wall,

$$\hat{n} \cdot \underline{B} = 0 \quad (\text{III.7.1.1})$$

and

$$\hat{n} \times \underline{E} = 0 \quad , \quad (\text{III.7.1.2})$$

where $\hat{n}$ is the unit normal vector outward from the wall. That is, the normal magnetic field and tangential electric fields vanish. For the rest of this section, we assume that the wall exists at $x_1 = x_w$ where x_1 is some arbitrary orthogonal curvilinear coordinate. The results, of course, are true for any coordinate we choose. Equation (III.7.1.1) gives us, then, that

$$B_{1w} = 0 \quad . \quad (\text{III.7.1.3})$$

Next, we write Ohm's law and cross it with $\hat{n}$ to give us

$$\hat{n} \times \underline{E}_w = \hat{n} \times \left(\underline{v} \times \underline{B} - \frac{\eta}{S} \nabla \times \underline{B} \right)_w = 0 \quad . \quad (\text{III.7.1.4})$$

Looking at the tangential components of this yields (remembering that $\hat{n}$ is in the x_1 direction)

$$E_{2w} = \left(v_3 B_1 - v_1 B_3 - \frac{\eta}{S} (\nabla \times \underline{B})_2 \right)_w = 0 \quad (\text{III.7.1.5.a})$$

and

$$E_{3_w} = \left(v_1 B_2 - v_2 B_1 - \frac{\eta}{S} (\nabla \times \underline{B})_3 \right)_w = 0 \quad . \quad (\text{III.7.1.5.b})$$

We may use Eq. (III.7.1.3) to eliminate the B_{1_w} terms from (III.7.1.5) leaving

$$\left(v_1 B_3 + \frac{\eta}{S} (\nabla \times \underline{B})_2 \right)_w = 0 \quad (\text{III.7.1.6.a})$$

and

$$\left(v_1 B_2 - \frac{\eta}{S} (\nabla \times \underline{B})_3 \right)_w = 0 \quad . \quad (\text{III.7.1.6.b})$$

Since we have a solid wall, we may write

$$\hat{n} \cdot \underline{v}_w = 0 \quad , \quad (\text{III.7.1.7})$$

giving us

$$v_{1_w} = 0 \quad (\text{III.7.1.8})$$

which further simplifies (III.7.1.6) to

$$(\nabla \times \underline{B})_2 = (\nabla \times \underline{B})_3 = 0 \quad . \quad (\text{III.7.1.9})$$

Expanding (III.7.1.9) and remembering that $B_{13} = 0$ for all values of x_2 and x_3 yields

$$\frac{\partial h_2 B_2}{\partial x_1} = \frac{\partial h_3 B_3}{\partial x_1} = 0 \quad (\text{III.7.1.10})$$

or, more generally,

$$\frac{\partial h_T B_T}{\partial n} = 0 \quad , \quad (\text{III.7.1.11})$$

where the T subscript refers to the component of the field tangential to the wall.

Next, we evaluate the normal component of the momentum equation at the wall, obtaining

$$\begin{aligned} \frac{\partial \rho v_1}{\partial t} + \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial}{\partial x_1} (h_2 h_3 \rho v_1^2) + \frac{\partial}{\partial x_2} (h_1 h_3 \rho v_1 v_2) \right. \\ \left. + \frac{\partial}{\partial x_3} (h_1 h_2 \rho v_1 v_3) + h_3 \rho v_1 v_2 \frac{\partial h_1}{\partial x_2} + h_2 \rho v_1 v_3 \frac{\partial h_1}{\partial x_3} \right. \\ \left. - \left[h_3 \rho v_2^2 \frac{\partial h_2}{\partial x_1} + h_2 \rho v_3^2 \frac{\partial h_3}{\partial x_1} \right] \right\} + \frac{1}{2h_1} \frac{\partial P}{\partial x_1} \\ + \frac{B_2}{h_1 h_2} \left\{ \frac{\partial}{\partial x_1} (h_2 B_2) - \frac{\partial}{\partial x_2} (h_1 B_1) \right\} \\ + \frac{B_3}{h_1 h_3} \left\{ \frac{\partial}{\partial x_3} (h_1 B_1) - \frac{\partial}{\partial x_1} (h_3 B_3) \right\} = 0 \quad . \quad (\text{III.7.1.12}) \end{aligned}$$

Using Eqs. (III.7.1.3), (III.7.1.7) and (III.7.1.11) reduces (III.7.1.12) to

$$-\frac{1}{h_1 h_2 h_3} \left\{ h_3 \rho v^2 \frac{\partial h_2}{\partial x_1} + h_2 \rho v^2 \frac{\partial h_3}{\partial x_1} \right\}_w + \frac{1}{2h_1} \left(\frac{\partial P}{\partial x_1} \right)_w = 0, \quad (\text{III.7.1.13})$$

which is a boundary condition on pressure. We take the well known "free slip" boundary condition (see Roache⁶⁸) to fix the velocity tangential to the wall,

$$\frac{\partial h_T v_T}{\partial n} = 0. \quad (\text{III.7.1.14})$$

Finally, we use the adiabaticity of the wall which allows no heat flow through the wall,

$$\frac{\partial T}{\partial n} = 0, \quad (\text{III.7.1.15})$$

coupled with our normal thermodynamic relationship

$$P = \rho T, \quad (\text{III.7.1.16})$$

to give

$$\frac{\partial \left(\frac{P}{\rho} \right)}{\partial n} = 0. \quad (\text{III.7.1.17})$$

We now have a full set of nonlinear boundary conditions for u.

In summary then the boundary conditions to be applied at a perfectly conducting, adiabatic, inviscid wall are:

$$B_n = 0 ;$$

$$\frac{\partial B_n}{\partial n} = 0 ;$$

$$v_n = 0 ;$$

$$\frac{\partial v_n}{\partial n} = 0 ;$$

$$\left(\frac{p}{\rho} \right)_n = 0 ;$$

$$\frac{1}{2} \left(\frac{p}{\rho} \right)_n = \frac{1}{h_1 h_2 h_3} \left\{ h_{T1} \cdot v_{T2}^2 \frac{h_{T2}}{x_n} + h_{T2} \cdot v_{T1}^2 \frac{h_{T1}}{x_n} \right\} = 0 .$$

(III.7.1.18)

By applying the averaging and differencing operators of Section III.3 to Eqs. (III.7.1.18) we have a set of equations which represent our boundary condition. We then use these equations and form our cell interface Jacobians which yields, at the $i = 1$ boundary,

$$G_L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{31} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{31} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -P_2 & \omega_2 \\ 0 & 0 & 0 & 0 & A_L & B_L & C_L & 1 \end{pmatrix}, \quad (\text{III.7.1.19})$$

where

$$\begin{aligned} A_L &= \frac{2\Delta \bar{v}_2}{h_2} \frac{\partial h_2}{\partial x_1}, \\ B_L &= \frac{2\Delta \bar{v}_3}{h_3} \frac{\partial h_3}{\partial x_2}, \\ C_L &= \frac{2\Delta}{h_2 h_3} \left\{ \bar{h}_3 \bar{v}_2^2 \frac{\partial h_2}{\partial x_1} + \bar{h}_2 \bar{v}_3^2 \frac{\partial h_3}{\partial x_1} \right\}; \end{aligned} \quad (\text{III.7.1.20})$$

and

$$H_L = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{32} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{32} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & D_L & E_L & F_L & 1 \end{pmatrix}, \quad (\text{III.7.1.21})$$

where

$$\begin{aligned} D_L &= \frac{-2\Delta \bar{\rho} \bar{v}_2}{\bar{h}_2} \frac{\partial h_2}{\partial x_1}, \\ E_L &= \frac{-2\Delta \bar{\rho} \bar{v}_3}{\bar{h}_3} \frac{\partial h_3}{\partial x_1}, \\ F_L &= \frac{-2\Delta}{\bar{h}_2 \bar{h}_3} \left\{ \bar{h}_3 \bar{v}_2 \frac{\partial h_2}{\partial x_1} + \bar{h}_2 \bar{v}_3 \frac{\partial h_3}{\partial x_1} \right\}, \end{aligned} \quad (\text{III.7.1.22})$$

and

$$J_L = 0. \quad (\text{III.7.1.23})$$

Similarly, for the $i = I$ boundary, we have

$$G_R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{2I} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{3I} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{2I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{3I} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -p_{I-1} & \rho_{I-1} \\ 0 & 0 & 0 & 0 & A_R & B_R & C_R & 1 \end{pmatrix}, \quad (\text{III.7.1.24})$$

where

$$\begin{aligned} A_R &= \frac{-2\Delta \bar{\rho} \bar{v}_2}{\bar{h}_2} \frac{\partial h_2}{\partial x_1}, \\ B_R &= \frac{-2\Delta \bar{\rho} \bar{v}_3}{\bar{h}_3} \frac{\partial h_2}{\partial x_1}, \\ C_L &= \frac{-2\Delta}{h_2 h_3} \left(\bar{h}_2 \bar{v}_3^2 \frac{\partial h_3}{\partial x_1} + \bar{h}_3 \bar{v}_2^2 \frac{\partial h_2}{\partial x_1} \right); \end{aligned} \quad (III.7.1.25)$$

and

$$H_R = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{2I-1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{3I-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{2I-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{3I-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & D_R & E_R & F_R & 1 \end{pmatrix}, \quad (III.7.1.26)$$

where

$$\begin{aligned} D_R &= \frac{2\Delta \bar{\rho} \bar{v}_2}{\bar{h}_2} \frac{\partial h_2}{\partial x_1}, \\ E_R &= \frac{2\Delta \bar{\rho} \bar{v}_3}{\bar{h}_3} \frac{\partial h_2}{\partial x_1}, \end{aligned}$$

$$F_R = \frac{2\Delta}{h_2 h_3} \left(\bar{h}_2 \bar{v}_3^2 \frac{\partial h_3}{\partial x_1} + \bar{h}_3 \bar{v}_2^2 \frac{\partial h_2}{\partial x_1} \right), \quad (\text{III.7.1.27})$$

and

$$\underline{J}_R = 0. \quad (\text{III.7.1.28})$$

III.7.2 Flux Surface Boundary Conditions

Another approach for setting the boundary conditions is to consider the physical interpretation of the boundary. Since we are modeling a perfectly conducting, adiabatic, inviscid wall which lies on a flux surface of the plasma, we can make the following statements:⁵⁴

1. The wall allows no fluxes into or out of the computational region.
2. The wall exerts a force that exactly balances any residual $P + B^2$ force.

We take a mesh which has its last point half a cell away from the wall (See Fig. III.4). The values of the state vector, $\underline{u}$, are not needed at the wall, only the fluxes and forces are required there. The differencing techniques outlined in Section III.3 were chosen to take advantage of this property. The conditions of statements 1 and 2 above are implemented merely by setting the symmetric and antisymmetric matrices $\underline{A}$ and $\underline{S}$ of Section III.5 to zero at the wall-interface. We thus have a very easily implemented boundary condition that is physically motivated. It is this physically motivated boundary condi-

tion that is most often used when running IMP and we have consistently seen good results when using it. A more general form of this physical boundary condition is used by Lindemuth in the ANIMAL⁶⁹ code. In ANIMAL, the plasma $P + B^2$ force is also checked to detect plasma separating from the wall. When this occurs, a background plasma is jetted in to fill the void. This wall-separation type of boundary condition may eventually be incorporated into the IMP code.

III.8 Miscellaneous Computation Problems

III.8.1 Advection Terms

As was pointed out by Brackbill,⁴⁰ the nonlinear advection terms $\left(\frac{\partial}{\partial t} + \underline{v} \cdot \nabla\right)$ in the MHD equations cause a large number of problems. While the Crank-Nicholson and leapfrog approximation of the advection terms are stable according to linear theory, they are "explosively unstable when numerically solved". The source of the instability is traced to the truncation error in the difference equations causing antidiffusion. In order to offset this antidiffusion, small, purely numerical, diffusion terms are added to the continuity equation, the force equation and the energy equation. The form of these terms is

$$\frac{\partial u}{\partial t} + \nabla \cdot (F(u) - c \nabla u) = 0 \quad (III.8.1.1)$$

where c is a constant which is typically of order 1×10^{-4} . These terms are differenced as FLUX terms in Section III.3. Experience has shown that the inclusion of these artificial diffusion terms has resulted in

the ability to run with much larger timestep sizes and with increased numerical stability.

III.8.2 Iteration Controls

The current version of IMP advances the mesh one row at a time. In this manner, we are able to allow rows with large changes to iterate many times while rows that have little or no change either do not iterate at all or only iterate once or twice. We are able to do this because our choice of ADI techniques, along with the method of differencing the mixed derivative and product of derivative terms, decouples the rows of the mesh. The iterations are carried to convergence by testing for the maximum variation between iterations versus the average value of the iterations

$$\underline{\epsilon} = \text{MAX} [5(\underline{u}_1^{\ell} - \underline{u}_1^{\ell-1})/(\underline{u}_1^{\ell} + \underline{u}_1^{\ell-1})] \quad (\text{III.8.2.1})$$

These are subjected to a floor value such that if $\underline{u}_1^{\ell-1}$ is less than the floor, then floor value is used for $\underline{u}_1^{\ell}$ in the denominator of III.8.2.1. Finally, the maximum value of ϵ is compared with the allowed convergence criterion and, if ϵ is less than the criterion, the row is declared converged. Typical values for the convergence criterion is $\epsilon < 1 \times 10^{-5}$.

III.8.3 Timestep Controls

The main purpose of using implicit techniques was to allow the use of large timesteps. Early versions of IMP used a static timestep.

They experienced the difficulty that the problem's timestep was limited by the timesteps needed during the extreme nonlinear phases of the code's run. In order to bypass this constraint, a dynamic timestepping algorithm was implemented. This algorithm allowed the input of an initial timestep and maximum and minimum allowable timesteps. The code has a number of ways to choose its timestep (Δt).

The first method monitors the maximum number of iterations required (N) to converge the rows of the mesh. This number is compared with an input allowed number of iterations (M). If the number needed is less than the input number ($N < M$), then the timestep is increased by some factor (usually 10%). If the Δt is increased for a number of consecutive timesteps, the increment factor is doubled. This doubling continues until the "ideal" timestep has been found. If $N > M$, then the timestep is decreased. If $N > M + 1$, then a recycle is performed. That is, the new timestep is rejected and we redo the timestep with a smaller Δt . If $N = M$, we also increment Δt by a small amount to try and find the largest possible Δt .

The second method is to monitor the maximum change of the variables on the mesh (subject to some floor condition below which we do not check the change). In this method, we have a number of sub-controls. We want the maximum variation on the mesh, which is calculated as

$$\underline{v}_{\max} = \sum_{i,j,k} \max \left(\frac{\underline{u}_{i,j,k}^{n+1} - \underline{u}_{i,j,k}^n}{\underline{u}_{i,j,k}^n} \right), \quad (\text{III.8.3.1})$$

to be as close as possible to some allowed change c . If $V_{\max}$ is less than $.85c$ we increase the timestep. If $V_{\max}$ is greater than $1.5c$ we recycle. Otherwise if $c < V_{\max} < 1.5c$, we decrease the timestep by the formula

$$\Delta t = .8 \Delta t (c/V_{\max}) \quad . \quad (\text{III.8.3.2})$$

The subcontrols in this method allow one to choose to check the variation of momentum rather than the change of velocity. They also allow for time variations in the velocity/momentum floor values. The reason for allowing this variation is that we are interested in following the evolution of instabilities. In instabilities, the velocity is always increasing and, where we initially had the velocity floor set to 5% of the maximum on the mesh, we can end up being limited by the change in the slowest velocity on the mesh. By constantly revising the floor value we are able to hold it to 5% of the maximum velocity. This has resulted in increases of 70-150% in our running values of Δt .

The aforementioned timestep controls are only first approximations at a general timestep control algorithm. Other factors that can be tested are the energy conservation, changes in interface fluxes, or truncation error analysis. Which of these are necessary and, in the case of the truncation error analysis, the method of implementation are not currently understood. Future work in this area may result in even more dramatic increases in timestep size.

CHAPTER IV

THE INTERNAL KINK IN CARTESIAN GEOMETRY

IV.1 Introduction

The first three-dimensional application of our model is the simulation of the $m = 1$, $n = 1$ internal kink instability in Cartesian coordinates. Figure IV.1 shows the computational region that is used in this chapter.

As has been discussed in Chapter I, the internal kink instability is the most dangerous to plasma confinement. The mode is unstable whenever the $q = 1$ surface lies inside the plasma. Figure IV.2 shows typical radial profiles of the current $j_z(r)$, safety factor $q(r)$, and the lowest order radial eigenfunction of the displacement $\xi(r)$.⁶² The displacement for the mode is entirely contained within the singular surface at $r = r_S$. The linear growth rate of this mode is given analytically to be of order $k_z^3 r^2 v_A$. In the simulations to be presented, we have chosen $k_z = n/R = 1$ and $r = r_S \approx .8$. Thus, we can expect growth rates to be of order $.5 v_A$. This shows that the kink mode is growing on the Alfvén timescale in the problem.

The internal kink mode has been the subject of a great deal of computational study, both in the linear and nonlinear regimes. These studies have been performed by Bateman et al.⁹ and Hicks⁵⁵ in the limit of ideal MHD. The results of our model is compared with these studies as an independent check.

The first case run is the use of a small velocity field to perturb an analytic equilibrium. The resistivity in our model is set to zero. The

perturbation is allowed to evolve until pure exponential growth is observed. This rate of growth and the form of the eigenmode is compared with the linear code of Bateman, which has been shown to give good agreement with theory. Our model produces growth rates that are within 2% of the linear results. The perturbation is then allowed to continue its growth until nonlinear saturation of the mode occurs. The amplitudes of the velocity at saturation are then compared with those obtained by Hicks and are found to be in good agreement.

Next, an eigenmode obtained from the linear code is used as the perturbation in IMP. The object is to determine if the eigenmodes of the linear code produce an immediate exponential growth in the nonlinear model. The linear eigenmodes, started at relatively large magnitudes, are to be used as the initial perturbations for IMP. This allows the bypassing of most of the initial linear growth regime in future saturation studies. The eigenmodes from the linear code do display the desired immediate exponential growth.

After performing the ideal MHD comparisons, we introduce a finite (Spitzer⁶⁵) resistivity. This causes both resistive diffusion of the magnetic field and Ohmic heating of the plasma. Both of these effects cause spontaneous flows in the plasma. In order to allow the maintenance of a constant current in the plasma, a background electric field can be imposed. This external field exactly balances the resistive diffusion of the equilibrium magnetic fields. Once determined, the external field remains constant for the remainder of the simulation. In a like fashion, a nonphysical cooling term can be added to the energy equation to balance

the Ohmic heating. While the imposition of the external electric field can be justified in some cases, the nonphysical cooling cannot be justified and is added only to allow the use of the velocity flow field and the kinetic energy as diagnostics. A simulation is also performed without the cooling term and also one without the external electric field. In these cases, the eigenmode grows to dominate the spontaneous flows and the growth rate of the instability is only slightly modified by the inclusion of the non-physical terms. The resistivity is found to enhance the growth of mode while the final saturation velocities are slightly depressed due to energy going into heating the plasma.

IV.2 Equilibrium

The equilibrium configuration is determined by the solution of the momentum equation (II.2.12.b) under the condition of a stationary steady state,

$$\frac{1}{2} \nabla P = (\mathbf{v} \times \mathbf{B}) \times \mathbf{B} . \quad (\text{IV.2.1})$$

The values of the magnetic field and pressure that satisfy this are given by²¹

$$B_x = -\frac{\pi}{2} \psi_c \cos\left(\frac{\pi}{2} x\right) \sin\left(\frac{\pi}{2} y\right) ; \quad (\text{IV.2.2.a})$$

$$B_y = \frac{\pi}{2} \psi_c \sin\left(\frac{\pi}{2} x\right) \cos\left(\frac{\pi}{2} y\right) ; \quad (\text{IV.2.2.b})$$

$$B_z = 1 ; \quad (\text{IV.2.2.c})$$

$$P = \frac{1}{2} \left(\frac{\pi}{2} \right)^2 \psi_c^2 \cos^2 \left(\frac{\pi}{2} x \right) \cos^2 \left(\frac{\pi}{2} y \right). \quad (\text{IV.2.2.d})$$

We also assume a constant initial density $\rho = 1$. The safety factor per unit wavelength on the axis can be expressed as

$$q_c = \frac{2B_{z_c}}{\pi \lambda J_{z_c}} \quad (\text{IV.2.3})$$

where J_{z_c} is the current on axis and $\lambda \equiv \lambda/2\pi$ is the wavelength of the instability. The central current is obtained by evaluating $\nabla \times B$ at $x = y = 0$ yielding

$$J_{z_c} = 2 \left(\frac{\pi}{2} \right)^2 \psi_c. \quad (\text{IV.2.4})$$

We are able specify our equilibrium by choosing λ and q_c . We consider here a short pipe such that $\lambda = 1$ and $q_c = .6$.

IV.3 Initial Conditions

The initial equilibrium can be perturbed by two methods. The first method is to generate two counter-rotating vortices in x-y plane. The sense of the vortices are then twisted as we proceed along in the z direction. This is accomplished by first specifying the velocities on the $z = 0$ and $z = \pi/4$ planes. These velocities are

$$v_{x,z=0}(x,y) = v_{y,z=\pi/4}(x,y) = \frac{xy}{|xy|} \sin^2 \pi x \sin^2 \pi y \quad (\text{IV.3.1})$$

$$v_{y,z=0}(x,y) = v_{y,z=\pi/4}(y,x) = \begin{cases} \cos^2 \frac{3\pi}{2} x \cos^2 \frac{\pi}{2} y & |x| \leq 1/3 \\ \cos^2 \frac{3\pi}{2} x \cos^2 \frac{\pi}{2} y & |x| > 1/3 \end{cases} \quad \begin{matrix} (\text{IV.3.1}) \\ (\text{continued}) \end{matrix}$$

The velocities are then combined by

$$\left. \begin{aligned} v_x(x,y,z) &= C \left(v_{x,z=0}(x,y) \cos 2\pi z - v_{x,z=\pi/4}(x,y) \sin 2\pi z \right) \\ v_y(x,y,z) &= C \left(v_{y,z=0}(x,y) \cos 2\pi z - v_{y,z=\pi/4}(x,y) \sin 2\pi z \right) \end{aligned} \right\} \quad (\text{IV.3.2})$$

to obtain the final perturbation velocities where C is a constant which determines the initial amplitude. We have generally used $C \approx 10^{-4}$. The sense of these velocity vortices spiral at the same pitch as the magnetic field lines, thus assuring us that the perturbation will align itself with the magnetic field.

The second method for perturbing the equilibrium is to use the eigenmodes of $\underline{B}_1$, $\underline{v}_1$, and $\underline{P}_1$, where the 1 subscript denotes a perturbation quantity, generated by the linear code. These eigenmodes are generated on the $z = 0$ and $z = \pi/4$ planes. We therefore use a combination technique that is similar in form to (IV.3.2):

$$\phi(x,y,z) = C'(\phi_0(x,y) \cos 2\pi z - \phi_1(x,y) \sin 2\pi z) \quad , \quad (\text{IV.3.3})$$

where ϕ is any of the perturbation quantities, ϕ_0 is its value on the $z = 0$ plane and ϕ_1 is its value on the $z = \pi/4$ plane, and C' is a constant that sets the magnitude of the perturbation to be used.

IV.4 Boundary Conditions and Normalization

Since the walls are a flux surface we may use the adiabatic, perfectly conducting wall boundary conditions given in Chapter III. We have checked the consistency of these boundaries by rerunning the same problems with the "ghost" points of Chapter III to see if there are any discrepancies. The ghost point conditions used are the ones given by

$$\left. \begin{aligned} \frac{\partial B_T}{\partial n} \Big|_w &= \frac{\partial v_T}{\partial n} \Big|_w = 0 \\ B_n \Big|_w &= v_n \Big|_w = 0 \\ \frac{\partial T}{\partial n} &= \frac{\partial P}{\partial n} = 0 \end{aligned} \right\} \text{(IV.4.1)}$$

The scale factors for Cartesian coordinates are all constant. The internal coordinate system used is normalized to be

$$\left. \begin{aligned} -1 &\leq x_1, x_2 \leq +1 \\ 0 &\leq x_3 \leq +1 \end{aligned} \right\} \text{(IV.4.2)}$$

where x_1 corresponds to the x direction, x_2 to the y direction and x_3 to the z direction. The normalization is chosen such that the half width in the x direction is unity. This is accomplished by setting

$$\left. \begin{aligned} h_1 &= 1 \\ h_2 &= b/a \quad , \\ h_3 &= 2\pi\kappa \end{aligned} \right\} \text{(IV.4.3)}$$

where a is the half width in the x direction, b is the half width in the y direction and λ is the wavelength in units of a (see Fig. IV.1).

IV.5 Diagnostics

The principle diagnostic tools used in IMP are time histories of the kinetic energy of the system and the Fourier components of the pressure along the z direction. The growth rate γ is calculated from these time histories. At specific points in time, vector plots of the velocity and magnetic fields on x - y planes are generated, as well as contour plots of the pressure, density, temperature, and current density j_z on x - y planes. Efficiency of the computation is monitored by time history plots of the timestep size and Courant number (where $C = 1$ is the maximum step size for an explicit code).

As was stated above, the growth rate is calculated from the time histories of the kinetic energy of the system and from the Fourier components of the pressure. The growth rate of a quantity u at a point in time, based on a function f ($= f(u^2)$), is given by

$$\gamma = \frac{1}{2} \frac{d \ln f}{dt} = \frac{1}{2} \frac{1}{f} \frac{df}{dt} . \quad (\text{IV.5.1})$$

The factor of $1/2$ is to take into account the fact that the function f depends on a square of a plasma state function (e.g., $f = \text{kinetic energy} \propto \rho v^2$).

The Fourier analysis of the pressure in the periodic (x_3) direction is

$$P(x_1, x_2, x_3) = p_0(x_1, x_2) + \sum_{n=1}^N (p_n(x_1, x_2) \cos 2\pi n x_3 + q_n(x_1, x_2) \sin 2\pi n x_3) , \quad (\text{IV.5.2})$$

where

$$\left. \begin{aligned} p_0(x_1, x_2) &= \int_0^1 P(x_1, x_2, x_3) h_3 dx_3 \\ p_n(x_1, x_2) &= \int_0^1 P(x_1, x_2, x_3) \cos (2\pi n x_3) h_3 dx_3 \\ q_n(x_1, x_2) &= \int_0^1 P(x_1, x_2, x_3) \sin (2\pi n x_3) h_3 dx_3 \end{aligned} \right\} \quad (\text{IV.5.3})$$

The power in a given mode is

$$E_n = \alpha \iint (p_n^2 + q_n^2) h_1 h_2 dx_1 dx_2 , \quad (\text{IV.5.4})$$

where α is a constant of proportionality. Thus, the growth rates in specific n modes are given by

$$\gamma_{F_n} = \frac{1}{2E_n} \frac{dE_n}{dt} . \quad (\text{IV.5.5})$$

The two growth rate calculations are used for comparison with the linear code results. The growth rate based on the kinetic energy γ_{KE} and

the velocity field plots are not able to follow the early time growth of instabilities in the cases of a) finite resistivity and b) lack of absolute force balance in the equilibrium. Case (a) has been discussed. Case (b) can arise even when we start from an analytic equilibrium. This is due to the inherent error ($O(\Delta x^2)$) in the finite difference representation. A set of force correction terms, based on equilibrium force balance only, have been added to the momentum equation to alleviate this problem. Simulations with identical initial conditions, only varying by the inclusion of these terms, have been performed. The inclusion of the force balance terms did not affect either the linear growth rate or the form of the velocity fields as compared to those found once the instability had grown to dominate the background flow in the case without force balance terms.

The Fourier mode plots and growth rates, on the other hand, are able to follow the growth of the instability even in the early times. This is because the lack of force balance and the effect of resistivity are axisymmetric and, thus, their effects are seen only in the $n = 0$ mode.

IV.6 Results

IV.6.1 Velocity Field Perturbation, Ideal MHD

In this case, C in Eq. IV.3.2 is set to 10^{-4} . The equilibrium is chosen to have the q per unit wavelength on axis to be .6, and the wavelength $\lambda = 1$. The growth rate calculated for this equilibrium by the linear code is $\gamma_{lin} = .49$. Figure IV.3 shows the initial velocity field perturbation on the $z = 0$ plane (IV.3.a) and the $z = \lambda/4$ plane (IV.3.b). In Fig. IV.4, the total energy (trace labeled E), internal

energy (trace I), the magnetic field energy (trace B), and the kinetic energy (trace K) are plotted versus time on a semilog graph. In this simulation, the timestep is kept at a small constant value. The oscillations in the kinetic energy at early times can be attributed to magnetoacoustic waves transiting the system. As time progresses, the $m = 1, n = 1$ mode establishes itself and the energy being deposited in the mode by the magnetic field dominates the energy fluctuations caused by the waves. During this period of time ($t = 7$ to $t = 19$) the kinetic energy time becomes linear. The growth rate calculated from the kinetic energy is given in Fig. IV.5, which converges at $t = 14$, to a value of $\gamma_K = .48$, which is within 2% of the linear code's result. Figure IV.6 shows the velocity fields on the $z = 0$ and $z = 3/4$ planes during the pure exponential growth period, while Fig. IV.7 shows the values of the state variables across a line defined by $-1 \leq x \leq 1, y = z = 0$. The mode then ceases exponential growth at $t = 18$, where the kinetic energy is 1% of the total energy in the problem. The velocity fields at this time are given in Fig. IV.8 while the final value attained after 23 transits is shown in Fig. IV.9. The poloidal velocity attained by Hicks was of order .5 which is in good agreement with the final velocity attained in our model.

IV.6.2 Perturbation by Linear Eigenmodes, Ideal MHD

The eigenmodes obtained from the linear code are shown in Fig. IV.10. The spatial dependence of these modes agrees quite well with those obtained in the previous section. The constant C' in Eq. (IV.3.3) is set to 10^{-4} in order to assure the perturbation is in the

linear regime. The mode grows exponentially immediately, as can be seen in Fig. IV.11, which gives the kinetic and Fourier mode energies. The growth rates based on these energies are shown in Fig. IV.12. They initially display variations from the linear growth rates but after a few Alfvén transits the growth rate, based on both diagnostics, converges to $\gamma = .53$. This is within 2% of the value obtained by the linear code of .54. The initial jitter in the growth rates in our model can be traced to the differences in the linear versus nonlinear equations and to different finite difference techniques used in the two codes.

IV.6.3 Resistive Plasma Long Time Simulation

The first case run with finite resistivity used only the velocity field perturbation ($v_{\max} = 10^{-4}$) with $S = 1000$ and the external electric field and nonphysical cooling terms enabled. Figure IV.13 shows the time history of the energy. Initially energy is taken from the perturbation and deposited in the plasma. By $t = 2$ this trend is reversed as the $m = 1, n = 1$ mode begins to grow. The exponential growth is well established by $t = 5$. Fig. IV.14 shows the velocity fields on the $z = 0$ and $z = \pi/4$ planes at $t = 9.6$. This is midway through the exponential growth regime. Growth continues until $t = 20$ at which point nonlinear saturation occurs. At this point, the wall is stabilizing the mode. Peak poloidal velocities of order $.4 v_A$ are attained. After saturation of the 1,1 mode, higher toroidal modes can be detected in the Fourier energy plots. Finally, the plasma relaxes to a state with an extremely slowly growing $m = 3, n = 1$ mode at $t = 90$. Figure IV.15 shows the velocity fields of this 3,1 mode on the z

= 0 and $z = \lambda/4$ planes. The Courant number versus time for this case is shown in Fig. IV.16. The average Courant number was 10 with peak values of 40-50.

IV.6.4 Resistive Plasma Dependence of Growth Rate on S

A series of cases were run in which the only parameter varied was the magnetic Reynolds number. The linear, ideal eigenmodes were used as the initial perturbation ($C' = 10^{-4}$) in our model. The code was allowed to evolve for 5 Alfvén transit times in order to allow the linear mode to become a mode of the nonlinear resistive equations. We, then, restarted the code with a fixed, small Δt ($\sim .01$) and ran for 10 timesteps to calculate the mode's growth rate. The growth rates versus $1/S$ were plotted in Fig. IV.17. The mode was found to grow faster as the resistivity increased. This is expected since the resistivity now allows the fluid to move across magnetic field lines. Thus, the fluid does not have to perform as much work on the magnetic field as in the case of ideal MHD. This was in qualitative agreement with the predictions of Coppi et al.⁷⁰

IV.6.5 Resistive Plasma Without Balancing Electric Field and Cooling Terms

A plasma with $S = 250$ was run without the external electric field and the cooling being enabled. As can be seen in Fig. IV.18, spontaneous flows appeared immediately as the equilibrium magnetic field began to diffuse and heat the plasma. This spontaneous flow completely masked the initial perturbation on the velocity field

diagnostics; but the growth of the 1/1 mode was evident in the Fourier analyzed energy plots (Fig. IV.19). The 1/1 mode reappeared in the velocity fields only after it has grown by 2 orders of magnitude and began to dominate the spontaneous flows (Fig. IV.20).

IV.7 Summary

We have shown agreement with Bateman⁹ and Hick⁵⁵ both with the form of the linear ideal eigenfunctions and with their growth rates. The addition of resistivity was shown to enhance the ideal growth rates without changing appreciably the form of the eigenfunctions. A simulation which extended for 90 Alfvén transit times was presented which displayed a new plasma state that was characterized by only an extremely slowly growing 3,1 mode. Finally, the terms added to balance the effects of finite resistivity were shown not to affect the calculated growth rates.

All the above simulations were performed at Courant numbers substantially greater than unity.

Figure IV.1

The computational region used in Cartesian coordinates.
The origin is at x and b/a is the squareness ratio.

Figure 1V.2

Radial profiles of the linear eigenfunctions of current $j_z(r)$, safety factor $q(r)$ and radial displacement $\xi(r)$. The singular surface ($k \cdot B = 0$) is at r_s .

Maximum velocity in plane (arrows) = $1.04097633\text{E-}04$
Maximum perpendicular velocity (circles) = 0.

Figure IV.3a

The initial velocity field used to perturb the plasma on the $z = 0$ plane. The length of each arrow is proportional to the relative velocity at that point, *normalized* to the maximum velocity on the plane.

Maximum velocity in plane (arrows) = 1.04037633E-04
Maximum perpendicular velocity (circles) = 0.

Figure IV.3b

The initial velocity perturbation on the $z = \pi/4$ plane.

Figure IV.4

The various components of the energy summed across the entire mesh are plotted as functions of time. The trace labeled K is the kinetic energy, the B trace is the magnetic energy, the I trace is the internal energy, and the E trace is the total energy.

Figure IV.5

The growth rate based on kinetic energy $\gamma_{KE} = \frac{1}{2} \frac{d(\ln K)}{dt}$ plotted as a function of time. The initial oscillations are followed by a period of exponential growth which then ceases as nonlinear saturation occurs.

Maximum velocity in plane (arrows) = 2.33030233E-01
 Maximum perpendicular velocity (circles) = 1.74644917E-01

Figure 1.6a

The velocity field on the $z = 0$ plane during the exponential growth phase. The velocity in the z direction is represented by the circles. The magnitude of the z velocity is proportional to the radius of the circle while the direction of the velocity is indicated by the presence of a cross inside the circle (negative v_z) or its absence (positive v_z).

Maximum velocity in plane (arrows) = 2.32781400E-01
 Maximum perpendicular velocity (circles) = 1.79158183E-01

Figure IV.6b

The velocity field on the $z = \lambda/4$ plane during the exponential growth phase.

Figure IV.7a

The state variables along a line $-1 \leq x \leq 1$, $y = 0$, $z = 0$.

Figure IV.7b

The state variables along a line $-1 \leq x \leq 1$, $y = 0$, $z = 0$.

Figure IV.7c

the state variables along a line $-1 \leq x \leq 1$, $y = 0$, $z = 0$.

Figure IV.8

The velocity field at the onset of saturation of the 1/1 mode on the $z = \lambda/4$ plane.

Figure IV.9

The velocity field at saturation on the $z = \lambda/4$ plane.

Maximum velocity in plane (arrows) = $9.92154827\text{E-}05$
 Maximum perpendicular velocity (circles) = $4.61674548\text{E-}05$

Figure IV.10a The velocity eigenfunction projected on the $z = 0$ plane.

$z = \lambda/4$

Maximum velocity in plane (arrows) = 1.00000000E-04
 Maximum perpendicular velocity (circles) = 4.67603787E-05

Figure IV.10b

The velocity eigenfunction projected on the $z = \lambda/4$ plane.
 Note the comparison of these velocity fields with the
 velocity fields found by IMP given in Figure IV - 6a and b.

Figure IV.11a

The energy components plotted versus time for the initial perturbation by linear eigenfunctions. The kinetic energy displays immediate exponential growth.

Figure IV.11b

The energy contained the $n = 0$ and $n = 1$ Fourier modes. Here again immediate exponential growth of an $n = 1$ mode can be observed.

Figure IV.12a The growth rate based on the kinetic energy versus time.

Figure IV.1zb . The growth rate based on the $n = 1$ Fourier mode displayed versus time.

Figure IV.13a

The kinetic energy plotted versus time for the long time resistive simulation.

Figure IV.13b

The Fourier mode energies versus time for the long time resistive simulation.

Maximum velocity in plane (arrows) = $1.88202761E-03$

Maximum perpendicular velocity (circles) = $9.78616857E-04$

Figure IV.14a

The velocity field on the $z = 0$ plane during the exponential growth phase of the resistive simulation.

Maximum velocity in plane (arrows) = 1.93540822E-03

Maximum perpendicular velocity (circles) = 9.87186103E-04

Figure IV.14b The velocity fields on the $z = \pi/4$ plane.

Maximum velocity in plane (arrows) = $4.56829917\text{E-}02$

Maximum perpendicular velocity (circles) = $5.73983576\text{E-}02$

Figure IV.15a

The velocity field at $t = 90$ on the $z = 0$ plane. The $m = 3$ character of the mode can be seen by the presence of 6 velocity vortices.

Maximum velocity in plane (arrows) = 4.79212243E-02

Maximum perpendicular velocity (circles) = 5.42713987E-02

Figure IV.15b The velocity field at $z = \pi/4$.

Figure IV.16

The time step size Δt and the Courant numbers used for the long time resistive simulation.

Figure IV.17

The growth rate plotted versus the inverse of the magnetic Reynolds number S . Note the increase in the growth rate with decreasing resistivity.

Maximum velocity in plane (arrows) = $7.09450652\text{E-}03$

Maximum perpendicular velocity (circles) = $4.05016837\text{E-}03$

Figure IV.18a

The spontaneous velocity field caused by magnetic field diffusion. The initial perturbation has effectively disappeared from the velocity field.

Figure IV.18b

Contours of constant density at the $z = 0$ plane are displayed. Note the steep gradients caused by the spontaneous velocity flows.

Figure IV.19a

The kinetic energy versus time for the resistive plasma with no balance terms.

Figure IV.19b

The growth rate versus time based on kinetic energy for the resistive plasma with no balance terms. The large initial growth hides the growth of the instability.

Figure IV.19c The energy in the $n = 1$ Fourier mode versus time for the same simulation. Note that the mode exhibits immediate exponential growth.

Figure IV.19d

The growth rate of the $n = 1$ Fourier mode plotted versus time. The mode exhibits immediate exponential growth at a rate that is larger than that of the ideal plasma.

Maximum velocity in plane (arrows) = 1.75669538E-02

Maximum perpendicular velocity (circles) = 1.49386683E-02

Figure IV.20a

The 1/1 mode can once again be seen in the velocity field at $t = 9.45$.

Figure IV.20b

The density isoplot displays a $m = 1$ island that has emerged at $t = 9.45$.

Figure IV.20c

The 1/1 mode has saturated by $t = 13.7$. The velocity field now shows a considerable nonlinear deformation.

Figure IV.20d

The $t = 13.7$ density in which the plasma displays a considerable deformation towards the wall.

CHAPTER V

THE INTERNAL KINK IN A SQUARE CROSS SECTION TORUS

V.1 Introduction

In the preceding chapter, the study of the internal kink was limited to the approximation of a large aspect ratio torus which was then treated in a straight Cartesian coordinate system. In this chapter, the effects of curvature are included by adopting the cylindrical coordinate system depicted in Fig. V.1.

This is done for three reasons. First, real toroidal devices do not have infinitely large aspect ratios. Typically, devices operate with aspect ratios from 3 to 5. Therefore, we wish to see the error that has been made by the large aspect ratio assumption. Second, the Cartesian system of the last chapter does not verify the correct inclusion of the "Coriolis" terms in IMP's orthogonal curvilinear coordinate system. Comparison of IMP results with another toroidal code can be used for this verification. Finally, we wish to see if the curvature affects the final plasma state in a long time simulation.

The linear code of Bateman has been extended by Hicks and Wooten⁷¹ to include the effects of curvature on linear ideal MHD modes. This code is used to generate the linear eigenmodes used as perturbations in our code. The initial linear behavior of these modes in IMP is used to verify the correct inclusion of the "Coriolis" terms in our orthogonal curvilinear representation.

The first case studied was an ideal $m = 1$, $n = 4$ internal mode in an aspect ratio (R/a) 4 torus with the safety factor per unit wavelength on axis equal to .6. This corresponds to the first case in the previous chapter. The growth rate determined in our model is within 1% of the predictions of the linear code.

An $m = 1$, $n = 2$ ideal internal mode is also simulated. This is a slowly growing mode and our growth rate differs from the linear value by 10%.

Finally, a simulation was performed which followed the long term development of the resistive plasma while allowing the ohmic heating to affect the plasma dynamics. An $m = 1$, $n = 1$ mode was used to perturb a plasma in an aspect ratio 3 torus with a magnetic Reynolds number of 10^4 . The evolution of the perturbation was followed for 1000 Alfvén transit times. The plasma, after initial motion caused by the resistive heating, exhibited growth of the $m = 1$, $n = 1$ mode. This saturated and the plasma finally relaxed to a new axisymmetric equilibrium state that included a finite flow field which displayed a pair of counter-rotating vortices at the outer radius (an $m = 1$ characteristic).

V.2 Equilibrium and Initial Conditions

The equilibrium used in this chapter is obtained numerically in the linear Hicks and Wooten code by the specification of an aspect ratio $A = R/a$, where R is the major radius of the torus and a is its minor radius. The safety factor per unit wavelength q_c on the magnetic axis of the torus of the

equilibrium is then rescaled to give the desired q_c . This numeric equilibrium is not exact. Rather, the equilibrium has been iterated until the residual error is below some required value. This error causes no problems in the linear code but induces a spontaneous flow in the nonlinear dynamic code. This flow masks the detection of low level perturbations by some of our diagnostics (e.g., the velocity field plots and the growth rates based on kinetic energy). In order to alleviate this problem, a set of fictitious forces are added to the momentum equation. These forces are calculated to exactly balance the errors in the equilibrium and, as such, do not vary in time. These forces allow us to observe the growth of the perturbation's velocity field and monitor its growth in the kinetic energy plots. Simulations have also been performed without the force balance terms which have shown that the instability growth rate, as monitored in the Fourier mode plots, is unchanged by these terms.

The equilibrium was once again perturbed by using the eigenmodes of B_1 , v_1 , and P_1 that were generated by the linear code. These eigenmodes were calculated on the $z = 0$ and $z = \pi/4$ planes, combined via Eq. IV.3.3, and added to the equilibrium values.

V.3 Boundary Conditions and Normalization

The adiabatic, perfectly conducting wall boundary conditions of Section III.7.2 are used for the r and z coordinates since the wall is once again a flux surface of the plasma. The angular coordinate θ has periodic boundary conditions applied.

The cylindrical coordinate system shown in Fig. V.1 corresponds to an ordering of $\underline{x}$ as

$$\left. \begin{aligned} x_1 &= z \quad , \\ x_2 &= r \quad , \\ x_3 &= \theta \quad . \end{aligned} \right\} \quad (V.3.1)$$

The coordinate ranges are normalized to

$$\left. \begin{aligned} -1 &\leq x_1 \leq +1 \quad , \\ A-1 &\leq x_2 \leq A+1 \quad , \\ 0 &\leq x_3 \leq 1 \quad . \end{aligned} \right\} \quad (V.3.2)$$

This gives us the set of scale factors

$$\left. \begin{aligned} h_1 &= b/a \quad , \\ h_2 &= 1 \quad , \\ h_3 &= 2\pi r/n \quad , \end{aligned} \right\} \quad (V.3.3)$$

where b/a is the squareness ratio of the torus and n is the toroidal mode number.

V.4 Results

V.4.1 Equilibrium Test

The ideal MHD subset of our model was used to observe spontaneous flows in the unperturbed plasma caused by the lack of equilibrium

force balance. These flows attained velocities of $10^{-2} v_A$, two orders of magnitude above the normal input perturbation levels. Next, the force balance terms were activated and the code was rerun for 100 cycles. During this run, the spurious velocities generated were found to be of order of the machine roundoff (v 's $\sim 1 \times 10^{-16}$).

V.4.2 $m = 1, n = 4$ Ideal Kink Mode

The $1/4$ ideal kink mode was run in an aspect ratio 4 torus whose safety factor per unit wavelength on the axis was chosen to be .6. This corresponded to the case treated in Section IV.6.2. The growth rate obtained from the linear code was $\gamma_{LIN} = .41$, 20% less than that given in the straight geometry. However, this large growth rate still made the $1/4$ mode an attractive first candidate for simulation in the three-dimensional code. Figure V.2 displays the initial equilibrium configuration of the plasma while Fig. V.3 depicts the velocity field linear eigenfunction (generated by the linear code) that was used as an initial perturbation. The constant C' of Eq. (IV.3.3) was set to 10^{-4} and the mode was allowed to evolve. The plots of kinetic energy versus time (Fig. V.4) and energy in the $n = 4$ mode versus time (Fig. V.5) show that the mode began immediate exponential growth. The growth rate versus time based on the above energies (Fig. V.6) converged to a value $\gamma_{IMP} = .38$. This was within 7% of the linear result. The simulation was continued until saturation was obtained at $t \sim 13$ transits. The velocities are of order $.29 v_a$ at this time.

Next, the simulation was run to the point where the growth rate had converged to .38. At this point, the timestep size was cut to 10^{-2} to increase the accuracy of the simulation and the growth rate

calculation. This resulted in a calculated growth rate $\gamma_{IMP} = .41$ which was within 1% of the linear code's result.

A resistive case was also run with a magnetic Reynolds number (S) of 1000. The growth rate and the final velocity attained at saturation was enhanced due to the effects of the resistivity, but the form of the eigenfunctions remained unchanged (see Fig. V.7).

V.4.3 $m = 1, n = 2$ Ideal Kink Mode

An $m = 1, n = 2$ internal mode in an aspect ratio 4 torus was also simulated in IMP. This longer wavelength mode has a much lower growth rate ($\gamma_{LIN} = .08$) as it is better wall stabilized than the $1/4$ mode. This mode required over 2000 timesteps for the linear code to converge on a 41×41 mesh. The resultant eigenmodes were then injected into the $19 \times 19 \times 24$ mesh used in IMP. The agreement between the linear code and our nonlinear one was not as good as in the $1/4$ mode ($\gamma_{IMP} = .06$); however, the simulation was performed at a large Δt which did not give the best resolution of the growth rate. The kinetic energy and growth rate versus time and the velocity field at saturation ($t \approx 60$) are given in Figs. V.8 and V.9. Note that the final velocities are of order $.03 v_a$ --an order of magnitude below the $1/4$ mode's final result. IMP required only 280 cycles to follow the plasma evolution through over 60 Alfvén transit times. The Courant number for this run peaked at 5 and averaged 2.5. The maximum timestep used was $\Delta t = .9$

V.4.4 Long Time Resistive Simulation

An $m = 1$, $n = 1$ ideal mode was started in an aspect ratio 3 torus with a magnetic Reynolds number of 10^4 . Magnetic diffusion of the equilibrium fields and ohmic heating of the plasma due to the equilibrium current was allowed to occur. The initial velocity field perturbation (Fig. V.10) immediately had its form eroded by the effects of the finite resistivity of the equilibrium fields (Fig. V.11). There was an immediate jump in kinetic energy which was then followed by the growth of the $m = 1$, $n = 1$ mode. This growth was easily visible on the Fourier mode plots (Fig. V.12) but was undistinguishable in the velocity and kinetic energy diagnostics (Figs. V.11, V.13). The growth rate calculated by IMP was $\gamma_{IMP} = .06$ while the linear, ideal growth rate was $\gamma_{LIN} = .015$. This large discrepancy can be attributed to the timestep size not having been limited to be a small fraction of an Alfvén transit time during the period of linear growth ($\Delta t \sim 1-2$ Alfvén transit times). These timesteps corresponded to Courant numbers of 10-20. During the latter parts of the simulation, the maximum timestep of 5 Alfvén transit times was attained (Fig. V.14). This corresponded to a Courant number of 60. The average Courant number for this problem was 40. At $t = 58$, the 1,1 mode again became visible in the velocity field plots (Fig. V.15), while saturation of the mode began at approximately $t = 70$.

As the simulation progressed, the interaction of the higher n modes caused the plasma to relax to a final axisymmetric equilibrium that possessed an $m = 1$, $n = 0$ flow field (Figs. V.16, V.17).

V.5 Summary

Our model has been applied to ideal and resistive plasmas in a toroidal geometry. Good agreement has been displayed between the growth rates predicted by the linear code and those calculated with IMP. In addition, a long term simulation which displayed the relaxation of a resistive plasma to an axisymmetric equilibrium with a finite flow field was presented.

Once again, the ability of our model to run at Courant numbers substantially greater than unity was displayed.

Figure V.1

The cylindrical coordinate system used in this chapter. The major radius is R and the minor radius is a or r . The squareness ratio is given by b/a . All lengths are measured in units of the minor radius a .

Figure V.2

The equilibrium pressure contours for an aspect ratio 4 torus are shown as found numerically by the equilibrium solver in the linear code. Note that the pressure peak is displaced toward the outer wall. Contours of constant magnetic flux are identical in form to these pressure contours.

Figure V.3a

The velocity field generated by the linear code and projected on the $\phi = 0$ plane.

Maximum velocity in plane (arrows) = 1.29026849E-02

Maximum perpendicular velocity (circles) = 7.36848347E-03

Figure V.3b

The velocity field generated by the linear code and projected on the $\theta = \pi/4$ plane.

Figure V.4

The energy is plotted versus time for the 1/4 ideal kink mode simulation.

Figure V.5

The energy in the $n = 4$ Fourier mode versus time is given for the $1/4$ ideal kink simulation. The mode displays an immediate exponential growth.

Figure V.6a

The growth rate based on the kinetic energy
(Figure V.4).

Figure V.6b

The growth rate based on the energy in the $n = 4$ Fourier mode (Figure V.5).

Figure V.7a

The growth rate versus time for the $1/4$ mode in a $s = 1000$ plasma based on the energy in the $n = 4$ fourier mode.

Maximum velocity in plane (arrows) = 3.50269972E-01
 Maximum perpendicular velocity (circles) = 4.57162242E-01

Figure V.7b

The velocity field on the $\theta = 0$ plane at $t = 25$ for the $1/4$ mode in a $s = 1000$ plasma.

Figure V.Ca

The energy plotted versus time for the 1/2 ideal kink simulation.

Figure V.1b

the growth rate of the kinetic energy plotted versus time for the 1/2 ideal kink simulation.

Figure V.9a

The velocity field on the $\eta = 0$ plane at saturation are shown for the $1/2$ ideal kink simulation at $t = 72$ Alfvén transit times.

Maximum velocity in plane (arrows) = 1.75713354E 02

Maximum perpendicular velocity (circles) = 1.85697924E 02

Figure V.9b

the velocity field on the $\theta = \pi/4$ plane in the $1/2$ ideal kink simulation at $t = 72$ Alfvén transit times.

Maximum velocity in plane (arrows) = 7.88063238E 05
Maximum perpendicular velocity (circles) = 1.47352917E 04

Figure V.10 the initial velocity field eigenfunction generated by the linear code as projected on the $x-y$ plane.

Maximum velocity / in plane (arrows) = 3.58553255E-03

Maximum perpendicular velocity (circles) = 2.98479588E-04

Figure V.11

The velocity field on the $z = 0$ plane at $t = .46$ Alfvén transit times into the simulation. The initial velocity perturbation (Fig. V.10) has disappeared due to the effects of the finite ($\eta = 10^{-4}$) resistivity.

Figure V.12a

The energy in the first five Fourier modes plotted versus time for the resistive ($S = 10^h$) simulation.

Figure V.12b

The growth rates γ_N for the Fourier modes depicted in Fig. V. 12a.

Figure V.13a

The kinetic energy plotted versus time for the resistive ($S = 10^4$) simulation.

Figure V.13b

The growth rate γ_{KE} calculated from the kinetic energy in Fig. V.12a.

Figure V.14

The timestep size used plotted versus a) time; and b) timestep number. Also, the Courant number to which these Δt 's correspond plotted versus c) time, and d) timestep number.

Maximum velocity in plane (arrows) = $1.76190346E-01$

Maximum perpendicular velocity (circles) = $4.603367E-01$

Figure V.1b

The velocity field on the $u = \pi/4$ plane at $t = 58$ Alfvén transit times. The twin counterrotating vortices characteristic of the $m = 1$ mode are once again visible.

Figure V.16a

The velocity field at $t = 1000$ Alfvén transits on the $\theta = 0$ plane.

Maximum velocity in plane (arrows) = 4.16385436E-02

Maximum perpendicular velocity (circles) = 1.59099000E-02

Figure V.16b

The velocity field at $t = 1000$ Alfvén transits on the $\theta = \pi/4$ plane.

Maximum velocity in plane (arrows) = $4.37184582E-7$

Maximum perpendicular velocity (circles) = $1.328853E-02$

Figure V.17a

The velocity field at $t = 1500$ Alfvén transits on the $\theta = 0$ plane.

Maximum velocity in plane (arrows) = 4.20433193E-02

Maximum perpendicular velocity (circles) = 1.32444421E-02

Figure V.17b

The velocity field at $t = 150^\circ$ Alfvén transits on the $\theta = \pi/4$ plane.

CHAPTER VI

SPONTANEOUS REVERSED FIELD PINCH

VI.1 Introduction

The spontaneous production of a reversed toroidal field in pinches in which the toroidal flux is conserved has been observed in the ZETA and HBTX experiments.⁷² Taylor⁷³ has shown that this is a relaxation to a minimum energy state of a moderately resistive plasma subject to the constraint that

$$K = \int_V \underline{A} \cdot \underline{B} \, d\tau \quad (\text{VI.1.1})$$

be a constant ($\underline{A}$ is the vector potential, $\underline{B}$ is the magnetic flux density, and V is the total plasma volume). The final plasma state then satisfies the condition

$$\nabla \times \underline{B} = \mu \underline{B} \quad (\text{VI.1.2})$$

where μ is a constant throughout the plasma. This final state is termed "force-free" due to the vanishing of the Lorentz force term ($\underline{J} \times \underline{B} = 0$). Stable final states can exist for plasmas with pinch ratios $\chi \leq A^{-1}$ (the aspect ratio) and $\chi \geq 1$. The pinch ratio χ is defined as

$$\chi \equiv \frac{2I}{r_0 B_0} \quad (\text{VI.1.3})$$

where I is the current in the plasma; B_0 is the initial toroidal magnetic

field; and r_0 is the minor radius of the torus. In a Cartesian geometry, the pinch ratio may be defined as

$$\chi = \frac{\oint \frac{B d\ell}{\langle B_z \rangle}}{\oint d\ell} = \frac{I/8a}{\langle B_z \rangle} \quad (\text{VI.1.4})$$

The spontaneous reversal of the toroidal field is demonstrated by three simulations performed in Cartesian coordinates. In the first, the evolution of a high current equilibrium is traced. The plasma undergoes a very quickly growing $m = 1$, $n = 1$ kink that leads to field reversal on the boundary. This is in agreement with the result obtained by Pritchett.^{74,75} In the second and third cases, low current density plasmas are subjected to an external electric field that drives the plasma into the $\chi > 1$ regime. In these cases, a strong field reversal occurs. The reversal then decays on the resistive timescale. The temporal variation of the current, kinetic energy and field reversal are in good qualitative agreement with the work of Sykes and Wesson,⁴⁵ and Gowers, et al.⁴⁶ One important difference in our physical model as opposed to that of Sykes and Wesson is that we obtain the field reversal using a scalar resistivity while they use a tensor model.

VI.2 Initial Conditions

The equilibrium specified in Eq. IV.2.2 is used for all three simulations in this chapter. The high initial χ simulation (Case 1) is characterized by a $q = .15$, $\chi_0 = 2.53$, and $\star = 1$. It is perturbed by the velocity vortices described by Eq. IV.3.1,2 with $C = 10^{-4}$. The initial plasma state is shown in Fig. VI.1.

The first low initial χ simulation (Case 2) is characterized by $q_0 = .8$, $\chi_0 = .98$ and $\star = .5$. The second simulation of low λ (Case 3)

has $q_0 = 1.1$, $x_0 = .72$ and $\tau = 1$. The perturbations for these cases are generated by the linear code and are added to the equilibrium configuration using Eq. IV.3.3 with $C' = .01$.

VI.3 Boundary Conditions and Zoning

The adiabatic, perfectly conducting wall boundary conditions (see Chapter: III and IV) are once again used, as are the scale factors given in Eqs. IV.4.2 and IV.4.3.

VI.3.1 Case 1

Since we are running at high currents, the singular layer ($\underline{k} \cdot \underline{B} = 0$) is close to the wall. In order to keep the number of mesh points to a minimum and yet to resolve any large functional variations at the singular layer, a variable mesh spacing is used. The mesh spacings are chosen by using a geometric ratio, R , to connect the zone sizes by

$$\frac{x_{i+1} - x_i}{x_i - x_{i-1}} = R \quad . \quad (VI.3.1.1)$$

The ratio is chosen so that the zones near the wall are approximately ten times smaller than the central zones. This is also a check on the nonuniform zoning capabilities in IMP.

VI.3.2 Case 2 and Case 3

In order to impose an external electric field, a time dependent boundary condition is required. The conservation of magnetic flux

equation (II.2.12.a) is written as

$$\frac{\partial \underline{B}}{\partial t} + \nabla \times \underline{E} = 0 \quad (\text{VI.3.2.1})$$

where $\underline{E}$ is a normalized electric field. For the poloidal field this becomes

$$\frac{\partial B}{\partial t} + \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = 0 \quad (\text{VI.3.2.2.a})$$

and

$$-\frac{\partial B}{\partial t} + \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = 0 \quad (\text{VI.3.2.2.b})$$

The normal value for the tangential electric field at the boundary is zero since the wall is assumed to be a perfect conductor. We now let the tangential electric field at the wall be

$$\underline{E} = E_z(t) \hat{z} \quad (\text{VI.3.2.3})$$

Using the spatial finite difference approximations given in Chapter III, we now write (VI.3.3) as

$$\frac{\partial B}{\partial t} + \frac{\bar{E}_z(y+) - \bar{E}_z(y-)}{2\Delta} = 0 \quad (\text{VI.3.2.4.a})$$

and

$$\frac{\partial B}{\partial t} = \frac{\bar{E}_z(x+) - \bar{E}_z(x-)}{1} = 0 \quad . \quad (\text{VI.3.2.4.b})$$

Depending on which boundary we are at, the appropriate $\bar{E}_z$ is given the value of $E_z(t)$. The time dependent electric field in the z direction is specified by

$$E_{z\text{wall}}(t) = \begin{cases} C_E(1 - \cos \pi t') & , t_{\min} \leq t \leq t_{\max} \\ 0 & , \text{otherwise} \end{cases} \quad (\text{VI.3.2.5})$$

where

$$t' = \frac{2}{t_{\max} - t_{\min}} \quad , \quad (\text{VI.3.2.6})$$

$$t' = t - t_{\min} \quad , \quad (\text{VI.3.2.7})$$

and C_E is constant of order unity. For case 2 C_E is .4, while for Case 3 C_E is .5. In Fig. VI.2, the magnitude of E_z at the wall versus time is shown in units of C_E .

VI.4 Artificial Viscosity

The electric field shown in Fig. VI.2 causes an increase in the current flowing in the plasma, thus pinching the plasma. The pinching causes a compression of the plasma that leads to numeric difficulties. These difficulties are resolved by the inclusion of a Von Neumann^{5b} artificial viscosity in the momentum and energy equations. In the nomen-

closure of Chapter III, a viscous flux is added to the momentum equation,

$$\frac{\partial \rho \underline{v}}{\partial t} + \nabla \cdot (\rho \underline{v} \underline{v} + \underline{q}) + \underline{B} \times (\nabla \times \underline{B}) + \frac{1}{2} \nabla P = 0, \quad (\text{VI.4.1})$$

and a viscous or shock heating force is added to the energy equation

$$\frac{\partial P}{\partial t} + \gamma \nabla \cdot P \underline{v} - (\gamma - 1) \underline{v} \cdot \nabla P + \frac{2\eta}{S} j^2 + (\underline{q} \cdot \nabla) \cdot \underline{v} = 0, \quad (\text{IV.4.2})$$

where

$$\underline{q} = \begin{cases} -C_1 \rho \left| \frac{\partial v_1}{\partial x_1} \right| \frac{\partial v_1}{\partial x_1} & 0 & 0 \\ 0 & -C_2 \rho \left| \frac{\partial v_2}{\partial x_2} \right| \frac{\partial v_2}{\partial x_2} & 0 \\ 0 & 0 & -C_3 \rho \left| \frac{\partial v_3}{\partial x_3} \right| \frac{\partial v_3}{\partial x_3} \end{cases} \quad (\text{VI.4.3})$$

and

$$C_i = \begin{cases} C_q, & \frac{\partial v_i}{\partial x_i} < 0; \quad i = 1, 2, 3 \\ 0, & \text{otherwise} \end{cases} \quad (\text{VI.4.4})$$

Thus, the artificial viscosity only effects compression and does not effect rarification. Typical values of C_q are .5.

VI.5 Results

VI.5.1 Case 1: High Initial γ

In this case, as in all cases presented in this chapter, the plasma is allowed to react to the effects of resistive diffusion and

ohmic heating ($S = 250$ in this case) by setting the external electric field and the pseudo cooling terms in the magnetic field and pressure equations to zero. This causes an immediate flow of plasma toward the walls. The kinetic energy exhibits rapid growth in the first few tenths of an Alfvén transit due to these effects (Fig. VI.3). Once this flow is established, the kinetic energy remains relatively constant until an $m = 1$, $n = 1$ mode begins to dominate the problem. The mode grows exponentially from $t = 2$ to $t = 8.5$. At $t = 8.5$, the $m = 1$, $n = 1$ mode saturates while an $n = 3$ mode continues to grow until it saturates at $t = 10$. This can be observed in the plots of the energy in the Fourier modes given in Fig. VI.4. The late time reversal of the toroidal magnetic field is illustrated in Fig. VI.5 which shows the B_z field on a number of lines across the mesh. The original value for B_z was 1 everywhere, while these late time plots show B_z dipping to values of -2 in some positions.

VI.5.2 Case 2: Externally Applied Electric Field, $q_0 = .8$

The plasma initially displays the flows caused by resistive diffusion and heating ($S = 50$ in Cases 2 and 3). These effects are first balanced and then overcome by the effects of the impressed electric field at the boundaries. The velocity field during the pinch phase is given in Fig. VI.6, while isoplots of the initially uniform density are given in Fig. VI.7 which display circular contours that are caused by the magnetic pinch. Velocity field plots during the kinking phase of the simulation are shown in Fig. VI.8, while isoplots of the density are given in Fig. VI.9. The flow due to the kink is shown to

be tightly spirally around the center of the pipe. The pinch ratio rises from an initial value of .98 to a peak of 2.88 (see Fig. VI.10). This drops rapidly to values of 2.3, followed by a smaller drop to 2.19. Following these rapid drops, γ then slowly falls as the current decays due to the effects of resistivity.

Time history plots of energy and Fourier mode energy (Fig. VI.11) show growth in kinetic energy due to the external electric field from $t = 0.5$ to $t = 2$. The growth of kinetic energy then ceases while the plasma continues to heat. By $t = 4$ transits, the $m = 1$, $n = 1$ and the $m = 1$, $n = 2$ modes have grown to a level that causes the kinetic energy to again exhibit growth. At this point, the current contained in the plasma has peaked and shows a rapid drop from $t = 6$ to $t = 7.5$. At the same time, the average value of B_z at the wall, $\langle B_z \rangle$, drops to a value of $-.67$, a strong field reversal (see Fig. VI.12). $\langle B_z \rangle$ then begins a rapid rise back to $-.2$ at which point the kinetic energy begins growth due to an $n = 4$ mode. This stabilizes the rapid decay of the reversed field at $t = 10$. For the remainder of the simulation the field reversal decays, on the resistive diffusion timescale until, at $t = 40$, it again passes through zero.

These results are in good qualitative agreement with the simulation of Sykes and Wesson⁴⁵ (SW) especially since our simulation did not contain as complete a physical model. SW included the effects of a tensor resistivity and "radiation" cooling. The tensor resistivity model used by SW assumed that $\eta_{\perp} = 2\eta_{\parallel}$. This had the effect of peaking

the current along the axis of the pinch. We, on the other hand, were able to obtain field reversal without this peaking of the current. The "radiation" cooling terms in SW were a simple model which scaled with pressure and inversely with radius. They had the effect of balancing ohmic heating and dissipating the high temperatures generated during the pinch, allowing the central pressure to drop to its pre-pinch level.

VI.5.3 Case 3: Externally Applied Electric Field, $q_0 = 1.1$

The initial plasma configuration used here has $\chi = .72$. The current is driven to a peak $\chi = 3$ at $t = 6$ (see Fig. VI.13). The current then resistively decays until $t = 11$. At this time, there is a sharper drop as the $m = 1, n = 1$ mode causes a slight field reversal. This is followed at $t = 16$ by a sharper drop as the $1/1$ mode is again destabilized by interactions with high n modes. Maximum field reversal is now observed (Fig. VI.14) as $\langle B_z \rangle_w = -.18$. This lesser reversal compared to Case 2 is due to the smaller amount of fluid (plasma) contained in the device (the ratio of P/B_z^2 is lower now) initially.

The lag time in $\langle B_z \rangle$ observed here corresponds to that seen in the Gowers report in as much as $\langle B_z \rangle$ is: 1) brought quickly to a level near zero; 2) remains here for a number of transit times; and 3) then displays a rapid reversal followed by decay back to the non-reversed regime.

VI.6 Summary

We have displayed a number of simulations which exhibit a spontaneous field reversal of a plasma with a large χ . In the first case, agreement

with Pritchett^{74,75} is obtained given a high χ equilibrium. In the second and third simulations, qualitative agreement with the work of Sykes and Wesson⁴⁵ and of Gowers⁴⁶ is obtained while using our more idealized model (scalar resistivity and no radiation cooling).

All these runs were performed at timesteps that exceeded the Courant limits by average factors of 5 and peak factors of 40.

Figure VI.1a

The initial plasma state as viewed across a line
 $-1 \leq x \leq 1$, $y = 1$, $z = 0$.

Figure VI.1b

The initial plasma state as viewed across a line $-1 \leq x \leq 1$, $y = 1$, $z = 0$. These velocities are the initial perturbation.

Figure VI.1c

The initial plasma state as viewed across a line
 $-1 \leq x \leq 1$, $y = 1$, $z = 0$.

Figure VI.2

The time dependant electric field $E_z(t)$ that was

$$E_z(t) = C_E \left[1 - \cos \frac{2\pi(t - t_{\min})}{\tau} \right]$$

$t_{\min} \leq t \leq t_{\max}$; $E_z(t) = 0$, otherwise).

Figure VI.3

The energy versus time plots for Case 1.

Figure VI.4

The Fourier mode energy plots versus time for Case 1.

Figure VI.5

Plots of B_z versus distance across the grid on the $z = 0$ plane for Case 1. Shown are:
a) $-1 \leq x \leq 1$, $y = -.76$; b) $-1 \leq x \leq 1$, $z = 0$; and
c) $x = -.98$, $-1 \leq y \leq 1$.

Maximum velocity in plane (arrows) = $1.05049533E+00$

Maximum perpendicular velocity (circles) = $2.66125935E-02$

Figure VI.6

The velocity field during the pinch phase of Case 2 and 3. The plasma is being compressed toward the center of the grid. Only the magnitude of the velocity varies between the two cases, not its character.

Figure VI.7

Isoplots of the density for Cases 2 and 3 during the pinch phase of the simulation. While the actual values of contours may vary between the two cases, the circular topology is unchanged.

Maximum velocity in plane (arrows) = $7.58314778\text{E-}01$
 Maximum perpendicular velocity (circles) = $2.66125935\text{E-}02$

Figure VI.8

The velocity field on the $z = 0$ plane at $t = 9.4$ Alfvén transits into the simulation. Note that the characteristic $m = 1$ counterrotating vortices have now reappeared but are tightly wound near the center of the mesh.

Figure VI.9

Isoplots of density at $t = 9.4$ for Case 2. Note that the plasma has now been displaced by the effects of the kink.

Figure VI.10

Plot of current (or γ) versus time for Case 2.

Figure VI.11a

Plot of Fourier mode energies versus time for Case 2.

Figure VI.11b Plot of kinetic energy versus time for Case 2. This is plotted on a linear scale to better compare with the results of Sykes and Messon.⁴⁵

Figure VI.12 Plot of $\langle B_z \rangle_{\text{wall}}$ versus time for Case 2. Note the rapid drop in $\langle B_z \rangle_{\text{wall}}$ at $t \approx 6$. This corresponds to the jump in kinetic energy showing in Figure VI.11b. $\langle B_z \rangle_{\text{wall}}$ then rises rapidly until another instability (See VI.11b) causes a flattening of the slope.

Figure VI.13a Plot of current (or χ) versus time for Case 3. The current dips first at $t = 11$ due to a $1/1$ mode. This is followed by a sharper drop at $t = 16$.

Figure VI.13b The kinetic energy for Case 3 plotted versus time. Note the peaks at $t = 11$ and 16.

Figure VI.13c

The Fourier mode energy versus time for Case 3.

Figure VI.14

Plots of $\langle B_z \rangle_{\text{wall}}$ versus time. Once again the field reversal corresponds with the peaks in velocity.

CHAPTER VII

SUMMARY AND CONCLUSIONS

VII.1 Summary

The development of the computer program IMP, which traces the evolution of a plasma immersed within a magnetic field, has been detailed. In particular, the physical model used is the set of eight single fluid resistive MHD equations. These consist of a set of eight coupled, nonlinear partial differential equations that consistently describe the interaction of an ionized gas with the magnetic field. No assumptions have been made to remove the fast timescales (e.g., low β or Tokamak ordering of the equations^{28, 50-52}). The equations have been expressed in orthogonal curvilinear coordinates to allow for generality in the problems to which the code may be addressed. The equations have been solved numerically on a variably spaced Eulerian finite difference mesh. The equations are advanced temporally by an adaption of the Douglas-Gunn⁵ algorithm for alternating direction implicit differencing. This has avoided the limitations in timestep size that are imposed on explicit techniques. The full set of eight equations has been advanced simultaneously, thus avoiding synchronization errors that can occur when the equations are split for solution.

While the continuity and magnetic flux equations have been treated in full conservation form, the momentum and energy equations have been solved in non-conservation form. This formulation has given enhanced numeric stability by eliminating errors that are introduced by the assumption that $\nabla \cdot \mathbf{B}$ is zero on the finite difference mesh.⁴⁹ This has also allowed the simulation of low β plasmas as the pressure (by the assumption of an ideal gas equation of state), rather than the total energy density, is an independent variable.

The boundary conditions that have been permitted are quite general in form (Dirichlet, Neumann, and periodic are allowed). The conservation boundary condition based on the physical properties of the wall⁵⁴ has proven to provide excellent results.

The techniques for discretizing the various terms in the MHD equations have been described. The Newton-Raphson iteration procedure, which also provides a second order accurate linearization of the nonlinear algebraic equations that result from the discretization of the partial differential equations, has been fully described.

IMP was applied to a number of problems in varying geometries of interest to magnetic fusion researchers. Ideal and resistive kink instabilities were treated in Cartesian coordinates. After specifying an initial analytic equilibrium, an arbitrary--though carefully chosen--velocity field perturbation led to the emergence of the 1/1 ideal kink instability. This agreed both in form and in growth rate with previous work.^{9,55} Next, a linear eigenfunction, generated by the linear MHD code of Bateman,⁹ was injected into the equilibrium plasma. It began immediate exponential growth confirming that an eigenfunction of the linear code was indeed extremely close to an eigenfunction of the nonlinear code. The addition of resistivity was shown to enhance the ideal growth rates without changing appreciably the form of the eigenfunctions. A simulation which extended for 90 Alfvén transits displayed a new plasma state that was characterized by an extremely slowly growing 3/1 mode. A final simulation was performed which allowed the finite resistivity to affect the initial equilibrium. While the velocity and density showed marked response to the magnetic diffusion and ohmic heating, the 1/1 growth rate was unchanged.

Next, a cylindrical coordinate system was used to examine the effects of curvature on the kink growth rates. An initial numeric equilibrium that corresponded to the first Cartesian simulation was perturbed by eigenfunctions generated by the linear toroidal code of Hicks and Wooten.⁷¹ Once again, immediate exponential growth of the kink mode was observed, and growth rates were found to be within 1% of the linear values. A resistive simulation of a 1/1 mode in an aspect ratio 3 torus was allowed to progress for more than 1300 Alfvén transit times. This was a very slowly growing mode and we did not attempt to resolve its growth rate. Rather, we followed its evolution until a new axisymmetric equilibrium that possessed a 1/0 flow field near the outer radius appeared. Timesteps were attained that corresponded to Courant numbers in excess of 60.

Finally, the spontaneous reversal of the magnetic field about a high pinch ratio plasma was demonstrated. This proved to be the most difficult simulation for a number of reasons. In the case of an initial high pinch ratio plasma, the singular layer is quite close to the boundary. In order to minimize the number of mesh points while maintaining reasonable resolution near the wall, a variable mesh spacing was used ($\Delta x_{\text{wall}}/\Delta x_{\text{center}} \sim 10$). The plasma displayed a late time reversal of B_z brought about by a 1/1 resistive kink. This is in agreement with the results of Pritchett.^{74,75}

The most challenging problems that were simulated were the initially low pinch ratio plasmas that were subjected to time varying external electric fields. In these cases, the plasma was pinched or compressed by the magnetic fields. The compression led to numeric difficulties that had to be resolved

by the inclusion of a Von Neumann⁵⁶ artificial viscosity in the momentum and energy equations. Once the time dependant electric field and the artificial viscosity were included, good qualitative agreement with Sykes and Wesson,⁴⁵ and Gowers, et. al.⁴⁶ was obtained.

VII.2 Conclusions

For the internal kink modelled in a Cartesian coordinate system, it has been shown that IMP can accurately determine the linear growth rates and can trace the nonlinear evolution of the plasma through the saturation of the 1/1 mode. With the inclusion of resistivity in the model, the presence of a new plasma state that contains only a slowly growing 3/1 mode is detected. The variation of magnetic Reynolds number S simulations showed that increased resistivity enhanced the growth rate of the 1/1 mode. This was in agreement with the theory of Coppi, et. al.⁷

The simulations performed in a torus in cylindrical geometry have demonstrated the versatility of the computational model in IMP. The lowered growth rates and final velocities attained are due to the stabilizing effects of the curvature which causes the plasma column into closer proximity with the outer wall. IMP was able to trace the nonlinear evolution of the 1/2 mode in only 280 cycles and on a much coarser mesh than was used in the linear code. Finally, the existance of a final axisymmetric state with finite--though non-growing--flow fields shows the necessity for having fully non-linear models which can trace a plasma's state through long periods of time.

The reversed field pinch (RFP) calculations have led to independent confirmation of the simulations of Sykes and Wesson,⁴⁵ and Gowers, et. al.⁴⁶ The main difference in our models is that IMP uses a scalar resistivity which does not cause as much peaking of the current as does the tensor model of

Sykes and Wesson. However, the conclusion that the nonlinear $1/1$ resistive kink, coupled with higher n kink modes ($1/2$ and $1/4$), is the driving mechanism that leads to the spontaneous field reversal is born out in our calculation.

The use of variable timestep size controls and Newton-Raphson iterations to a convergence criterion have proven to be extremely valuable to the success of this code. Once again, the inclusion of an artificial viscosity has also been shown to be required when any compression is occurring. Finally, the general model in IMP has been shown to be a useful tool--although one whose use must be carefully considered--in the study of magnetized plasmas.

VII.3 Future Work

Much work lies ahead in the development of realistic three-dimensional codes. In our model, only the first non-ideal transport term, resistivity has been included. The next important term to include is thermal conductivity. Following this, a model to describe the energy losses due to radiation must be included.^{45,69} Also, one must consider the actual transport of radiation throughout the plasma if the plasma becomes optically thick.⁷⁶

A treatment of concentration points of coordinate systems must be included to allow the simulation of circular devices. Also, a better understanding of the effects of mixed derivatives on the time centering and stability of numeric techniques must be achieved.

While much is still to be done to improve the physics model contained in IMP, the implementation of the algorithm must also be considered.

The next generation of IMP, CRIMP (CRAY IMP), will be designed to run on the CRAY-1 computer. While the current IMP can execute on the CRAY, it is grossly inefficient for this single level memory, vector processor.

In this section we will be repeatedly referring to vectors and vectorizability. Therefore, we must have a working definition of a vector and what is vectorizable. The term vector on a computer refers to an array of n elements separated in core by some constant increment m . A vectorizable sequence of code is one in which the same operations are performed on all the elements of a vector. An example of this is

```
DO 10 I = 1,1000
```

```
    A(I) = B(I)*C(I) + D(I+1)*C(I+1)
```

```
10  CONTINUE      .
```

Here A, B, C, and D are vectors, and we are performing the same operations on all 1000 elements. The following loop is not vectorizable:

```
DO 20 I = 2,1000
```

```
    A(I) = A(I-1) + B(I)*C(I)
```

```
20  CONTINUE      .
```

The reason that this loop is not vectorizable is because the computation of $A(I)$ requires the value of $A(I-1)$. This is only known after the previous computation. The vector processor works by starting a string of up to 64 numbers (on the CRAY) through a vector functional unit. The first answer comes out after the same number of clock cycles as it would from a scalar unit with the same function. After the first answer comes out, each succeeding answer

is returned at the rate of 1 per clock period. In the case of loop 20, the input stream of numbers for A is unknown.

As was explained in Chapter III, the basic nonlinear algorithm solved is as follows. First we bring a row of our mesh into SCM/SSM.* Next we repeatedly use a block tridiagonal solver to advance as many Newton-Raphson iterations along the row as are required to achieve a convergence criterion. We then store the results back in LCM** and repeat the procedure on the next row. First of all, on the CRAY we do not need to move the information around in memory. Next, the solution of the block-tridiagonal matrix requires the inversion of smaller 8 by 8 submatrices at each grid point. This is accomplished via LU decomposition. The LU decomposition is inherently non-vectorizable since we must solve a recursion relation. The way to convert this to a vectorizable problem is to iterate n rows of our mesh simultaneously, where n is a number in the range 1 to 64. This vectorizes the block-tridiagonal solver and also vectorizes almost all calculations required to generate the elements of the matrix.

One other change that could lead to a great savings in time is to change our basic iteration technique. The Newton-Raphson iteration technique converges at an ϵ^2 rate,⁶¹ but it forces us to invert the block-tridiagonal system. The Cord method uses the value of the Jacobian at an older iteration to approximate the correct Jacobian and only requires a matrix multiplication to give us our next set of iterates. We can, therefore,

* Small Core or Semiconductor Memory

** Large Core Memory

use the full tridiagonal solver to get a Jacobian, then use this Jacobian for a number of iterations, and, perhaps, even for a number of timesteps, until the iterations fail to converge. We then update the Jacobian via the full block-tridiagonal solver. This new technique could lead to speed-ups of an order of magnitude or more by the elimination of most of the Jacobian inversion.

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APPENDIX A

2-D TEARING MODE SIMULATION

The two-dimensional tearing mode instability in a sheet pinch was simulated in the IMP code. The purpose of the simulation was to verify that the resistive terms in the MHD equations had been correctly incorporated into the code.

The tearing mode instability does not exist in ideal MHD since the instability is caused by the fluid detaching itself from the magnetic field lines (forbidden in ideal MHD) near a singular surface ($k \cdot B = 0$). The conditions can occur whenever the field is sheared or reversed. The fluid flow forces the magnetic field to change its topology near the singular surface. The field lines tear and reconnect about the singular surface forming magnetic islands.

The initial analytic studies on the tearing mode were done by Furth, Killeen and Rosenbluth.¹⁷ They gave a growth rate $\gamma \propto R^{-3/5}$ which was proportional to the magnetic Reynolds number $S^{2/5}$ (see Chapter II). The growth rate was slow compared to ideal MHD timescales but faster than the resistive diffusion timescale, $\tau_R \propto R^{-1/2}$. These results were also obtained and extended computationally into the nonlinear regime by Schnack.¹⁸

For the test of IMP, a copy of Schnack's code was obtained and both codes were started with identical initial conditions. Due to the sharpness of the tearing layer, both codes used identical nonuniform mesh spacing for better resolution in this region. This also, then, tested our nonuniform zoning capability. Figure A.1 shows the initial flux contours in both

codes, while Figure A.2 shows the cross section of the perturbation eigenfunctions which highlights the need for the nonuniform mesh. The problem was run three times in IMP. In each run we rotated the plane of the simulation to verify that the code would produce identical results no matter how the problem was run. We then compared the growth rates calculated by IMP to Schnack's code. The growth rate was determined in both codes by dividing the growth of the reconnected flux (see Schnack¹⁸) on the simulation plane by the growth rates from both codes agreed to four significant figures. The main difference found was that IMP's improved iteration scheme (Section III.5), coupled with the use of the non-conservation form of the momentum equation (Section II.2), allowed the successful use of a timestep 100 times larger than that used by Schnack's code. IMP was able to run this problem at Courant numbers of 120 to 150 and experienced no problems with numeric instabilities.

Figure A.3 shows the growth rate calculated by the reconnected flux versus time. The peak in this plot at $t = 7$ is found in both IMP and Schnack's code. Past $t = 7$ we see the growth rate decreasing due to nonlinear saturation of the mode. In Fig. A.4 a plot of Courant number versus time shows the ability of IMP to run at many times the Courant condition which would limit an explicit code. This 2-D run has traced the linear growth of the tearing mode and the onset of nonlinear saturation in 1.0 timesteps-- less than 10 minutes of CDC-7600 time.

Figure A.1

The initial magnetic flux contours used in both IMP and Schnack's code.

Figure A.2a

The perturbation eigenfunctions of magnetic field used in both IMP and Schnack's code. Note the strongly peaked nature of B_y as it crosses the origin.

Figure A.2b

The perturbation eigenfunctions of momentum that were used. Once again, note the highly localized nature of the perturbations near the axis.

Figure A.3

The growth rate of the tearing mode instability calculated by IMP. The peak at $t \sim 7$ was found in both our model and Schnack's.

Figure A.4

The Courant numbers are plotted versus time for IMP in the preceeding simulation. The traces, labeled 1-4, are for the Courant number for 1) x direction hydro, 2) y direction hydro, 3) z direction hydro, and 4) resistive diffusion.

APPENDIX B

The REDUCE Generator Code

The source code used to generate the Jacobian matrix elements via the REDUCE algebraic code system is listed below.

```

off echo$
write "starting definitions for mhd(3d) equations";

comment This file contains the definition of the MHD equations in
generalized orthogonal curvilinear coordinates. They have been time
and space discretised by the methods outlined in Chapter III. Only
the implicit terms are included here as they provide the only
contributions to the Jacobian.

off exp;
order hfac,hfacp,ffac,ffacp,reyni,rmagi,gam1,etab,delt1i,
dh2b2,dh3b3,swu;
factor hfac, nfacp, ffac, ffacp;
*cardno:=10$
operator fi,fx,v1b,v2b,v3b,b1b,b2b,b3b,rhob,ub,u2n,swu,presb,rs1,rs2,
press,etab,eta,al,be,ga,h12bi,h13bi,h23bi,h12i,h13i,h23i,fh12,
fh22,fh,delt1i,dh1dx2,dh2dx1,dh3dx1,dh3dx2,defadp,defadr,dh1a+3,
dh2dx3,s1,s2,s3,hfac,delt2i,delt3i,fh1a,fh2a,fh3a,h12a,h13a,h23a,
dh1b1,dh2b2,dh3b3,pb1,pb2,pb3,pb1b,pb2b,pb3b,
vsq,vsqb,b2b1,b3b1,fforce,d2hb1,d3hb1,ffac,hfacp,
dh12b3,dh13b2,dh23b1,cort1,cort2,cort3,bsq,hvolb,hvol,q1,q2,q3$

comment define f as f of u;

forall j let fu(1,j)=u2n(1,j)$
forall j let fu(2,j)=u2n(2,j)$
forall j let fu(3,j)=u2n(3,j)$
forall j let fu(4,j)=u2n(7,j)*u2n(4,j)$
forall j let fu(5,j)=u2n(7,j)*u2n(5,j)$
forall j let fu(6,j)=u2n(7,j)*u2n(6,j)$
forall j let fu(7,j)=u2n(7,j)$
forall j let fu(8,j)=u2n(8,j)$

comment define the f functions for the first timestep;

forall j let fx(1,j)=0$

```

```

forall j let fx(2,j)=b2b(j)*v1b(j)-b1b(j)*v2b(j)-reyni*etab(i)*
  del11(fj)*h12b1(j)*dh2b2(j)$
forall i let fx(3,i)=b3b(i)*v1b(i)-b1b(i)*v3b(i)-reyni*etab(i)*
  del11(fj)*h13b1(j)*dh3b3(j)$
forall j let fx(4,j)=rhob(i)*v1b(j)**2+q1(i)
  del11(fj)/fh1a1(i)*gnu*(u2n(4,i)-u2n(4,i-1))$
forall i let fx(5,i)=rhob(i)*v1b(i)*v2b(i)+q2(i)
  del11(fj)/fh1a1(i)*gnu*(u2n(5,i)-u2n(5,i-1))$
forall i let fx(6,i)=rhob(i)*v1b(i)*v3b(i)+q3(i)
  del11(fj)/fh1a1(i)*gnu*(u2n(6,i)-u2n(6,i-1))$
forall i let fx(7,i)=rhob(i)*v1b(i)
  del11(fj)/fh1a1(i)*gnurho*(u2n(7,i)-u2n(7,i-1))$
forall i let fx(8,i)=gamma*presb(i)*v1b(i)
  del11(fj)/fh1a1(i)*gnutherm*(u2n(8,i)-u2n(8,i-1))$

comment define the force functions;
for k=1:8 do forall j let fforce(k,j)=0$
forall i let fforce(1,i)=0$
forall i let fforce(2,i)=4*press(i)/z**fh1a1(j)
  del11(fj)/fh3b1(i)$
forall i let fforce(3,i)=b1b(i)*h12b1(j)*dh2b2(j)$
forall i let fforce(4,i)=b1b(i)*h13b1(j)*dh3b3(j)$
forall i let fforce(5,i)=gnu*(v1b(i)*(press(i)-press(i-1))
  fh1a1(i)*rhob(i)*etab(i)*dh3b3(j)*del11(fj)-d5nb1(i)*dh3b3(i)*
  rhob(i)*dh2b2(j)*del11(fj)-d2ho1(i)*dh2b2(j)*h12b1(j)**2))
  gnu*(v1b(i)*(u2n(4,i)-u2n(4,i-1)+q2(i))*(u2n(5,i)-u2n(5,i-1))
  +q3(i)*(u2n(6,i)-u2n(6,i-1))/fh1a1(j))$

comment define the colax terms;
for k=1:3 do forall i let corrt1(k,i)=0$
forall j let corrt1(1,j)=0$
forall i let
  corrt1(4,i)=dh2dx1(i)*h12b1(i)*rhob(i)*v2b(j)**2
  +dh3dx1(i)*h13b1(i)*rhob(i)*v3b(i)**2)
  +kap*rhob(i)*v1b(i)$
forall i let
  corrt1(5,i)=dh2dx1(i)*h12b1(i)*rhob(i)*v1b(i)*v2b(j)$
forall i let
  corrt1(6,i)=dh3dx1(i)*h13b1(i)*rhob(i)*v1b(i)*v3b(j)$
forall i let corrt1(8,i)=-kap*rhob(i)*vsqb(i)$

comment define the source functions sl;
for k=1:8 do forall j let sl(k,j)=0$

```


comment define the bar functions to the program var=swu;

```
forall j let press(j)=u2n(8,j)$
forall j let b1b(j)=swu(1,j)$
forall j let b2b(j)=swu(2,j)$
forall j let b3b(j)=swu(3,j)$
forall j let v1b(j)=swu(4,j)$
forall j let v2b(j)=swu(5,j)$
forall j let v3b(j)=swu(6,j)$
forall j let rhob(j)=swu(7,j)$
forall j let presb(j)=swu(8,j)$
```

comment define the proc. delt =the kronicker delta function;

```
integer procedure delt(i,k)$
begin if i=k then return 1 else return 0$ end$
```

comment define the proc. pointtoave =map the correspondance
of a value point to an average point\$

```
procedure pointtoave(i,j,k)$
begin if (j-k) or (j-k+1) then return 1/2 else return 0$ end$
```

comment define the derivatives of u and uaverage;

```
forall i,k,m,n let df(u2n(k,j),u2n(m,n))=delt(i,k,m)*delt(j,n)$
forall i,k,l,m let df(swu(k,j),u2n(l,m))=delt(i,k,l)*pointtoave(j,m)$
forall i,k,m,n let df(swu(k,j),swu(m,n))=delt(i,k,m)*delt(j,n,n+1)$
```

comment define the dnb arrays and their derivatives\$

```
forall j,k,l let df(dh1b1(j),u2n(k,l))=delt(j,k,l)*delt(l,l+1)*fn1$
-delt(l,l-1)*fn1(l,l-1,j)$
forall j,k,l let df(dh2b2(j),u2n(k,l))=delt(j,k,l)*delt(l,l+1)*fn2(l)
-delt(l,l-1)*fn2(l,l-1,j)$
forall j,k,l let df(dh3b3(j),u2n(k,l))=delt(j,k,l)*delt(l,l+1)*fn3(l)
-delt(l,l-1)*fn3(l,l-1,j)$
```

comment define the vsq and vsq derivatives\$

```
forall j,k,l let df(vsq(j),u2n(k,l))=delt(j,j,l)*2*delt(4,k)*u2n(4,l)
+delt(5,k)*u2n(5,l)+delt(6,k)*u2n(6,l))$
forall j,k,l let df(vsqb(j),swu(k,l))=delt(j,j,l)*2*(delt(4,k)*swu(4,l)
+delt(5,k)*swu(5,l)+delt(6,k)*swu(6,l))$
forall j,k,l let df(vsqb(j),u2n(k,l))=pointtoave(j,l)
*delt(vsqb(j),swu(k,j))$
```

```

comment define the bsq operator;

forall j,k,l let df(bsq(j),u2n(k,l))=delt(j,l)*2*(delt(1,k)*u2n(1,l)
+del(2,k)*u2n(2,l)+del(3,k)*u2n(3,l))$

comment define the b2b1, etc. derivatives
where b2b1 = b2b(j)*(fh22(j)*u2n(2,j)-fh22(j-1)*u2n(j-1))*h12i(j);

forall j,k,l let df(b2b1(j),u2n(k,l))=h12bi(j)*(dh2b2(j)*
df(b2b(j),u2n(k,l))+b2b(j)*df(dh2b2(j),u2n(k,l)))$
forall j,k,l let df(b3b1(j),u2n(k,l))=h13bi(j)*(dh3b3(j)*
df(b3b(j),u2n(k,l))+b3b(j)*df(dh3b3(j),u2n(k,l)))$

comment define the derivatives of eta and etab$

forall j,k,l let df(eta(j),u2n(k,l))=delt(j,l)*(detadp(l)*
df(press(l),u2n(k,l))+delt(k,7)*detadr(l))$
forall j,k,l let df(etab(j),swu(k,l))=delt(j,l)*(detadp(l)*
df(presb(l),swu(k,l))+delt(k,7)*detadr(l))$
forall j,k,l let df(etab(j),u2n(k,l))=pointtoove(j,l)
*df(etab(j),swu(k,j))$

comment define the artificial viscosity operators q1,q2,q3:

forall j let q1(j)=cz1*rhob(j)*(u2n(4,j)-u2n(4,j-1))**2$
forall j let q2(j)=cz2*rhob(j)*(u2n(5,j)-u2n(5,j-1))**2$
forall j let q3(j)=cz3*rhob(j)*(u2n(6,j)-u2n(6,j-1))**2$

comment define the derivatives of the pseudo-constant operators;

forall k,j let df(al(k),j)=0$
forall k,l let df(be(k),l)=0$
forall k,l let df(ga(k),l)=0$
forall k,l let df(h12bi(k),l)=0$
forall k,l let df(h13bi(k),l)=0$
forall k,l let df(h23bi(k),l)=0$
forall k,l let df(h12i(k),l)=0$
forall k,l let df(h13i(k),l)=0$
forall k,l let df(h23i(k),l)=0$
forall k,l let df(h12a(k),l)=0$
forall k,l let df(h13a(k),l)=0$
forall k,l let df(h23a(k),l)=0$
forall j,l let df(rs1(j),l)=0$
forall j,l let df(rs2(j),l)=0$
forall j,l let df(hvolb(j),l)=0$
forall j,l let df(hvol(j),l)=0$

```

```

forall j,l let df(ffac(j),l)=0$
forall j,l let df(hfacp(j),l)=0$
forall k,j,l let df(hfac(k,j),l)=0$
forall k,l let df(fh1a(k),l)=0$
forall k,l let df(fh2a(k),l)=0$
forall k,l let df(fh3a(k),l)=0$
forall k,l let df(fh12(k),l)=0$
forall k,l let df(fh22(k),l)=0$
forall k,l let df(fh32(k),l)=0$
forall k,l let df(delt1i(k),l)=0$
forall k,l let df(delt2i(k),l)=0$
forall k,l let df(delt3i(k),l)=0$
forall k,l let df(dh1dx2(k),l)=0$
forall k,l let df(dh2dx1(k),l)=0$
forall k,l let df(dh3dx1(k),l)=0$
forall k,l let df(dh3dx2(k),l)=0$
forall k,l let df(dh1dx3(k),l)=0$
forall k,l let df(dh2dx3(k),l)=0$
forall j,l let df(d2hb1(j),l)=0$
forall j,l let df(d3hb1(j),l)=0$
forall k,l let df(detadp(k),l)=0$
forall k,l let df(detadr(l),k)=0$

write "end definition of mhd equations "$

on rat,nat; order al,reyni,etab,swu;
array symj(8,8), asymj(8,8), symjp(8,8), asymjp(8,8);

comment procedure to write to disk;

procedure wrts();
begin
for k:=1:8 do for l:=1:8 do write symj(l,k):=symj(l,k);
for k:=1:8 do for l:=1:8 do write symjp(l,k):=symjp(l,k);
for k:=1:8 do for l:=1:8 do write asymj(l,k):=asymj(l,k);
for k:=1:8 do for l:=1:8 do write asymjp(l,k):=asymjp(l,k);
end;

operator symm, asymm;
write "begin forming the symmetric & antisym coefficients";

comment first we get the force and coriolus terms;
for all m let symm(m)=ffacp*fforce(m,j+1)+dtby2*cor1(m,j+1)/2;

comment then the flux terms;
for all m let asymm(m)=al(m)*fx(m,j+1);

```

```

comment now form the Jacobian matrix elements;
for m:=1:8 do begin write "m= ",m; for k:=1:8 do
begin
  symj(m,k):=df(symm(m),u2n(k,j));
  symjp(m,k):=df(symm(m),u2n(k,j+1));
  asymj(m,k):=df(asymm(m),u2n(k,j));
  asymjp(m,k):=df(asymm(m),u2n(k,j+1));
end; end;
write "coefficients arrays now complete";
out "sym.jac": off nat; wrts(), shut "sym.jac"; on nat;
write "coefficients written to disk--file= sym.jac ";

write "writing FORTRAN coding";

off nat; on nat,fort,herc;
in "indexed"; out "sym.for";
write "$cat 'me* c b'me$ l'me v1 + l',rom";
write "$a: out hsp l'me dest. box v1 jacobians";
write "      subroutine flx ( itj, itjp )";
write "      use comm3d";
write "      use kinkcom";
write "      data czzz / 8. /";
write "      j = itj";
write "      jp1 = itjp";
write "      h1p = ' / fh':fjp1";
write "      cz1 = cz2 = cz3 = 0."
write "      if ( u2n(v1)-u2n(v1m) .lt. 0. ) cz1 = czzz";
write "      if ( u2n(v2)-u2n(v2m) .lt. 0. ) cz2 = czzz";
write "      if ( u2n(v3)-u2n(v3m) .lt. 0. ) cz3 = czzz";
write "      ";
write "c.... calculate the jacobian of the j+1/2 interface";
write "      ";
for k:=1:8 do begin for l:=1:8 do begin
if (symj(l,k) neq 0 and symjp(l,k) neq 0) then begin
write symj(l,k):=symj(l,k);
if symjp(l,k)-symj(l,k)=0 then
  write "      symjp('l',' ',k,")=symj('l',' ',k,")";
if symjp(l,k)+symj(l,k)=0 then
  write "      symjp('l',' ',k,")=-symj('l',' ',k,")";
if (symjp(l,k)-symj(l,k) neq 0 and symjp(l,k)+symj(l,k) neq 0) then
write symjp(l,k):=symjp(l,k);
end;
if (asymj(l,k) neq 0 and asymjp(l,k) neq 0 ) then begin
write asymj(l,k):=asymj(l,k);
if asymjp(l,k)-asymj(l,k)=0 then
  write "      asymjp('l',' ',k,")=asymj('l',' ',k,")";

```

```

if asymjp(i,k)+asymj(i,k)=0 then
  write "      asymjp(",i,",",k,")=-asymj(",i,",",k,")";
if (asymjp(i,k)-asymj(i,k) neq 0 and asymjp(i,k)+asymj(i,k) neq 0) then
write asymjp(i,k):=asymj(i,k);
end;
end; end;
write "      return";
write " ";
write "      end";
shut "sym.for";
write "FORTRAN is written";

```

```

comment begin the file INUEXPED;

```

```

comment This file is used to remove the 2-dimensional indexing of
arrays and to change the names of some of the REDUCE program
variables into the notation used in the code;

```

```

off echo;
write "starting substitutions for indexes";

```

```

let swu(1,j)=swu(b1)$
let swu(2,j)=swu(b2)$
let swu(3,j)=swu(b3)$
let swu(4,j)=swu(v1)$
let swu(5,j)=swu(v2)$
let swu(6,j)=swu(v3)$
let swu(7,j)=swu(rho)$
let swu(8,j)=swu(en)$
let u2n(1,j)=u2n(b1)$
let u2n(2,j)=u2n(b2)$
let u2n(3,j)=u2n(b3)$
let u2n(4,j)=u2n(v1)$
let u2n(5,j)=u2n(v2)$
let u2n(6,j)=u2n(v3)$
let u2n(7,j)=u2n(rho)$
let u2n(8,j)=u2n(en)$
let hfac(1,j)=hfac(1)$
let hfac(2,j)=hfac(2)$
let hfac(3,j)=hfac(3)$
let hfac(4,j)=hfac(4)$
let hfac(5,j)=hfac(5)$
let hfac(6,j)=hfac(6)$
let hfac(7,j)=hfac(7)$
let hfac(8,j)=hfac(8)$
let swu(1,j+1)=swu(b1p)$
let swu(2,j+1)=swu(b2p)$

```

```

let swu(3, j+1)=swu(b3p)$
let swu(4, j+1)=swu(v1p)$
let swu(5, j+1)=swu(v2p)$
let swu(6, j+1)=swu(v3p)$
let swu(7, j+1)=swu(rhop)$
let swu(8, j+1)=swu(enp)$
let u2n(1, j+1)=u2n(b1p)$
let u2n(2, j+1)=u2n(b2p)$
let u2n(3, j+1)=u2n(b3p)$
let u2n(4, j+1)=u2n(v1p)$
let u2n(5, j+1)=u2n(v2p)$
let u2n(6, j+1)=u2n(v3p)$
let u2n(7, j+1)=u2n(rhop)$
let u2n(8, j+1)=u2n(enp)$
let hfac(1, j+1)=hfacp(1)$
let hfac(2, j+1)=hfacp(2)$
let hfac(3, j+1)=hfacp(3)$
let hfac(4, j+1)=hfacp(4)$
let hfac(5, j+1)=hfacp(5)$
let hfac(6, j+1)=hfacp(6)$
let hfac(7, j+1)=hfacp(7)$
let hfac(8, j+1)=hfacp(8)$
let swu(1, j-1)=swu(b1m)$
let swu(2, j-1)=swu(b2m)$
let swu(3, j-1)=swu(b3m)$
let swu(4, j-1)=swu(v1m)$
let swu(5, j-1)=swu(v2m)$
let swu(6, j-1)=swu(v3m)$
let swu(7, j-1)=swu(rhom)$
let swu(8, j-1)=swu(enm)$
let u2n(1, j-1)=u2n(b1m)$
let u2n(2, j-1)=u2n(b2m)$
let u2n(3, j-1)=u2n(b3m)$
let u2n(4, j-1)=u2n(v1m)$
let u2n(5, j-1)=u2n(v2m)$
let u2n(6, j-1)=u2n(v3m)$
let u2n(7, j-1)=u2n(rhom)$
let u2n(8, j-1)=u2n(enm)$
let hfac(1, j-1)=hfac(b1m)$
let hfac(2, j-1)=hfac(b2m)$
let hfac(3, j-1)=hfac(b3m)$
let hfac(4, j-1)=hfac(v1m)$
let hfac(5, j-1)=hfac(v2m)$
let hfac(6, j-1)=hfac(v3m)$
let hfac(7, j-1)=hfac(rhom)$
let hfac(8, j-1)=hfac(enm)$

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let fh1a(j+1)=fh1a(jp1)$
let fh2a(j+1)=fh2a(jp1)$
let fh3a(j+1)=fh3a(jp1)$
let fh12(j+1)=fh12(jp1)$
let fh22(j+1)=fh22(jp1)$
let fh32(j+1)=fh32(jp1)$
let h12i(j)=h12i$
let h13i(j)=h13i$
let h23i(j)=h23i$
let h12i(j+1)=h12ip$
let h13i(j+1)=h13ip$
let h23i(j+1)=h23ip$
let h12bi(j+1)=h12bi(jp1)$
let h13bi(j+1)=h13bi(jp1)$
let h23bi(j+1)=h23bi(jp1)$
let del11i(j+1)=del11i(jp1)$
let del12i(j+1)=del12i(jp1)$
let del13i(j+1)=del13i(jp1)$
let detadp(j+1)=detadp(jp1)$
let detadr(j+1)=detadr(jp1)$
let etab(j+1)=etab(jp1)$
let s1(j+1)=s1(jp1)$
let s2(j+1)=s2(jp1)$
let s3(j+1)=s3(jp1)$
let fh1a(j-1)=fh1a(jm1)$
let fh2a(j-1)=fh2a(jm1)$
let fh3a(j-1)=fh3a(jm1)$
let fh12(j-1)=fh12(jm1)$
let fh22(j-1)=fh22(jm1)$
let fh32(j-1)=fh32(jm1)$
let h12i(j-1)=h12im$
let h13i(j-1)=h13im$
let h23i(j-1)=h23im$
let h12bi(j-1)=h12bi(jm1)$
let h13bi(j-1)=h13bi(jm1)$
let h23bi(j-1)=h23bi(jm1)$
let del11i(j-1)=del11i(jm1)$
let del12i(j-1)=del12i(jm1)$
let del13i(j-1)=del13i(jm1)$
let detadp(j-1)=detadp(jm1)$
let detadr(j-1)=detadr(jm1)$
let etab(j-1)=etab(jm1)$
let eta(j+1)=eta(jp1)$
let eta(j-1)=eta(jm1)$
let dh2dx1(j+1)=dh2dx1(jp1)$
let dh2dx1(j-1)=dh2dx1(jm1)$

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let dh3dx1(j+1)=dh3dx1(jp1)$
let dh3dx1(j-1)=dh3dx1(jm1)$
let dh1dx2(j+1)=dh1dx2(jp1)$
let dh1dx2(j-1)=dh1dx2(jm1)$
let dh3dx2(j+1)=dh3dx2(jp1)$
let dh3dx2(j-1)=dh3dx2(jm1)$
let dh1dx3(j+1)=dh1dx3(jp1)$
let dh1dx3(j-1)=dh1dx3(jm1)$
let dh2dx3(j+1)=dh2dx3(jp1)$
let dh2dx3(j-1)=dh2dx3(jm1)$
let s1(j+1)=s1(jm1)$
let s2(j+1)=s2(jm1)$
let s3(j+1)=s3(jm1)$
let dh1b1(j+1)=dh1b1j$
let dh1b1(j-1)=dh1b1j$
let ffac(j+1)=ffacjp$
let ffac(j-1)=ffacjm$
let dh2b2(j+1)=dh2b2jp$
let dh2b2(j-1)=dh2b2jm$
let dh3b3(j+1)=dh3b3jp$
let dh3b3(j-1)=dh3b3jm$
let b2b1(j+1)=b2b1jp$
let b2b1(j-1)=b2b1jm$
let b3b1(j+1)=b3b1jp$
let b3b1(j-1)=b3b1jm$
let vsq(j+1)=vsqjp$
let vsq(j)=vsqj$
let vsq(j-1)=vsqjm$
let vsqb(j+1)=vsqbp$
let vsqb(j)=vsqbj$
let h12a(j)=h12aj$
let h12a(j+1)=h12ajp$
let h13a(j)=h13aj$
let h13a(j+1)=h13ajp$
let h23a(j)=h23aj$
let h23a(j+1)=h23ajp$
let rs1(7,j)=rs1rj$
let rs1(7,j+1)=rs1rjp$
let rs1(8,j)=rs1ej$
let rs1(8,j+1)=rs1ejp$
let rs2(7,j)=rs2rj$
let rs2(7,j+1)=rs2rjp$
let rs2(8,j)=rs2ej$
let rs2(8,j+1)=rs2ejp$
let bsq(j)=bsqj$
let bsq(j+1)=bsqjp$

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let dh12b3(j)=dh12b3$
let dh12b3(j+1)=dn12b3p$
let dh13b2(j)=dh13b2$
let dh13b2(j+1)=dn13b2p$
let dh23b1(j)=dh23b1$
let dh23b1(j+1)=dn23b1p$
let d2hb1(j+1)=d2hb1p$
let d2hb1(j)=d2hb1$
let d3hb1(j+1)=d3hb1p$
let d3hb1(j)=a3hb1$
let swu(rho)**(-2)=rhobm2$
let swu(rhop)**(-2)=rhobpm2$
let swu(en)**(-2)=enbm2$
let swu(enp)**(-2)=enpbm2$
let bsq(j)=bsq$
let bsq(j+1)=bsqp$
let bsq(j-1)=bsqm$
write "indexes compressed";
end "indexreq";

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