An Accurate Characteristics-Splitting Scheme for Numerical Solution of MHD Equations *

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Abstract

A new approach to accurately simulate plasma flows is presented. The approach has three notable features: self-consistent treatment of flow and magnetic field equations, conservation formulation of the problem, and a characteristics-splitting scheme. Characteristics-splitting has been proven to work reliably for Navier-Stokes equations, and is shown here to be well suited for MHD problems. Since the Rankine-Hugoniot jump conditions are exactly satisfied by characteristics-splitting, this allows for monotonic capturing of discontinuities. Shocks and MHD waves are therefore readily handled by this scheme. This approach has been validated against a Riemann type problem for the unsteady case, and the Taylor state problem for the steady state. It provides a robust numerical framework for accurate simulation of plasma thruster flows.

1 Introduction

In the continuing effort to numerically simulate continuum plasma flow for propulsion problems, there remains a need for robust and accurate numerical methods.

Kimura[1] *et al.* and Fujiwara[2] started developing single-fluid 2-D models on simple geometries, and have continued to make improvements to their models. Currently, the efforts of Fujiwara[3] *et al.* are directed at studying the onset phenomenon using multi-fluid models. Caldo and Choueiri[4] have developed a multi-fluid model to study the effects of anomalous transport, described in ref. [5], on MPD flows. The effort by LaPointe[6] focused on studying the effect of geometry on performance. Sleziona[7] *et al.* have developed a numerical model for MPD thrusters and have refined it over a decade. This numerical model now works on an unstructured adaptive grid, and contains detailed models for many transport processes and multiple levels of ionization. Martinez-Sanchez[8],[9] *et al.* have developed multi-fluid 2-D/axisymmetric numerical models to study various aspects of the flow. Turchi[10] *et al.* use MACH2, an unsteady MHD solver developed for high power plasma gun simulation, to model PPTs and MPD thrusters in many geometries. MACH3[11], the next generation of MACH2, is also used to simulate possible 3-D effects in specific situations.

With the exception of refs. [9], [12] and [11], the codes described above solve the flow and magnetic field equations separately. Moreover, none of these codes solve all the equations in conservation form. Using conservation form, however, allows accurate capturing of any discontinuities, such as shocks and MHD waves, that may be of interest in many MHD flows.

The approach presented in this paper has three important features:

1. Self-consistent treatment of flow and magnetic field equations,

2. Conservative formulation of the problem,

3. Characteristics-splitting.

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These features will be described in the ensuing sections. The advantages of these three features is described in Section 2. The implementation methodology is described in Section 3 using a simple plasma flow model. Section 4 describes the tests that were performed to validate the scheme. The steps involved in applying the scheme to simulate propulsive plasma flows are described in Section 5.

2 Guiding Principles

The approach presented here is based on both physical and numerical considerations. Magnetic Reynolds' numbers in typical plasma thruster flows indicate that both convective and resistive diffusion of the magnetic field are important. The Alfvèn and fluid time scales are not very disparate. This implies that the full set of equations describing the flow field and magnetic field evolution have to be computed self consistently. Moreover, solving Maxwell's equations consistently with compressible gasdynamics equations naturally produces waves physically associated with the problem, such as Alfvèn and magnetosonic waves, as eigenvalues. Not doing so could lead to misleading conclusions about time step constraints.

Whenever possible, these equations should be solved in their conservation form. Apart from its physical meaning of global conservation of mass, momentum, magnetic flux, and energy, the conservation form possesses certain numerical advantages. Specifically, the treatment of boundaries is more transparent. More importantly, conservative formulation is necessary for accurately capturing discontinuities.

Conservative formulation, however, carries a penalty in cases where magnetic pressure is several orders of magnitude larger than thermodynamic pressure. Fortunately, it is not the case in most plasmas of interest to propulsion.

Furthermore, the conservation formulation allows the use of characteristics-splitting techniques for capturing discontinuities, without excessive numerical dissipation.

The resulting scheme would be time dependent, and can be used as a basis to simulate unsteady electromagnetic acceleration or, to simulate steady state MHD flows by solving unsteady equations to march towards steady state.

A scheme based on the principles described above is expected to be robust and can accommodate the addition of more complex physics. However, a simple plasma flow model will be used to illustrate the scheme.

3 Methodology of the New Solver

A sample MHD flow problem of a fully ionized, quasi-neutral plasma in thermal equilibrium and satisfying the validity of continuum approximation is used to illustrate the scheme. Subsequent physical models can be added as deemed appropriate, without significant changes to the underlying numerical building blocks of the solver. The governing equations for this problem can be written in the form:

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho\mathbf{u} \\ \mathbf{B} \\ \epsilon \end{bmatrix} + \nabla\cdot\begin{bmatrix} \rho\mathbf{u} \\ \rho\mathbf{u}\mathbf{u} + \bar{\bar{\mathrm{p}}} - \bar{\bar{\mathcal{B}}}_M \\ \mathbf{u}\mathbf{B} - \mathbf{B}\mathbf{u} \\ (\epsilon + P)\,\mathbf{u} - \frac{\mathbf{B}}{\mu_{\mathbf{o}}}(\mathbf{u}\cdot\mathbf{B}) \end{bmatrix} = \mathbf{S}, \quad (1)$$

where, $\bar{\bar{p}}$ is the pressure tensor, $\bar{\bar{\mathcal{B}}}_M$ is the Maxwell stress tensor, ϵ is the energy density, P is the total pressure, and $\mathbf{S}$ the vector of source terms. Other symbols have their usual MHD meaning. The source terms are due to round-off errors ($\nabla\cdot\mathbf{B}$) and physical dissipative effects:

$$\mathbf{S}_{\nabla\cdot\mathbf{B}} = (\nabla\cdot\mathbf{B})\begin{bmatrix} 0 \\ \frac{\mathbf{B}}{\mu_o} \\ \mathbf{u} \\ \frac{\mathbf{B}}{\mu_o}\cdot\mathbf{u} \end{bmatrix} \; and \; \mathbf{S}_{dis} = \nabla\cdot\begin{bmatrix} 0 \\ \bar{\bar{\tau}}_{vis} \\ \bar{\bar{\mathcal{E}}}_{res} \\ \mathbf{q} \end{bmatrix}. \quad (2)$$

Here, $\bar{\bar{\tau}}_{vis}$ is the viscous stress tensor, and $\bar{\bar{\mathcal{E}}}_{res}$ the resistive diffusion tensor.

The momentum equation contains the body force per unit volume, $\mathbf{j}\times\mathbf{B}$, written as the divergence of the Maxwell stress tensor $\bar{\bar{\mathcal{B}}}_M$, as described in ref. [13].

The convective diffusion of the magnetic field is written as a divergence of the antisymmetric tensor $\mathbf{u}\mathbf{B}-\mathbf{B}\mathbf{u}$. The resistive diffusion appears in the source term, also as divergence of a tensor, as in ref. [14],

$$\nabla\cdot\bar{\bar{\mathcal{E}}}_{res} = -\frac{1}{\mu_o}\nabla\times\left[\bar{\bar{\eta}}\cdot(\nabla\times\mathbf{B})\right],$$

in which $\bar{\bar{\eta}}$ is the full resistivity tensor.

The energy equation is written in terms of the energy density, whose parts are the internal energy, kinetic energy and the energy in magnetic field (per unit volume):

$$\epsilon = \frac{p}{\gamma - 1} + \frac{1}{2}\rho \mathbf{u}\cdot\mathbf{u} + \frac{\mathbf{B}\cdot\mathbf{B}}{\mu_{\mathbf{o}}},$$

with the definitions:

$$\begin{aligned} P &= p + \frac{\mathbf{B}\cdot\mathbf{B}}{2\mu_o}, \\ \mathbf{q} &= (\bar{\bar{\tau}}_{vis}\cdot\mathbf{u}) - (\bar{\bar{\eta}}\cdot(\mathbf{j}\times\mathbf{B})) + (\bar{\bar{\kappa}}_{th}\cdot\nabla T). \end{aligned}$$

Under some physical conditions, when the magnetic pressure is several orders of magnitude larger than thermodynamic pressure, the conservation form of the energy equation may not be suitable. In these cases, since p is calculated from subtraction of one large number ($B^2/2\mu_o$) from another (ϵ), the associated errors could be large. However, for the conditions that are of interest to plasma propulsion, the magnetic pressure is seldom two to three orders of magnitude greater than thermodynamic pressure. Thus the conservation form of the energy equation is, in general, numerically suitable here.

The treatment of the $\nabla\cdot\mathbf{B}$ terms are important, since they could be a cause of numerical instabilities, as explained in ref. [15]. The technique of Powell[16] to absorb this into the Jacobian ensures that any artificial source is convected away as,

$$\frac{\partial}{\partial t}(\nabla\cdot\mathbf{B}) + \nabla\cdot(\mathbf{u}\nabla\cdot\mathbf{B}) = 0. \tag{3}$$

Since the physical dissipation is written in the divergence form, the entire set of equations can be written in the form,

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla\cdot\left[\bar{\bar{\mathcal{F}}}_{conv} - \bar{\bar{\mathcal{F}}}_{dis}\right] = \mathbf{0}, \tag{4}$$

where, $\bar{\bar{\mathcal{F}}}_{conv}$ is the convective flux tensor, and $\bar{\bar{\mathcal{F}}}_{dis}$ the dissipative flux tensor.

3.1 Spatial Discretization

The numerical solution to this set of hyperbolic equations is based on techniques that are extensively used in computational fluid dynamics. In particular, the non-oscillatory scheme developed in terms of local extremum diminishing (LED) principle by Jameson[17] is used. In 2-D, the conservation law given by Eqn. (1) is expressed as,

$$\frac{d\mathbf{U}_{j,k}}{dt} + \left[\frac{\mathbf{Hr}_{j+\frac{1}{2},k} - \mathbf{Hr}_{j-\frac{1}{2},k}}{\Delta r} + \frac{\mathbf{Hz}_{j,k+\frac{1}{2}} - \mathbf{Hz}_{j,k-\frac{1}{2}}}{\Delta z}\right] = 0, \tag{5}$$

where, $\mathbf{U}$ is the vector of conserved variables, $\mathbf{Hr}$ is the approximation of flux in the $\hat{r}$ direction, and $\mathbf{Hz}$ the approximation of flux in the $\hat{z}$ direction.

The true flux, obtained from Eqn. (4), in the $\hat{r}$ direction can be split as,

$$\mathbf{Fr}(\mathbf{U}) = \mathbf{Fr}(\mathbf{U})^+ + \mathbf{Fr}(\mathbf{U})^-, \tag{6}$$

where the eigenvalues of $d\mathbf{Fr}^+/d\mathbf{U}$ are all non-negative, and the eigenvalues of $d\mathbf{Fr}^-/d\mathbf{U}$ are all non-positive. Then, the approximation of flux is estimated as,

$$\mathbf{Hr}_{j+\frac{1}{2},k} = \mathbf{Fr}^+_{j,k} + \mathbf{Fr}^-_{j+1,k}.$$

Using Eqn. (6), this can be rewritten as,

$$\mathbf{Hr}_{j+\frac{1}{2},k} = \frac{1}{2}\left(\mathbf{Fr}_{j,k} + \mathbf{Fr}_{j+1,k}\right) - \mathbf{Dr}_{j+\frac{1}{2},k},$$

where

$$\mathbf{Dr}_{j+\frac{1}{2},k} = \frac{1}{2}\left[\left(\mathbf{Fr}^+_{j+1,k} - \mathbf{Fr}^+_{j,k}\right) + \left(\mathbf{Fr}^-_{j+1,k} - \mathbf{Fr}^-_{j,k}\right)\right]. \tag{7}$$

There still remains a question of how $\mathbf{Fr}^+$ and $\mathbf{Fr}^-$ can be evaluated. This evaluation is possible if there is a matrix $\mathbf{A}$, such that

$$\mathbf{Fr}_{j+1,k} - \mathbf{Fr}_{j,k} = \mathbf{A}\cdot\left(\mathbf{U}_{j+1,k} - \mathbf{U}_{j,k}\right). \tag{8}$$

Note that, in the case the points $j+1$ and j are on opposite sides of a discontinuity, Eqn. (8) indicates that this scheme satisfies the Rankine-Hugoniot jump conditions *exactly*.

For a hyperbolic system of equations, $\mathbf{A}$ can be diagonalized as:

$$\mathbf{A} \equiv \mathbf{R}\mathbf{\Lambda}\mathbf{R}^{-\mathbf{1}}, \tag{9}$$

where $\mathbf{R}$ contains the right eigenvectors of $\mathbf{A}$ as its columns, and $\mathbf{R}^{-1}$ contains the left eigenvectors of $\mathbf{A}$ as its rows. $\mathbf{\Lambda}$ is the diagonal matrix of eigenvalues of $\mathbf{A}$. Since $\mathbf{\Lambda}$ can be easily split into,

$$\mathbf{\Lambda} = \mathbf{\Lambda}^+ + \mathbf{\Lambda}^-,$$

using Eqn. (9), $\mathbf{A}$ can be split. Thus if there exists an $\mathbf{A}$ such that Eqn. (8) is true, then $\mathbf{F}$ can be split. For the Euler equations, this matrix was derived by Roe[18]. However, this is not necessarily applicable to MHD equations. There have been efforts by Cargo[19] to derive such matrices for MHD equations. The literature[20] suggests that various forms of averaged matrices work satisfactorily.

Away from the discontinuities, the spatial accuracy of the scheme can be improved by including limiters, described in ref. [17]:

$$\mathbf{Dr}_{j+\frac{1}{2},k} = \frac{1}{2}\left|\mathbf{A}\right|[\Delta\mathbf{U}_{j+\frac{1}{2},k} - \mathbf{Lr}\left(\Delta\mathbf{U}_{j+\frac{3}{2},k},\Delta\mathbf{U}_{j-\frac{1}{2},k}\right)]. \quad (10)$$

Similar equations can be written for the corresponding terms in the $\hat{z}$ direction.

An alternative to characteristics-splitting for solving conservation form of the equations is to use artificial viscosity. In this formalism, the equivalent expression for Eqn. (7) is,

$$\mathbf{Dr}_{j+\frac{1}{2},k} = \frac{1}{2}\left|\lambda\right|_{max}\left(\Delta\mathbf{U}_{j+\frac{1}{2},k}\right). \quad (11)$$

However, as described in ref. [17], this tends to artificially smooth out the solution.

3.2 Temporal Discretization

Unlike in fluid mechanics, the equations of MHD allow many different types of waves to exist. Even though physically the flow velocity is the sought quantity of most interest to propulsion, numerically the velocity of the fastest wave is what determines the time-step constraints. In plasmas of propulsion interest, the fluid velocity is $\mathcal{O}(10^4)$ m/s. For a plasma with charge density $\mathcal{O}(10^{19})/m^3$ and thermodynamic pressures of $\mathcal{O}(10^{-1})$ Torr and magnetic pressure of $\mathcal{O}(10^1)$ Torr, the fast magnetosonic wave speed is typically of the same order of magnitude as the flow velocity. This indicates that an explicit time marching scheme is suitable. From the CFL criterion, the time step for such a problem would be $\mathcal{O}(10^{-8})$ s.

The physical dissipation, given by Eqn. (2), brings in a parabolic nature to the equations. It also bring in different characteristic time scales into the problem. They are:

Viscous diffusion: $= \frac{\rho\Delta r^2}{\eta_{visc}} \sim 10^{-8}$ s

Magnetic diffusion: $= \mu_o\sigma\Delta r^2 \sim 10^{-9}$ s

Heat conduction: $= \frac{\rho k_B\Delta r^2}{m\kappa_{th}} \sim 10^{-9}$ s

If these were vastly different, that would call for an implicit treatment of time stepping. That is not the case here, and an explicit time-stepping scheme was chosen.

4 Validation of the Scheme

4.1 Unsteady Case

Riemann problem The test problem chosen was of the classical Riemann problem type, which consists of a single jump discontinuity in an otherwise smooth initial conditions. In 1-D the problem is:

$$\mathbf{U}(x,0) = \begin{cases} \mathbf{U}_L & \text{if } x < \frac{L}{2} \\ \mathbf{U}_R & \text{if } x \geq \frac{L}{2} \end{cases}. \quad (12)$$

The Riemann problem was chosen because it is one of the very few that have an analytical solution. This problem provides an excellent illustration of the wave nature of the equations. The solution to the Riemann problem is useful to verify the capturing of both smooth waves (characteristics) as well as non-smooth waves (shocks).

The initial states used were very similar to the Sod's[21] problem for Euler equations. They were:

$$Left: \begin{cases} \rho = 1.0 \\ V_x = 0.0 \\ V_y = 0.0 \\ V_z = 0.0 \\ B_x = \frac{3}{4} \\ B_y = 1.0 \\ B_z = 0.0 \\ p = 1.0 \end{cases} \quad Right: \begin{cases} \rho = \frac{1}{8} \\ V_x = 0.0 \\ V_y = 0.0 \\ V_z = 0.0 \\ B_x = \frac{3}{4} \\ B_y = -1.0 \\ B_z = 0.0 \\ p = \frac{1}{10} \end{cases}. \quad (13)$$

Some sample results are shown in Fig. (1).

Results from characteristics-splitting and the artificial viscosity method are seen in Fig. (1). It is clear the characteristics-splitting captures the discontinuities more accurately.

In these figures, the fast rarefaction (FR) wave can be seen on the far right and the far left, as it is the fastest of the waves present in the problem. The slow shock (SS) and the compound wave (SM) have speeds less than that of the FR wave.

As shown in these figures, the scheme successfully captures the time-dependent discontinuities. A 2-D extension of this problem was tested, and the solver worked satisfactorily.

4.2 Steady State Case

Taylor state In order to simulate steady state MHD flows, this solver can be used to solve the unsteady equation to steady state. Then, an important question is whether it remains in that steady state. To answer this question, a test problem was chosen, whose

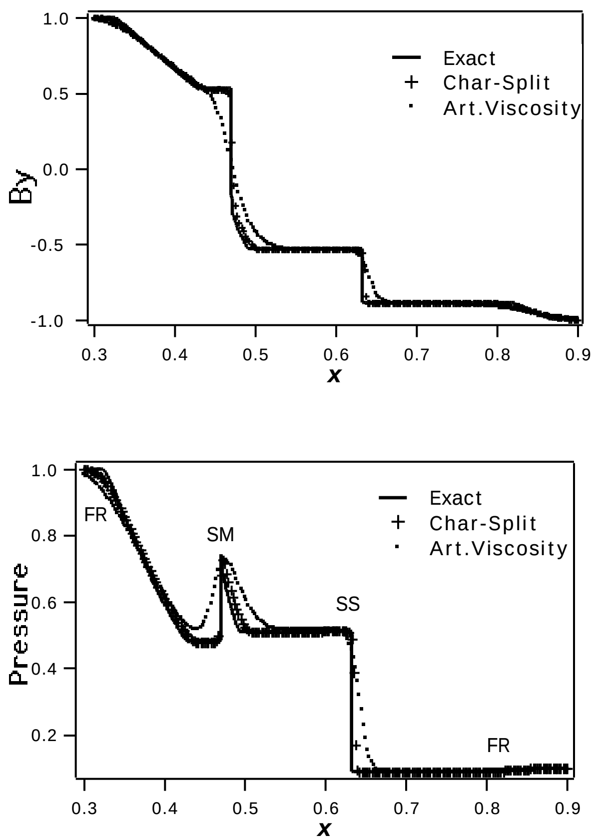

Figure 1: Comparison of exact magnetic field and pressure profiles with numerical solutions.

equilibrium solution is known analytically. This equilibrium solution is given as the initial condition for the solver. After marching several hundreds or thousands of time steps, a check is performed if the variables have changed from the initial conditions.

The test problem chosen for this simulation was the Taylor State[22] configuration. When a perfectly conducting plasma in an arbitrary initial condition is allowed to evolve, it will move quickly and dissipate energy before coming to rest. This stable equilibrium configuration can be analytically found using the minimum energy principle, and is of the form:

$$\nabla \times \mathbf{B} = \lambda \mathbf{B}, \tag{14}$$

where λ is an eigenvalue.

Since the current is parallel to the magnetic field, the $\mathbf{j} \times \mathbf{B}$ body force is identically zero. Furthermore, if there are no thermodynamic pressure gradients, the plasma is in a state of force-free equilibrium. For an axisymmetric geometry, the resulting magnetic field profile is:

$$B_\theta = B_0 J_1(\lambda r);\ B_z = B_0 J_0(\lambda r), \tag{15}$$

where B_o is a constant amplitude, J_0 and J_1 are Bessel functions of the first kind, of orders 0 and 1 respectively.

For a Cartesian grid of dimensions $L_x \times L_z$, with symmetry along the $\hat{y}$ direction, the magnetic field distribution satisfying Eqn. (14) is:

$$\begin{aligned} B_x &= -B_0\ \sin\left(\frac{m\pi x}{L_x}\right)\cos\left(\frac{n\pi z}{L_z}\right), \\ B_y &= B_0\ \sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi z}{L_z}\right), \\ B_z &= B_0\ \sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi z}{L_z}\right), \end{aligned} \tag{16}$$

where m and n are eigenvalues.

The code was run for several thousand time steps with this $\mathbf{B}$ profile and uniform pressure and density as initial conditions. The maximum local deviation from the equilibrium solution, for any of the variables, was less than 0.5% on a 50×50 grid, and even better on a finer grid.

5 Application to MHD Propulsion Flows

As already mentioned, the physical model adapted to illustrate the scheme is simplistic. Specifically, the equations described above assume a fully ionized plasma, with ideal equation of state, in thermal equilibrium, and with simplistic form of transport coefficients, and lack the description of many energy sinks. Furthermore no sheath models are included. However, as stated above, such physical effects can be added without affecting the numerical foundation.

The extension to include the effect of two temperatures and finite ionization can be done in two steps:

1. Adding a continuity equation for electrons:

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}_e) = m_e \dot{n}_e, \tag{17}$$

   where $\dot{n}_e$ is the net ionization/recombination rate, and $\mathbf{u}_e = \mathbf{u} - \mathbf{j}/en_e$,

2. Adding a separate energy equation for electrons.

Including ionization reactions will bring in a different time scale to the problem, and the time-stepping scheme has to be implicit. However, this does not conflict with the characteristics-splitting scheme.

Another improvement that could be implemented easily is to include a realistic equation of state, as there is no fundamental change in the scheme to have $p/\rho = f(T)$.

On the numerical side, it would be helpful to implement this scheme on an unstructured adaptive grid, as done in ref. [7], to make this applicable to an arbitrary geometry.

Accurate expressions for classical transport coefficients, such as thermal conductivity and viscosity, obtained from ref. [23], and anomalous coefficients, obtained from ref. [5], can easily be introduced. This is presently being implemented in a code to simulate self-field MPD thrusters.

6 Conclusion

An accurate numerical method for solving the MHD system has been validated against test problems. The scheme exhibits good accuracy in smooth regions and captures discontinuities monotonically. The scheme can be extended to include complicated physical models without affecting the underlying numerical foundation. This method is currently being implemented in a code to simulate plasma propulsion problems.

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