CFD Notes

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These notes are a supplement to the main repository and provide references to equations and formulas used in the code. There are also some scattered comments on other matters of interest.

1 Generalized Ohm's Law

Magnetohydrodynamic (MHD) physics is contained in the generalized Ohm's law. We define the electron mass m_e, ion mass m_i, electric charge e, speed of light c, current density $\mathbf{J}$, mass density ρ, flow velocity $\mathbf{u}$, pressure tensor P, electric field $\mathbf{E}$, magnetic field $\mathbf{B}$, and conductivity σ. Then the generalized Ohm's law reads as

$$\frac{m_e m_i}{\rho e^2}\frac{\partial \mathbf{J}}{\partial t} - \frac{m_i}{\rho e}\boldsymbol{\nabla}\cdot\mathsf{P} = \mathbf{E} + \frac{1}{c}\mathbf{u}\times\mathbf{B} - \frac{m_i}{\rho e c}\mathbf{J}\times\mathbf{B} - \frac{1}{\sigma}\mathbf{J}, \tag{1}$$

where the terms are interpreted from left to right as the electron inertia, electron pressure, electric field, convective field, Hall term, and the conductivity.

The electron inertia can be neglected at length scales longer than the electron inertial length and time scales longer than an electron cyclotron period. The conductivity can be neglected for plasmas with very high conductivity, e.g. for many fully ionized plasmas. The Hall and electron pressure terms can be neglected at length scales longer than the ion inertial length and time scales longer than an ion cyclotron period. When all of these are assumed, we are left with ideal MHD.

2 Euler equations

2.1 Conservation form

The mass density ρ, flow velocity $\mathbf{u}$, and pressure P are the primitive variables. The equation of state of an ideal gas $P = (\gamma-1)\rho\mathcal{E}$ is used, where γ is the adiabatic index and $\mathcal{E}$ is the specific internal energy. From here, we define the momentum density $\rho\mathbf{u}$ and the energy density

$$E = \frac{P}{\gamma-1} + \frac{1}{2}\rho u^2. \tag{2}$$

The notation $u^2 = \|\mathbf{u}\|^2 = \mathbf{u}\cdot\mathbf{u}$ is a Euclidean norm, and we take $\gamma = 7/5$. Then the Euler equations of fluid dynamics read as

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ \rho\mathbf{u} \\ E\end{pmatrix} + \boldsymbol{\nabla}\cdot\begin{pmatrix}\rho\mathbf{u} \\ \rho\mathbf{u}\otimes\mathbf{u} + P\mathsf{I} \\ \mathbf{u}(E+P)\end{pmatrix} = 0. \tag{Euler equations}$$

2.2 Eigensystem

We define an abstract state vector $\mathbf{Q} = (\rho, \rho\mathbf{u}, E)^T$ of conserved variables and their associated fluxes $\mathsf{F}(\mathbf{Q})$. The sound speed is $c_s = \sqrt{\gamma P/\rho}$. Then the Jacobian in 1D is

$$\frac{\partial \mathbf{F}}{\partial \mathbf{Q}} = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{3-\gamma}{2}u^2 & (3-\gamma)u & \gamma-1 \\ \frac{\gamma-2}{2}u^3 - \frac{u c_s^2}{\gamma-1} & \frac{c_s^2}{\gamma-1} + \frac{3-2\gamma}{2}u^2 & \gamma u \end{pmatrix}. \tag{3}$$

In 2D, the x Jacobian is

$$\frac{\partial \mathbf{F}_x}{\partial \mathbf{Q}} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -\frac{3-\gamma}{2}u_x^2 + \frac{\gamma-1}{2}u_y^2 & (3-\gamma)u_x & (1-\gamma)u_y & \gamma-1 \\ -u_x u_y & u_y & u_x & 0 \\ \frac{\gamma-2}{2}u_x u^2 - \frac{u_x c_s^2}{\gamma-1} & \frac{c_s^2}{\gamma-1} + \frac{3-2\gamma}{2}u_x^2 + \frac{1}{2}u_y^2 & (1-\gamma)u_x u_y & \gamma u_x \end{pmatrix}. \tag{4}$$

It has eigenvalues $u_x - c_s$, u_x, u_x, and $u_x + c_s$ with corresponding right eigenvectors

$$R_x = \begin{pmatrix} 1 & 1 & 0 & 1 \\ u_x - c_s & u_x & 0 & u_x + c_s \\ u_y & u_y & 1 & u_y \\ H - c_s u_x & \frac{1}{2}(u_x^2 + u_y^2) & u_y & H + c_s u_x \end{pmatrix} \tag{5}$$

where $H = (E+P)/\rho$. The y Jacobian is

$$\frac{\partial \mathbf{F}_y}{\partial \mathbf{Q}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ -u_x u_y & u_y & u_x & 0 \\ -\frac{3-\gamma}{2}u_y^2 + \frac{\gamma-1}{2}u_x^2 & (1-\gamma)u_x & (3-\gamma)u_y & \gamma-1 \\ \frac{\gamma-2}{2}u_y u^2 - \frac{u_y c_s^2}{\gamma-1} & (1-\gamma)u_x u_y & \frac{c_s^2}{\gamma-1} + \frac{3-2\gamma}{2}u_y^2 + \frac{1}{2}u_x^2 & \gamma u_y \end{pmatrix}. \tag{6}$$

It has eigenvalues $u_y - c_s$, u_y, u_y, and $u_y + c_s$ with corresponding right eigenvectors

$$R_y = \begin{pmatrix} 1 & 1 & 0 & 1 \\ u_x & u_x & 1 & u_x \\ u_y - c_s & u_y & 0 & u_y + c_s \\ H - c_s u_y & \frac{1}{2}(u_x^2 + u_y^2) & u_x & H + c_s u_y \end{pmatrix}. \tag{7}$$

2.3 Gravity

In the Rayleigh-Taylor instability bubble, the momentum equation contains a source term $\rho\mathbf{g}$, where $\mathbf{g} = (0, -g)^T$ and g is the gravitational acceleration, while the energy equation contains a source term $\rho\mathbf{g}\cdot\mathbf{u}$. They read as

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho\mathbf{u} \\ E \end{pmatrix} + \boldsymbol{\nabla}\cdot\begin{pmatrix} \rho\mathbf{u}\otimes\mathbf{u} + P\mathsf{I} \\ \mathbf{u}(E+P) \end{pmatrix} = \begin{pmatrix} \rho\mathbf{g} \\ \rho\mathbf{g}\cdot\mathbf{u} \end{pmatrix}. \tag{8}$$

3 Ideal MHD

3.1 Conservation form

We use Gaussian units in this section. The conversion to SI is easily made by replacing $4\pi \to \mu_0$ whenever they arise. The generalized Ohm's law gives an electric field

$$\mathbf{E} = -\frac{1}{c}\mathbf{u}\times\mathbf{B}, \tag{9}$$

which we substitute into the induction equation and the expression for the Poynting vector that contributes an energy flux density due to the electromagnetic fields. Thus, once we introduce the dynamics of $\mathbf{B}$, the dynamics of $\mathbf{E}$ are not independent. The energy density is modified to be

$$E = \frac{P}{\gamma-1} + \frac{1}{2}\rho u^2 + \frac{B^2}{8\pi}, \tag{10}$$

which includes the contribution from the magnetic field. For convenience and to more clearly see the analogous form of the fluxes, we also define the total pressure to include the magnetic pressure

$$P_{\text{tot}} = P + \frac{B^2}{8\pi}. \tag{11}$$

We take $\gamma = 5/3$. Then the equations of ideal MHD read as

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ \rho\mathbf{u} \\ E \\ \mathbf{B}\end{pmatrix} + \boldsymbol{\nabla}\cdot\begin{pmatrix}\rho\mathbf{u} \\ \rho\mathbf{u}\otimes\mathbf{u} + P_{\text{tot}}\mathsf{I} - \dfrac{1}{4\pi}(\mathbf{B}\otimes\mathbf{B}) \\ \mathbf{u}(E+P_{\text{tot}}) - \dfrac{1}{4\pi}\mathbf{B}(\mathbf{u}\cdot\mathbf{B}) \\ \mathbf{u}\otimes\mathbf{B} - \mathbf{B}\otimes\mathbf{u}\end{pmatrix} = 0. \tag{Ideal MHD}$$

The eigensystem is treated as described in [1], and we do not repeat it for brevity. However, we point out a typo in one of the left eigenvectors. The correct $L_{1,7}$ is

$$L_{1,7}^T = \frac{1}{2a^2}\begin{pmatrix}\gamma_1\alpha_f u^2 \pm \Gamma_f \\ (1-\gamma)\alpha_f u_x \mp \alpha_f c_f \\ (1-\gamma)\alpha_f u_y \pm c_s\alpha_s\beta_y\,\text{sgn}(B_x) \\ (1-\gamma)\alpha_f u_z \pm c_s\alpha_s\beta_z\,\text{sgn}(B_x) \\ (1-\gamma)\alpha_f B_y + \sqrt{\rho}\,a\alpha_s\beta_y \\ (1-\gamma)\alpha_f B_z - \sqrt{\rho}\,a\alpha_s\beta_z \\ (\gamma-1)\alpha_f\end{pmatrix} \tag{12}$$

with the typo in the sign of the fifth element (should be plus, not minus). The definition

$$\text{sgn}(B) = \begin{cases} +1 & B \geq 0 \\ -1 & B < 0 \end{cases} \tag{13}$$

which assigns $\text{sgn}(0) = 1$ is particularly important in ensuring that the eigenvectors are nonsingular.

3.2 Divergence constraint

Numerical simulations solving these equations must also ensure that $\boldsymbol{\nabla}\cdot\mathbf{B} = 0$ at every time step. We opt for the constrained transport method, described in [2], which we summarize below. In 2D (spatial dependence on x and y), the constraint in Cartesian coordinates is that we only need to evolve the z component of the magnetic potential A_z via the advection equation

$$\frac{\partial A_z}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})A_z = 0 \tag{14}$$

while identifying the components $B_x = \partial_y A_z$ and $B_y = -\partial_x A_z$. Given the MHD state vector $\mathbf{Q} = (\rho, \rho\mathbf{u}, E, \mathbf{B})^T$ and A_z with initial conditions $\mathbf{Q}(0)$ and $A_z(0)$, we write

$$\begin{aligned}\frac{\partial\mathbf{Q}}{\partial t} &= \mathcal{L}(\mathbf{Q}), \quad \mathcal{L} = -\boldsymbol{\nabla}\cdot\mathsf{F} \\ \frac{\partial A_z}{\partial t} &= \mathcal{H}(A_z, \mathbf{u}), \quad \mathcal{H} = -(\mathbf{u}\cdot\boldsymbol{\nabla})A_z\end{aligned} \tag{15}$$

as the dynamical equations. The procedure is then given as follows.

1. Discretize $\mathcal{L}$ and $\mathcal{H}$ using the WENO scheme. The operator $\mathcal{L}$ is discretized in the usual way. However, $\mathcal{H}$ is modified to be

$$\mathcal{H}(A_z, \mathbf{u}) = -u_x\left(\frac{\partial_x A_z^+ + \partial_x A_z^-}{2}\right) - u_y\left(\frac{\partial_y A_z^+ + \partial_y A_z^-}{2}\right) + \alpha_x\left(\frac{\partial_x A_z^+ - \partial_x A_z^-}{2}\right) + \alpha_y\left(\frac{\partial_y A_z^+ - \partial_y A_z^-}{2}\right) \tag{16}$$

   where $\alpha_x = \max|u_x|$ and $\alpha_y = \max|u_y|$ and the maximum is taken across the global stencil. Of note is that we identify $\partial_x A_z^\pm$ and $\partial_y A_z^\pm$ with $\hat{f}_{i+1/2}^\mp$ to correctly calculate the nonlinear weights.

2. Evolve $\mathbf{Q}$ and A_z in time using the TVD RK-3 method. We obtain a new $\mathbf{Q}^*$, which contains a magnetic field $\mathbf{B}^*$ that in general does not satisfy $\nabla \cdot \mathbf{B} = 0$, as well as an energy E^*.

3. Replace $\mathbf{B}^*$ by a discretized curl of A_z. In other words,

$$\begin{pmatrix} B_x^{n+1} \\ B_y^{n+1} \end{pmatrix} = \begin{pmatrix} +\partial_y A_z \\ -\partial_x A_z \end{pmatrix}. \tag{17}$$

   The derivatives on the right are discretized using 6th order central differencing

$$\frac{\mathrm{d}A_i}{\mathrm{d}x} = \frac{1}{\Delta x}\left[\frac{1}{60}A_{i+3} - \frac{3}{20}A_{i+2} + \frac{3}{4}A_{i+1} - \frac{3}{4}A_{i-1} + \frac{3}{20}A_{i+2} - \frac{1}{60}A_{i-3}\right]. \tag{18}$$

   Ref. [2] opts for the 4th order central differencing; however, this loses the 5th order accuracy of the WENO scheme in smooth regions. We also might as well make use of the three ghost cells required for the WENO scheme with flux splitting.

4. Conserve the total energy. This means that we do not do anything to the calculated energy: $E^{n+1} = E^*$. Another option is to conserve the thermal pressure

$$E^{n+1} = E^* + \frac{\left\|\mathbf{B}^{n+1}\right\|^2 - \left\|\mathbf{B}^*\right\|^2}{2} \tag{19}$$

   which may help in low β plasmas to prevent the pressure from becoming negative, but this comes at the cost of conservation of energy.

It is important to note that in 2D, this correction only changes B_x and B_y; B_z can be left unchanged because it does not contribute to the $\nabla \cdot \mathbf{B} = 0$ condition.

4 Hall MHD

4.1 Conservation form

The generalized Ohm's law gives an electric field

$$\mathbf{E} = -\frac{1}{c}\mathbf{u} \times \mathbf{B} + \frac{m_i}{\rho e c}\mathbf{J} \times \mathbf{B}. \tag{20}$$

The last term is known as the Hall term, which introduces an electric field transverse to the current density and the magnetic field. Physically, the magnetic field lines are frozen only in the ion fluid; ion and electron motions are decoupled on ion inertial length scales [3]. To more clearly see the analogous form of the flow velocity, we define the Hall velocity as

$$\mathbf{u}_H = -\frac{m_i}{\rho e}\mathbf{J} \tag{21}$$

which is interpreted to be the electron velocity in the ion reference frame. Since the electron inertia term in the generalized Ohm's law is neglected (and therefore the displacement current is neglected), the dynamics of $\mathbf{J}$ are not independent and are found from Ampere's law

$$\mathbf{J} = \frac{c}{4\pi}\nabla \times \mathbf{B}. \tag{22}$$

Then the equations of Hall MHD read as

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho\mathbf{u} \\ E \\ \mathbf{B} \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho\mathbf{u} \\ \rho\mathbf{u} \otimes \mathbf{u} + P_{\text{tot}}\mathsf{I} - \frac{1}{4\pi}(\mathbf{B} \otimes \mathbf{B}) \\ \mathbf{u}(E+P) + (\mathbf{u}+\mathbf{u}_H)\frac{B^2}{8\pi} - \frac{1}{4\pi}\mathbf{B}((\mathbf{u}+\mathbf{u}_H)\cdot\mathbf{B}) \\ (\mathbf{u}+\mathbf{u}_H) \otimes \mathbf{B} - \mathbf{B} \otimes (\mathbf{u}+\mathbf{u}_H) \end{pmatrix} = 0. \tag{Hall MHD}$$

5 AdaWENO scheme

The AdaWENO-Z scheme as proposed in [4] makes use of the smoothness functions

$$G^{\pm} = \rho + \rho u^2 + P \pm \alpha \rho u \tag{23}$$

where α is the Lax-Friedrichs parameter often taken to be the largest speed in the local stencil. The smoothness functions seem to be a phenomenological guess whose weights are only calculated in smooth regions. According to the authors, the choice of $G^{\pm}$ is such that any discontinuities in any of the variables, primitive or conserved, are included in the shared variables. We experiment with a smoothness function

$$G^{\pm} = \rho + E \pm \alpha \rho u \tag{24}$$

where E takes into account the discontinuities in pressure and velocities. In 2D, we extend it to

$$G^{\pm} = \rho + E \pm \alpha(\rho u_x + \rho u_y). \tag{25}$$

When ρu_z is included and the energy in (10) is used, the smoothness function above can be used for ideal MHD as well.

While the results for Euler and ideal MHD in 1D are good using this method, they are less effective in 2D.

References

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[4] Peng, J., Zhai, C., Ni, G., Yong, H., and Shen, Y., "An adaptive characteristic-wise reconstruction weno-z scheme for gas dynamic euler equations", Comput. Fluids **179**, 34–51 (2019).