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A new 3D MHD algorithm: the distribution function method

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A new three-dimensional (3D) magnetohydrodynamic (MHD) algorithm is described. The 3D MHD equations are solved in conservative form using a finite-volume scheme. The hydrodynamic variables in a cell are updated by calculating fluxes across the cell interfaces. The fluxes of mass, momentum and energy across cell interfaces are calculated by integrating a Boltzmann-like distribution function over velocity space. The novel feature of the method is that the distribution function incorporates most of the electromagnetic terms. In addition, the electric field along cell edges, which is used to update the magnetic field at cell faces, is also calculated using the Boltzmann-like distribution function. An important aspect of the method is that it provides a theoretical framework to incorporate additional terms in the 3D MHD equations (e.g. an anisotropic ion stress tensor and anisotropic temperature distributions).

1. Introduction

The concept of using a Boltzmann-like distribution function to solve hydrodynamic equations is not new (Chu 1965; Sanders and Prendergast 1974; Pullin 1980; Macrossan 1989); these numerical techniques are also referred to as 'gas-kinetic' schemes. In recent years the gas-kinetic method has been applied to the Euler and Navier–Stokes equations using the collisional BGK model (Prendergast and Xu 1993; Xu and Prendergast 1994; Xu et al. 1995).

The basic idea of the method is described as follows. Consider the continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{V} = 0. \tag{1.1}$$

Integrating over a cell width Δx and a time step Δt, and applying Gauss' law, gives

$$\rho_T^{t+\Delta t} = \rho_T^t - \Delta t \int (\rho \mathbf{V})^{t+\Delta t/2} \cdot \mathbf{n}\, d^2x, \tag{1.2}$$

where ρ_T is the total mass in the cell, $\mathbf{n}$ is the outward normal to a cell face, and the flux $\rho \mathbf{V}$ is evaluated at the intermediate time step $t + \frac{1}{2}\Delta t$. Thus (1.2) updates the mass in a cell by summing the mass fluxes across each cell face. The flux at each interface is calculated using the distribution function method. This is easily understood by considering a single interface $i + \frac{1}{2}$ as shown in Fig. 1. The mass flux $\mathscr{F} = \rho V$ at interface $i + \frac{1}{2}$ is written as $\mathscr{F}_{i+1/2} = \mathscr{F}_L + \mathscr{F}_R$, where $\mathscr{F}_L$ is the flux

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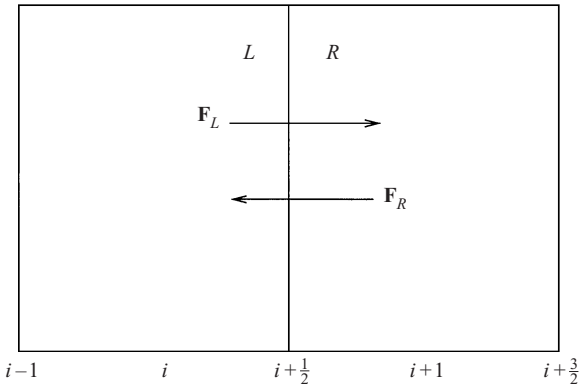


Figure 1. Left (L) and right (R) states at interface i, and the corresponding fluxes.

associated with particles moving from the left side (L) of the interface to the right side (R) of the interface, and $\mathscr{F}_R$ is the flux associated with particles moving from the right side (R) of the interface to the left side (L) of the interface. The flux is defined as

$$\mathscr{F} = \rho V = \int v f(v)\, dv, \tag{1.3}$$

so that

$$\mathscr{F}_L = \int_0^\infty v f_L(v)\, dv, \tag{1.4}$$

$$\mathscr{F}_R = \int_\infty^0 v f_R(v)\, dv, \tag{1.5}$$

where $f_L(v)$ and $f_R(v)$ are the velocity space distributions representative of the left- and right-hand states of the interface. Thus, once an appropriate velocity space distribution function $f(v)$ has been determined, it is used to calculate fluxes at cell interfaces.

In this paper we present a distribution function method relevant to ideal 3D MHD theory. The 3D MHD equations are solved in conservative form using a finite-volume scheme. The hydrodynamic variables are updated by calculating fluxes across the cell interfaces. The fluxes of mass, momentum and energy across cell interfaces are calculated by integrating a Boltzmann-like distribution function over velocity space. The novel feature of the method is that the distribution function incorporates most of the electromagnetic terms. The electric field along cell edges, which is used to update the magnetic field at cell faces, is also calculated using the Boltzmann-like distribution function. An important aspect of the method is that it can be generalized to incorporate additional terms in the 3D MHD equations (e.g. an anisotropic ion stress tensor and anisotropic temperature distributions).

The organization of the paper is as follows. In Sec. 2 we write down the 3D MHD equations in conservative form and the velocity space distribution function $f(v)$ used to calculate the fluxes. In Sec. 3 we demonstrate that the 3D ideal MHD equations can be recovered using the distribution function $f(v)$. In Sec. 4 we describe the details of calculating the mass, momentum and energy fluxes. In Sec. 5 we demonstrate that the distribution function method can also be used to calculate the electric field and can be used to update the magnetic field. An example of the

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3D MHD code is given in Sec. 6, where the Brio–Wu shock problem is solved. The results of this paper are summarized in Sec. 7.

2. MHD equations

The 3D MHD equations are written in conservative form as

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{V}) = 0, \tag{2.1}$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \boldsymbol{\nabla} \cdot \left[\rho \mathbf{V}\mathbf{V} + \left(P + \frac{B^2}{8\pi} \right) \mathbf{I} - \frac{\mathbf{B}\mathbf{B}}{4\pi} \right] = 0, \tag{2.2}$$

$$\frac{\partial \epsilon}{\partial t} + \boldsymbol{\nabla} \cdot \left[\mathbf{V} \left(\epsilon + P + \frac{B^2}{8\pi} \right) - \frac{\mathbf{B}}{4\pi} (\mathbf{V} \cdot \mathbf{B}) \right] = 0, \tag{2.3}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \boldsymbol{\nabla} \times (\mathbf{V} \times \mathbf{B}), \tag{2.4}$$

where

$$\epsilon = \frac{1}{2} \rho V^2 + \frac{3}{2} P + \frac{B^2}{8\pi}. \tag{2.5}$$

The equations are closed by assuming an adiabatic equation of state:

$$P/\rho^{\gamma} = \text{constant}.$$

We consider the following generalized transport equation

$$\frac{\partial n \langle \chi \rangle}{\partial t} + \boldsymbol{\nabla} \cdot n \langle \chi \mathbf{v} \rangle - n \left\langle \mathbf{a} \cdot \frac{\partial \chi}{\partial \mathbf{v}} \right\rangle = 0, \tag{2.6}$$

where

$$\mathbf{a} = \frac{1}{8\pi\rho} \frac{\partial B_x^2}{\partial x} \hat{\mathbf{e}}_x + \frac{1}{8\pi\rho} \frac{\partial B_y^2}{\partial y} \hat{\mathbf{e}}_y + \frac{1}{8\pi\rho} \frac{\partial B_z^2}{\partial z} \hat{\mathbf{e}}_z, \tag{2.7}$$

and the angular brackets are defined by

$$\langle \mathscr{G} \rangle = \int d\mathbf{v}\, \mathscr{G}(\mathbf{v})\, F(\mathbf{v}), \qquad \text{with} \qquad 1 = \int d\mathbf{v}\, F(\mathbf{v}).$$

The continuity equation is obtained from (2.6) by setting $\chi = m$, the momentum equation by setting $\chi = m\mathbf{v}$, and the energy equation by setting $\chi = \frac{1}{2} m v^2$. The question to be answered is the following: Can a distribution function $F(\mathbf{v})$ be found such that, when it is substituted into the transport equation (2.6), the ideal 3D MHD equations (2.1)–(2.3) are recovered?

The following distribution function satisfies this requirement:

$$F = F_1 + F_2, \tag{2.8}$$

where

$$F_1 = \frac{\exp(-u_1^2)}{(\pi v_{1x}^2)^{1/2}} \frac{\exp(-v_1^2)}{(\pi v_{1y}^2)^{1/2}} \frac{\exp(-w_1^2)}{(\pi v_{1z}^2)^{1/2}}, \tag{2.9}$$

$$F_2 = -(u_2 v_2 + u_2 w_2 + v_2 w_2) \frac{\exp(-u_2^2)}{(\pi v_{2x}^2)^{1/2}} \frac{\exp(-v_2^2)}{(\pi v_{2y}^2)^{1/2}} \frac{\exp(-w_2^2)}{(\pi v_{2z}^2)^{1/2}} \tag{2.10}$$

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and

$$u_\alpha = \frac{v_x - V_x}{v_{\alpha x}}, \qquad v_\alpha = \frac{v_y - V_y}{v_{\alpha y}}, \qquad w_\alpha = \frac{v_z - V_z}{v_{\alpha z}},$$

$$v_{1x}^2 = \frac{2C_s^2}{\gamma} + V_{Ay}^2 + V_{Az}^2, \qquad v_{1y}^2 = \frac{2C_s^2}{\gamma} + V_{Ax}^2 + V_{Az}^2, \qquad v_{1z}^2 = \frac{2C_s^2}{\gamma} + V_{Ax}^2 + V_{Ay}^2,$$

$$v_{2x}^2 = 4V_{Ax}^2, \qquad v_{2y}^2 = 4V_{Ay}^2, \qquad v_{2z}^2 = 4V_{Az}^2,$$

$$C_s^2 = \frac{\gamma P}{\rho}, \qquad V_{A\alpha}^2 = \frac{B_\alpha^2}{4\pi\rho}.$$

The MHD equations (2.1)–(2.3) are recovered from the transport equation (2.6) using the distribution function defined by (2.8), as is shown in the next section. The point is that the distribution function F now contains the pressure and all of the magnetic forces except those associated with $\mathbf{a}$. Thus, by calculating the mass, momentum and energy fluxes using F, the plasma pressure and most of the electromagnetic terms are calculated directly.

3. Moments of the distribution function F

3.1. Continuity equation

The moments of F associated with $\chi = m$ and $\chi\mathbf{v} = m\mathbf{v}$ are the following:

$$n \int d^3v\, mF_1(v_x, v_y, v_z) = \rho, \tag{3.1}$$

$$n \int d^3v\, mF_2(v_x, v_y, v_z) = 0, \tag{3.2}$$

$$n \int d^3v\, m\mathbf{v}F_1(v_x, v_y, v_z) = \rho\mathbf{V}, \tag{3.3}$$

$$n \int d^3v\, m\mathbf{v}F_2(v_x, v_y, v_z) = 0. \tag{3.4}$$

The first-moment equation is the continuity equation

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{V}) = 0, \tag{3.5}$$

since $\langle \partial m/\partial\mathbf{v}\rangle = 0$.

3.2. Momentum equation

The moments of F associated with $\chi = m\mathbf{v}$ and $\chi\mathbf{v} = m\mathbf{v}\mathbf{v}$ are the following:

$$n \int d^3v\, m\mathbf{v}F_1(v_x, v_y, v_z) = \rho, \tag{3.6}$$

$$n \int d^3v\, m\mathbf{v}F_2(v_x, v_y, v_z) = 0, \tag{3.7}$$

$$n \int d^3v\, m\mathbf{v}\mathbf{v}F_1(v_x, v_y, v_z) = \rho\mathbf{V}\mathbf{V} + \mathbf{P}_1, \tag{3.8}$$

$$n \int d^3v\, m\mathbf{v}\mathbf{v}F_2(v_x, v_y, v_z) = -\mathbf{P}_2, \tag{3.9}$$

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where

$$\mathbf{P}_1 = \begin{pmatrix} P + \dfrac{B_y^2 + B_z^2}{8\pi} & 0 & 0 \\ 0 & P + \dfrac{B_x^2 + B_z^2}{8\pi} & 0 \\ 0 & 0 & P + \dfrac{B_x^2 + B_y^2}{8\pi} \end{pmatrix}, \tag{3.10}$$

$$\mathbf{P}_2 = \begin{pmatrix} 0 & \dfrac{B_x B_y}{4\pi} & \dfrac{B_x B_z}{4\pi} \\ \dfrac{B_y B_x}{4\pi} & 0 & \dfrac{B_y B_z}{4\pi} \\ \dfrac{B_z B_x}{4\pi} & \dfrac{B_z B_y}{4\pi} & 0 \end{pmatrix}, \tag{3.11}$$

The last term on the left-hand side of (2.6) for $\chi = m\mathbf{v}$ is

$$n\left\langle \mathbf{a} \cdot \frac{\partial \chi}{\partial \mathbf{v}} \right\rangle = -\boldsymbol{\nabla} \cdot \mathbf{P}_N,$$

where

$$\mathbf{P}_N = \begin{pmatrix} \dfrac{B_x^2}{8\pi} & 0 & 0 \\ 0 & \dfrac{B_y^2}{8\pi} & 0 \\ 0 & 0 & \dfrac{B_z^2}{8\pi} \end{pmatrix}, \tag{3.12}$$

and $\langle \partial(m\mathbf{v})/\partial \mathbf{v} \rangle = m$ has been used. The momentum-conservation equation takes the form

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{V}\mathbf{V} + \mathbf{P}_1 - \mathbf{P}_2 - \mathbf{P}_N) = 0, \tag{3.13}$$

where (3.3) has been used. In (3.13), the moment associated with F_1 leads to the terms $\rho\mathbf{V}\mathbf{V} + \mathbf{P}_1$, the moment associated with F_2 leads to the term $-\mathbf{P}_2$, and the acceleration term in (2.6) leads to the term $-\mathbf{P}_N$. Finally, (3.12) can be written as

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \boldsymbol{\nabla} \cdot \left[\rho \mathbf{V}\mathbf{V} + \left(P + \frac{B^2}{8\pi} \right) \mathbf{I} - \frac{\mathbf{B}\mathbf{B}}{4\pi} \right] = 0, \tag{3.14}$$

in agreement with (2.2).

3.3. Energy equation

The moments of F associated with $\chi = \frac{1}{2}mv^2$ and $\chi\mathbf{v} = \frac{1}{2}mv^2\mathbf{v}$ are the following:

$$n \int d^3v \frac{1}{2} m v^2 F_1(v_x, v_y, v_z) = \frac{1}{2}\rho V^2 + \frac{3}{2}P + \frac{B^2}{8\pi}, \tag{3.15}$$

$$n \int d^3v \frac{1}{2} m v^2 F_2(v_x, v_y, v_z) = 0, \tag{3.16}$$

$$n \int d^3v \frac{1}{2} m v^2 \mathbf{v} F_1(v_x, v_y, v_z) = \frac{1}{2}\rho V^2 \mathbf{V} + \mathbf{P}_3, \tag{3.17}$$

$$n \int d^3v \frac{1}{2} m v^2 \mathbf{v} F_2(v_x, v_y, v_z) = -\mathbf{P}_4, \tag{3.18}$$

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where

$$\mathbf{P}_3 = \left(\frac{5}{2}P + \frac{B^2}{8\pi} + \frac{B_y^2 + B_z^2}{8\pi}\right) V_x \hat{\mathbf{e}}_x + \left(\frac{5}{2}P + \frac{B^2}{8\pi} + \frac{B_x^2 + B_z^2}{8\pi}\right) V_y \hat{\mathbf{e}}_y + \left(\frac{5}{2}P + \frac{B^2}{8\pi} + \frac{B_x^2 + B_y^2}{8\pi}\right) V_z \hat{\mathbf{e}}_z, \quad (3.19)$$

$$\mathbf{P}_4 = \left(\frac{B_y}{4\pi}V_y + \frac{B_z}{4\pi}V_z\right) B_x\, \hat{\mathbf{e}}_x + \left(\frac{B_x}{4\pi}V_x + \frac{B_z}{4\pi}V_z\right) B_y\, \hat{\mathbf{e}}_{yx} + \left(\frac{B_x}{4\pi}V_x + \frac{B_y}{4\pi}V_y\right) B_z\, \hat{\mathbf{e}}_z. \quad (3.20)$$

The last term on the left-hand side of (2.6) for $\chi = \frac{1}{2}mv^2$ is

$$n\left\langle \mathbf{a} \cdot \frac{\partial \chi}{\partial \mathbf{v}} \right\rangle = -\boldsymbol{\nabla} \cdot \mathbf{P}_5, \quad (3.21)$$

where

$$\mathbf{P}_5 = \frac{B_x^2}{8\pi} V_x\, \hat{\mathbf{e}}_x + \frac{B_y^2}{8\pi} V_y\, \hat{\mathbf{e}}_y + \frac{B_z^2}{8\pi} V_z\, \hat{\mathbf{e}}_z, \quad (3.22)$$

and $\langle \partial(\frac{1}{2}mv^2)/\partial \mathbf{v} \rangle = m\mathbf{V}$ has been used. The energy equation can be written as

$$\frac{\partial \epsilon}{\partial t} + \boldsymbol{\nabla} \cdot \left(\tfrac{1}{2}\rho V^2 \mathbf{V} + \mathbf{P}_3 - \mathbf{P}_4 - \mathbf{P}_5\right) = 0, \quad (3.23)$$

where the moment associated with F_1 leads to the terms $\frac{1}{2}\rho V^2\mathbf{V} + \mathbf{P}_3$, the moment associated with F_2 leads to the term $-\mathbf{P}_4$, and the acceleration term in (2.6) leads to the term $-\mathbf{P}_5$. Finally, rearranging terms gives the usual energy equation

$$\frac{\partial \epsilon}{\partial t} + \boldsymbol{\nabla} \cdot \left[\mathbf{V}\left(\epsilon + P + \frac{B^2}{8\pi}\right) - \frac{\mathbf{B}}{4\pi}(\mathbf{V} \cdot \mathbf{B})\right] = 0. \quad (3.24)$$

where

$$\epsilon = \frac{1}{2}\rho V^2 + \frac{3}{2}P + \frac{B^2}{8\pi}.$$

4. Computational algorithms

The MHD equations (2.1)–(2.3) are integrated over a cell volume $dx\,dy\,dz$ and written as

$$\frac{\partial \rho_T}{\partial t} = -\int \rho \mathbf{V} \cdot d\mathbf{A} = -\int \mathscr{F}_\rho \cdot d\mathbf{A}, \quad (4.1)$$

$$\frac{\partial (\rho \mathbf{V})_T}{\partial t} = -\int \left[\rho \mathbf{V}\mathbf{V} + \left(P + \frac{B^2}{8\pi}\right)\mathbf{I} - \frac{\mathbf{B}\mathbf{B}}{4\pi}\right] \cdot d\mathbf{A} = -\int \mathscr{F}_{\rho V} \cdot d\mathbf{A}, \quad (4.2)$$

$$\frac{\partial \epsilon_T}{\partial t} = -\int \left[\mathbf{V}\left(\epsilon + P + \frac{B^2}{8\pi}\right) - \frac{\mathbf{B}}{4\pi}(\mathbf{V} \cdot \mathbf{B})\right] \cdot d\mathbf{A} = -\int \mathscr{F}_\epsilon \cdot d\mathbf{A}, \quad (4.3)$$

where $\mathscr{F}_\alpha$ is the flux of α, the subscript T denotes the total mass, momentum, and

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energy in a cell, and $d\mathbf{A} = dy\,dz\,N_x\,\hat{\mathbf{e}}_x + dx\,dz\,N_y\,\hat{\mathbf{e}}_y + dx\,dy\,N_a\,\hat{\mathbf{e}}_z$, where $\mathbf{N}$ is the unit normal and is taken to be 'outward' from the cell face. The total mass, momentum and energy at time $t + \Delta t$ are then

$$\rho_T^{t+\Delta t} = \rho_T^t - \Delta t \int \mathscr{F}_\rho^{t+\Delta t/2} \cdot d\mathbf{A}, \tag{4.4}$$

$$(\rho\mathbf{V})_T^{t+\Delta t} = (\rho\mathbf{V})_T^t - \Delta t \int \mathscr{F}_{\rho V}^{t+\Delta t/2} \cdot d\mathbf{A}, \tag{4.5}$$

$$\epsilon_T^{t+\Delta t} = \epsilon_T^t - \Delta t \int \mathscr{F}_\epsilon^{t+\Delta t/2} \cdot d\mathbf{A}, \tag{4.6}$$

where the fluxes are calculated at the half-time step. The new feature of the algorithm is that the fluxes $\mathscr{F}$ are calculated by integrating a Boltzmann-like distribution function $F(\mathbf{v})$ over velocity space.

4.1. Continuity equation

The continuity equation is written as

$$\frac{\partial \rho_T}{\partial t} = -\sum \mathscr{F}_{\rho x}\,dA_x - \sum \mathscr{F}_{\rho y}\,dA_y - \sum \mathscr{F}_{\rho z}\,dA_z \tag{4.7}$$

where $\mathscr{F}_\rho = \rho\mathbf{V}$, and the summation is over the two cell faces in the x, y, and z directions. The variables ρ and $\mathbf{V}$ can be discontinuous across a cell face; in order to calculate the total flux across an interface, the 'left' and 'right' side values of ρ and $\mathbf{V}$ are needed. These are obtained using a high-order interpolation scheme and a flux limiter (e.g. a partial donor cell method; Hain 1987).

The flux in the x direction at an interface $i + \frac{1}{2}$ is calculated as follows:

$$\mathscr{F}_{\rho,x,i+1/2} = \mathscr{F}_{L,\rho,x,i+1/2} + \mathscr{F}_{R,\rho,x,i+1/2}, \tag{4.8}$$

where

$$\mathscr{F}_{L,\rho,x,i+1/2} = \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x\, v_x\, \rho_L F_L, \tag{4.9}$$

$$\mathscr{F}_{R,\rho,x,i+1/2} = \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x\, v_x \rho_R F_R, \tag{4.10}$$

with the subscripts L and R indicating that the variables used in F correspond to 'left-side' and 'right-side' states. The first term on the right-hand side of (4.8) transports mass across the interface from the 'left side'; only particles moving in the positive x direction contribute to the flux, so the integration limits on v_x are from 0 to ∞ in (4.9). The second term on the right-hand side of (4.8) transports mass across the interface from the 'right side'; only particles moving in the negative x direction contribute to the flux, so the integration limits on v_x are from $-\infty$ to 0 in (4.10). The sum of these two fluxes then gives the total flux across the interface $i + \frac{1}{2}$. The mass flux in the x direction at the interface $i - \frac{1}{2}$ is calculated in the same way. The mass fluxes in the y and z directions are calculated similarly.

The mass flux functions are found by substituting (2.8) into (4.9) and (4.10). Representative mass flux functions are given in the Appendix. In practice, these flux functions are not calculated explicitly every time step; rather, they are calculated once at the outset, and a table look-up is used during the running of the code.

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The mass at time $t = t + \Delta t$ is then given by

$$\rho_T^{t+\Delta t} = \rho_T^t - \Delta t \left(\mathscr{F}^{t+\Delta t/2}_{\rho,x,i+1/2} \, dA_{x,i+1/2} - \mathscr{F}^{t+\Delta t/2}_{\rho,x,i-1/2} \, dA_{x,i-1/2} \right)$$
$$-\Delta t \left(\mathscr{F}^{t+\Delta t/2}_{\rho,y,j+1/2} \, dA_{y,j+1/2} - \mathscr{F}^{t+\Delta t/2}_{\rho,y,j-1/2} \, dA_{y,j-1/2} \right)$$
$$-\Delta t \left(\mathscr{F}^{t+\Delta t/2}_{\rho,z,k+1/2} \, dA_{z,k+1/2} - \mathscr{F}^{t+\Delta t/2}_{\rho,z,k-1/2} \, dA_{z,k-1/2} \right). \tag{4.11}$$

4.2. Momentum equation

The momentum flux is calculated in a similar manner, except the term associated with the acceleration **a** needs to be treated separately. The momentum equation is

$$\frac{\partial(\rho \mathbf{V})_T}{\partial t} = -\int \boldsymbol{\mathscr{F}}_{\rho V} \cdot d\mathbf{A} \tag{4.12}$$

where

$$\boldsymbol{\mathscr{F}}_{\rho V} = \rho \mathbf{V}\mathbf{V} + \mathbf{P}_1 - \mathbf{P}_2 - \mathbf{P}_N.$$

The calculation of the flux associated with $\mathbf{P}_1$ is obtained by integrating over the distribution function F_1 and the flux associated with $\mathbf{P}_2$ is obtained by integrating over the distribution function F_2. The pressure term $\mathbf{P}_N$ is calculated directly; trying to incorporate this term into the distribution function leads to the possiblility of negative 'thermal' velocities, which is unphysical and computationally intractable.

Expanding the x component of (4.12) in Cartesian coordinates gives

$$\frac{\partial(\rho V_x)_T}{\partial t} = -\sum \mathscr{F}_{\rho V,xx} \, dA_x - \sum \mathscr{F}_{\rho V,xy} \, dA_y - \sum \mathscr{F}_{\rho V,xz} \, dA_z. \tag{4.13}$$

The fluxes at an interface are defined by

$$\mathscr{F}_{\rho V,xx,i+1/2} = \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x \, \rho_L v_x^2 F_{1L}$$
$$+ \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x \, \rho_R v_x^2 F_{1R}$$
$$- \frac{B^2_{x,i+1/2}}{8\pi}, \tag{4.14}$$

$$\mathscr{F}_{\rho V,xy,j+1/2} = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_y \, \rho_L v_x v_y (F_{1L} + F_{2L})$$
$$+ \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_y \, \rho_R v_x v_y (F_{1R} + F_{2R}), \tag{4.15}$$

$$\mathscr{F}_{\rho V,xz,k+1/2} = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_0^{\infty} dv_z \, \rho_L v_x v_z (F_{1L} + F_{2L})$$
$$+ \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{0} dv_z \, \rho_R v_x v_z (F_{1R} + F_{2R}). \tag{4.16}$$

Explicit expressions for the momentum flux functions are presented in the Appendix.

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The momentum flux in the x-direction at time $t + \Delta t$ is given by

$$
\begin{aligned}
(\rho V_x)_T^{t+\Delta t} = (\rho V_x)_T^t &- \Delta t\big(\mathscr{F}^{t+\Delta t/2}_{\rho V,xx,i+1/2}\, dA_{x,i+/12} - \mathscr{F}^{t+\Delta t/2}_{\rho V,xx,i-1/2}\, dA_{x,i-1/2}\big) \\
&-\Delta t\left(\mathscr{F}^{t+\Delta t/2}_{\rho V,xy,j+1/2}\, dA_{y,j+1/2} - \mathscr{F}^{t+\Delta t/2}_{\rho V,xy,j-1/2}\, dA_{y,j-1/2}\right) \\
&-\Delta t\left(\mathscr{F}^{t+\Delta t/2}_{\rho V,xz,k+1/2}\, dA_{z,k+1/2} - \mathscr{F}^{t+\Delta t/2}_{\rho V,xz,k-1/2}\, dA_{z,k-1/2}\right) \\
&+\Delta t\left(\frac{B^2_{x,i+1/2}}{8\pi}\, dA_{x,i+1/2} - \frac{B^2_{x,i-1/2}}{8\pi}\, dA_{x,i-1/2}\right). \qquad (4.17)
\end{aligned}
$$

An important aspect of (4.17) is the presence of a term proportional to B_x^2. Since this component of **B** is normal to the cell face, B_x is continuous across the interface, and the flux associated with this term is calculated directly. The y and z components of the momentum equation are calculated similarly but are not shown explicitly.

4.3. Energy equation

The energy flux calculation is similar to that of the momentum flux in that the acceleration **a** needs to be treated separately. The energy equation is written as

$$
\frac{\partial \epsilon_T}{\partial t} = -\sum \mathscr{F}_{\epsilon,x}\, dA_x - \sum \mathscr{F}_{\epsilon,y}\, dA_y - \sum \mathscr{F}_{\epsilon,z}\, dA_z \qquad (4.18)
$$

where

$$
\mathscr{F}_\epsilon = \tfrac{1}{2}\rho V^2 \mathbf{V} + \mathbf{P}_3 - \mathbf{P}_4 - \mathbf{P}_5.
$$

The flux in the x direction is defined as follows

$$
\begin{aligned}
\mathscr{F}_{\epsilon,x,i+1/2} = &\int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x\, \rho_L \frac{1}{2} m(v_x^2 + v_y^2 + v_z^2) v_x (F_{1L} + F_{2L}) \\
&+ \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x\, \rho_R \frac{1}{2} m(v_x^2 + v_y^2 + v_z^2) v_x (F_{1R} + F_{2R}) \\
&- \frac{V_{x,i+1/2} B^2_{x,i+1/2}}{8\pi}. \qquad (4.19)
\end{aligned}
$$

Explicit expressions for the energy flux functions are presented in the Appendix.

A concern is the calculation of the final term in the energy flux; unlike the momentum equation, this term is not continuous across the interface, because of the velocity component. However, making use of the fact that the normal component of the magnetic field is continuous, this term is calculated as follows:

$$
\begin{aligned}
\frac{V_{x,i+1/2} B^2_{x,i+1/2}}{8\pi} = &\frac{B^2_{x,i+1/2}}{8\pi} \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x\, v_x F_{1L} \\
&+ \frac{B^2_{x,i+1/2}}{8\pi} \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x\, v_x F_{1R}. \qquad (4.20)
\end{aligned}
$$

In essence, the flux of normal magnetic energy is being calculated, which cancels that included in the integrations over F_1 in (4.19).

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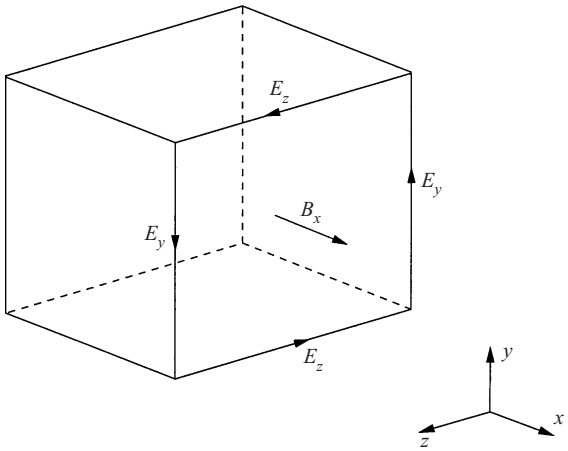


Figure 2. Cell geometry, showing the face-centred magnetic field B_x, and the edge-aligned electric fields E_y and E_z.

Finally, the energy at time $t = t + \Delta t$ is given by

$$\epsilon_T^{t+\Delta t} = \epsilon_T^t - \Delta t \left(\mathscr{F}_{\epsilon,x,i+1/2}^{t+\Delta t/2} \, dA_{x,i+1/2} - \mathscr{F}_{\epsilon,x,i-1/2}^{t+\Delta t/2} \, dA_{x,i-1/2} \right)$$
$$-\Delta t \left(\mathscr{F}_{\epsilon,y,j+1/2}^{t+\Delta t/2} \, dA_{y,j+1/2} - \mathscr{F}_{\epsilon,y,j-1/2}^{t+\Delta t/2} \, dA_{y,j-1/2} \right)$$
$$-\Delta t \left(\mathscr{F}_{\epsilon,z,k+1/2}^{t+\Delta t/2} \, dA_{z,k+1/2} - \mathscr{F}_{\epsilon,z,k-1/2}^{t+\Delta t/2} \, dA_{z,k-1/2} \right). \tag{4.21}$$

5. Magnetic field evolution

This technique is also used to update the magnetic field. The evolution of the magnetic field is governed by

$$\frac{\partial \mathbf{B}}{\partial t} = \boldsymbol{\nabla} \times (\mathbf{V} \times \mathbf{B}) = -c \boldsymbol{\nabla} \times \mathbf{E}. \tag{5.1}$$

The normal component of the field is integrated over a cell face:

$$\int d\mathbf{A} \cdot \frac{\partial \mathbf{B}}{\partial t} = -c \int d\mathbf{A} \cdot \boldsymbol{\nabla} \times \mathbf{E} = -c \int \mathbf{E} \cdot d\mathbf{l}, \tag{5.2}$$

where $\int d\mathbf{l}$ denotes a line integral around the cell face. The electric field is

$$\mathbf{E} = -\frac{1}{c}(V_y B_z - V_z B_y)\, \hat{\mathbf{e}}_x + \frac{1}{c}(V_z B_x - V_z B_x)\, \hat{\mathbf{e}}_y - \frac{1}{c}(V_x B_y - V_y B_x)\, \hat{\mathbf{e}}_z. \tag{5.3}$$

As an example, the x flux through each interface is

$$\frac{\partial \Phi_x}{\partial t} = -c \sum E_y \, dy - c \sum E_z \, dz, \tag{5.4}$$

where $\Phi_x = B_x \, dy \, dz$ and the summation is over the two faces associated with each cell (see Fig. 2). Thus the updated x flux is

$$\Phi_x^{t+\Delta t} = \Phi_x^t + c\Delta t \left(\sum E_y \, dy + \sum E_z \, dz \right)^{t+\Delta t/2}. \tag{5.5}$$

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The distribution method can also be used to calculate the electric field. For example, the z component of the electric field is found from

$$E_z = \frac{1}{c}(V_x B_y - V_y B_x)$$
$$= \frac{1}{c}\left(\int F(v) v_x B_y \, d^3v - \int F(v) v_y B_x \, d^3v\right). \tag{5.6}$$

The velocity integrations are more complicated than those associated with the hydrodynamic variables. In Fig. 3(a) we show the four cells in the (x, y) plane surrounding a 'corner' along which we want to determine the electric field E_z. The magnetic fields B_x and B_y are known at the 'cell-centred' face of each cell as shown. However, unlike the hydrodynamic variables ρ, V, and ϵ in which two states are needed (the left L and right R with respect to the cell interface), four states (I, II, III and IV) are needed to calculate the electric field along a vertex. One way to calculate the electric field E_z from (5.6) would be as follows:

$$\begin{aligned} cE_z = &\left[\int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_y \int_0^{\infty} F(v) v_x B_y \, dv_x \right. \\ &\left. - \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x \int_0^{\infty} F(v) v_y B_x \, dv_y \right]_{\mathrm{I}} \\ &+\left[\int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_y \int_{-\infty}^{0} F(v) v_x B_y \, dv_x \right. \\ &\left. - \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x \int_0^{\infty} F(v) v_y B_x \, dv_y \right]_{\mathrm{II}} \\ &+\left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} v_y \int_{-\infty}^{0} F(v) v_x B_y \, dv_x \right. \\ &\left. - \int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_x \int_{-\infty}^{0} F(v) v_y B_x \, dv_y \right]_{\mathrm{III}} \\ &+\left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{0} dv_y \int_0^{\infty} F(v) v_x B_y \, dv_x \right. \\ &\left. - \int_{-\infty}^{\infty} dv_z \int_0^{\infty} dv_x \int_{-\infty}^{0} F(v) v_y B_x \, dv_y \right]_{\mathrm{IV}}, \end{aligned} \tag{5.7}$$

where the subscript denotes which variable states are used in the integrations. These integrations are more complex than the mass, momentum and energy flux integrations, because only one of the three integations is from $-\infty$ to $+\infty$.

An easier calculation is to rotate the mesh through 45° in the (x, y) plane so that the new axes are x', y' (see Fig. 3b). The electric field E_z is now written as

$$E_z = \frac{1}{c}(V'_x B'_y - V'_y B'_x)$$
$$= \frac{1}{c}\left(\int F(v') v'_x B'_y \, d^3v' - \int F(v') v'_y B'_x \, d^3v'\right)$$

where

$$A'_x = A_x \cos \tfrac{1}{4}\pi + A_y \sin \tfrac{1}{4}\pi,$$
$$A'_y = -A_x \sin \tfrac{1}{4}\pi + A_y \cos \tfrac{1}{4}\pi.$$

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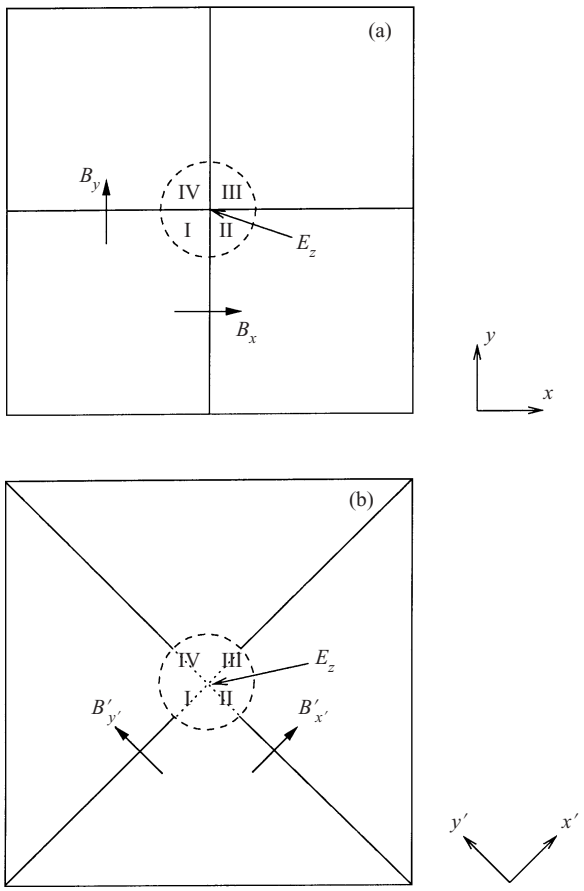


Figure 3. Configuration for calculating the electric field E_z in (a) the original geometry and (b) the rotated geometry.

In this coordinate system the calculation of E_z is much simpler:

$$
\begin{aligned}
cE_z = &\left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{\infty} dv'_y \int_{0}^{\infty} F(v')v'_x B'_y \, dv'_x\right]_{\mathrm{I}} \\
&+ \left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{\infty} dv'_x \int_{0}^{\infty} F(v')v'_y B'_x \, dv'_y\right]_{\mathrm{II}} \\
&+ \left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{\infty} v'_y \int_{-\infty}^{0} F(v')v'_x B'_y \, dv'_x\right]_{\mathrm{III}} \\
&+ \left[\int_{-\infty}^{\infty} dv_z \int_{-\infty}^{\infty} dv'_x \int_{-\infty}^{0} F(v')v'_y B'_x \, dv'_y\right]_{\mathrm{IV}} . \qquad (5.8)
\end{aligned}
$$

There are fewer terms to calculate and the integrals are simpler. The needed flux functions are similar to those used in the mass-flux calculation.

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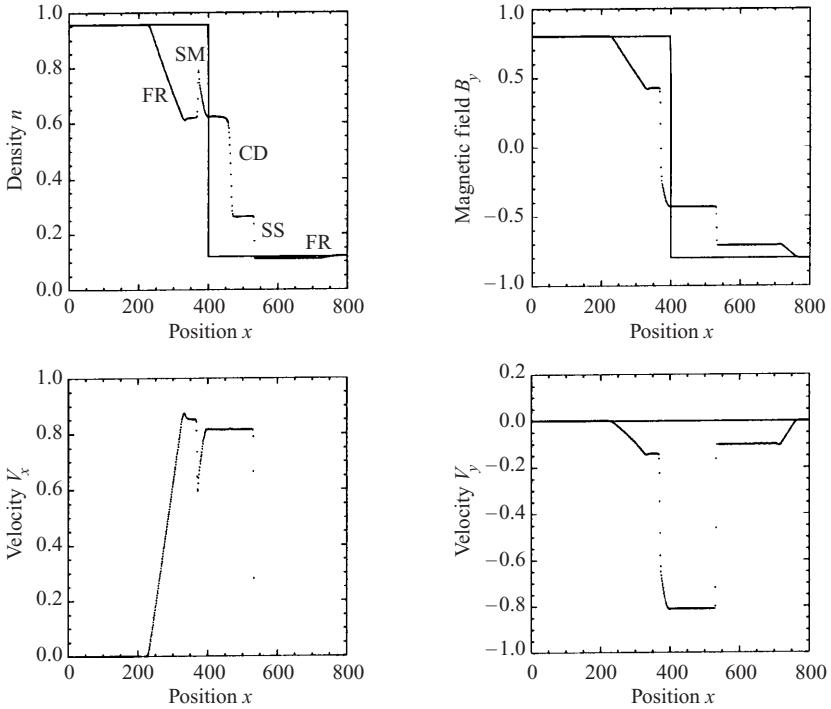


Figure 4. Solutions to the Brio–Wu problem.

6. Test case

As an example of this technique we present results for the Brio–Wu shock problem (Brio and Wu 1988). This problem is similar to the Sod shock problem (Sod 1978), except that both tangential and normal magnetic fields are included. The profiles of the density n, magnetic field B_y, and velocities V_x and V_y are shown in Fig. 4. The mesh is 800 cells and the initial conditions are as follows:

$$\rho_R = 0.12, \qquad \rho_L = 0.96, \qquad P_R = 0.1, \qquad P_L = 1,$$

$$B_{yR} = -0.8, \qquad B_{yL} = 0.8, \qquad B_x = 0.75 B_{yL}, \qquad \gamma = \tfrac{5}{3}.$$

The solid curves are the initial conditions. The important features of Fig. 4 are that the fast rarefaction waves (FR), slow compound wave (SM), contact discontinuity (CD) and slow shock (SS) are well resolved.

7. Summary

A new three-dimensional magnetohydrodynamic (3D MHD) algorithm has been developed. The fluxes of mass, momentum and energy across cell interfaces, as well as the electric field along cell edges, are calculated by integrating a Boltzmann-like distribution function over velocity space. The novel feature of the method is that the distribution function incorporates most of the electromagnetic terms. A nice feature of the distribution function method is that it can be used to solve more general forms of the MHD equations. For example, finite-Larmor-radius (FLR) effects and temperature anisotropies (e.g. $T_\perp$ and $T_\parallel$) can be included by choosing appropriate distribution functions. The 2D MHD FLR equations have been solved using this technique (Huba 1996).

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Appendix

We present several representative flux functions associated with the mass flux, momentum flux and energy flux. We only show expressions for the x direction; similar expressions can be derived for the y and z directions.

The mass flux in the x direction is given by

$$\mathscr{F}_{\rho,x} = \rho_L v_{1xL} F_{1xL} + \rho_R v_{1xR} F_{1xR},$$

where

$$F_{1xL} = \frac{1}{2}\left\{\frac{1}{\pi^{1/2}} e^{-V_{1xL}^2} + V_{1xL}\left[1 + \mathrm{erf}\left(V_{1xL}\right)\right]\right\},$$

$$F_{1xR} = \frac{1}{2}\left\{-\frac{1}{\pi^{1/2}} e^{-V_{1xR}^2} + V_{1xR}\left[1 - \mathrm{erf}(V_{1xR})\right]\right\}.$$

The momentum flux in the x direction is given by

$$\begin{aligned}\mathscr{F}_{\rho V,x} = {} & \rho_L v_{1xL}^2 F_{2xL} + \rho_L v_{1xL}\left(V_{1yL} + V_{1zL}\right) F_{1xL} \\ & + \rho_L v_{2xL}\left(v_{2yL} + v_{2zL}\right) G_{2xL} \\ & + \rho_R v_{1xR}^2 F_{2xR} + \rho_R v_{1xR}\left(V_{1xR} + V_{1zR}\right) F_{1Rx} \\ & + \rho_R v_{2xR}\left(v_{2yR} + v_{2zR}\right) G_{2xR} - \frac{B_x^2}{8\pi},\end{aligned}$$

where

$$F_{2xL} = \frac{1}{2}\left\{\frac{1}{\pi^{1/2}} V_{1xL} \exp(-V_{1xL}^2) + \left(\frac{1}{2} + V_{1xL}^2\right)\left[1 + \mathrm{erf}(V_{1xL})\right]\right\},$$

$$F_{2xR} = \frac{1}{2}\left\{-\frac{1}{\pi^{1/2}} V_{1xR} \exp(-V_{1xR}^2) + \left(\frac{1}{2} + V_{1xR}^2\right)\left[1 - \mathrm{erf}(V_{1xR})\right]\right\}$$

$$G_{2xL} = -\tfrac{1}{8}[1 + \mathrm{erf}(-V_{2xL})],$$

$$G_{2xR} = -\tfrac{1}{8}[1 + \mathrm{erf}(-V_{2xR})].$$

The energy flux in the x direction is given by

$$\begin{aligned}F_{\epsilon,x} = {} & \rho_L v_{1xL}^2 V_{1xL} F_{2xL} \\ & + \rho_L v_{1xL}[v_{1xL}^2 + \tfrac{1}{2}(v_{1yL}^2 + v_{1zL}^2) + (V_{1yL}^2 + V_{1zL}^2)] F_{1xL} \\ & + 2\rho_L v_{2xL}(v_{2yL} V_{1yL} + v_{2zL} V_{1zL}) G_{2xL} \\ & + \rho_R v_{1xR}^2 V_{1xR} F_{2xR} \\ & + \rho_R v_{1xR}[v_{1xR}^2 + \tfrac{1}{2}(v_{1yR}^2 + v_{1zR}^2) + (V_{1yR}^2 + V_{1zR}^2)] F_{1xR} \\ & + 2\rho_R v_{2xR}(v_{2yR} V_{1yR} + v_{2zR} V_{1zR}) G_{2xR} \\ & - \frac{B_x^2}{8/\pi}(v_{1xL} F_{1xL} + v_{1xR} F_{1xR}).\end{aligned}$$

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In the above equations the following definitions are used:

$$v_{1x} = \left(\frac{2C_s^2}{\gamma} + V_{Ay}^2 + V_{Az}^2\right)^{1/2}, \qquad v_{1y} = \left(\frac{2C_s^2}{\gamma} + V_{Ax}^2 + V_{Az}^2\right)^{1/2},$$

$$v_{1z} = \left(\frac{2C_s^2}{\gamma} + V_{Ax}^2 + V_{Ay}^2\right)^{1/2}, \qquad C_s^2 = \frac{\gamma P}{\rho},$$

$$V_{Ax}^2 = \frac{B_x^2}{4\pi\rho}, \qquad V_{Ay}^2 = \frac{B_y^2}{4\pi\rho}, \qquad V_{Az}^2 = \frac{B_z^2}{4\pi\rho},$$

$$v_{2x} = 2V_{Ax}, \qquad v_{2y} = 2V_{Ay}, \qquad v_{2z} = 2V_{Az},$$

$$V_{2x} = \frac{V_x}{v_{2x}}, \qquad V_{2y} = \frac{V_y}{v_{2y}}, \qquad V_{2z} = \frac{V_z}{v_{2z}},$$

and the subscripts L and R refer to the left and right states of the interface.

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