Multi-Ion Magnetohydrodynamics

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Abstract. We derive and numerically solve the full set of magnetohydrodynamic equations with multiple ion fluids. The numerical difficulties and the algorithmic solutions are discussed. We show some preliminary results for the interaction of Mars’ ionosphere with the solar wind.

1. Introduction

Most of the plasma in space- and astro-physical systems is collisionless to a very good approximation. The ions interact through the magnetic field only. If the plasma is dominated by a single type of ion, typically hydrogen, single fluid magnetohydrodynamics (MHD) provides a reasonably good description for the plasma dynamics. In some systems, however, ions of different molecular masses and sometimes of different electric charge are mixed together. In this case the single fluid approximation is not valid any more, and a multi-ion MHD approximation becomes necessary.

Examples include the Earth’s magnetosphere, where ionospheric O+ is a significant fraction of the magnetospheric plasma population, particularly during geomagnetic storms. The ionosphere of Mars contains O+, O2+ and CO2+ ions and it mixes with the hydrogen ions of the solar wind. In fact, the solar wind itself contains a mixture of hydrogen and helium ions.

The simplest approach of handling a mixture of ions, is multi-species MHD that solves the same equations as single-fluid MHD except that each ion species has its own continuity equation (see e.g. Glocer et al. 2009a; Ma et al. 2004) This is in contrast to the multi-fluid approach in which each ion has its own continuity, momentum, and energy equation. Moore et al. (2007) approached this problem by using a particle tracing code to track millions of particles of various origin (solar wind, polar wind, auroral wind) through a magnetic field calculated by an ideal MHD model. Winglee, Lewis, & Lu (2005) took a similar approach as us by solving the multi-fluid MHD model.

This paper presents the set of equations and the numerical techniques as implemented into the Block-Adaptive-Tree Solar-wind Roe-type Upwind Scheme (BATS-R-US) (Powell et al. 1999). A much longer and more application oriented paper will appear in the Journal of Geophysical Research (Glocer et al. 2009b).

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2. Multi-fluid MHD Equations

Here we give a brief derivation for the multi-fluid MHD equations. The electron number density \( n_e \) can be calculated from the charge neutrality condition as
\[
n_e = \frac{1}{e} \sum_s n_s q_s \]
where \( e \) is the electron charge, \( s \) indexes the ion fluids, \( n_s \) is ion number density, and \( q_s \) is the charge of ion fluid \( s \).

The momentum equations for the ion and electron fluids are
\[
\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + \mathbf{I} p_s) = + n_s q_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \mathbf{S}_{\rho_s \mathbf{u}_s},
\]
\[
\frac{\partial \rho_e \mathbf{u}_e}{\partial t} + \nabla \cdot (\rho_e \mathbf{u}_e \mathbf{u}_e + \mathbf{I} p_e) = - n_e e (\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) + \mathbf{S}_{\rho_e \mathbf{u}_e},
\]
where \( \rho_s \) and \( \rho_e \) are the ion and electron mass densities, \( \mathbf{u}_s \) and \( \mathbf{u}_e \) are the ion and electron velocities, \( p_s \) and \( p_e \) are the ion and electron pressures, \( \mathbf{E} \) and \( \mathbf{B} \) are the electric and magnetic field strengths, finally \( \mathbf{S}_{\rho_s \mathbf{u}_s} \) and \( \mathbf{S}_{\rho_e \mathbf{u}_e} \) are arbitrary source terms due to electron-ion collisions, charge exchange for ions, etc.

We can use the electron momentum equation (2) to express the electric field. Since the electron mass is much smaller than the ion mass, we may neglect terms proportional to the electron mass density and arrive at the generalized Ohm’s law:
\[
\mathbf{E} = - \mathbf{u}_e \times \mathbf{B} - \frac{1}{en_e} \nabla p_e + \eta \mathbf{J},
\]
where \( \eta \mathbf{J} \) is the resistivity term originating from the source term \( \mathbf{S}_{\rho_e \mathbf{u}_e} \) in the electron momentum equation. The current density can be written as \( \mathbf{J} = -en_e \mathbf{u}_e + \sum_s q_s n_s \mathbf{u}_s \), which can be rearranged to obtain the electron velocity as \( \mathbf{u}_e = - \mathbf{J} / (en_e) + \mathbf{u}_+ \), where \( \mathbf{u}_+ = \sum_s n_s q_s \mathbf{u}_s / (en_e) \) is the charge averaged ion velocity. We can substitute the electron velocity into Ohm’s law (3) to obtain the electric field, which is then substituted into the ion momentum equation (1) and the induction equation to arrive at the following multi-fluid MHD equations:
\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) = \mathbf{S}_{\rho_s},
\]
\[
\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + \mathbf{I} p_s) = n_s q_s (\mathbf{u}_s - \mathbf{u}_+) \times \mathbf{B} + \frac{n_s q_s}{n_e} (\mathbf{J} \times \mathbf{B} - \nabla p_e) + \mathbf{S}_{\rho_s \mathbf{u}_s},
\]
\[
\frac{\partial p_s}{\partial t} + \nabla \cdot \mathbf{p}_s \mathbf{u}_s = - (\gamma - 1) p_s \nabla \cdot \mathbf{u}_s + \mathbf{S}_{p_s},
\]
\[
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u}_+ \times \mathbf{B}) = 0,
\]
where \( \gamma \) is the adiabatic index. The units of the magnetic field are chosen such that magnetic permeability of vacuum is unity. We note the following: (i) the multi-ion MHD equations cannot be written into conservation form, (ii) resistivity is neglected, and (iii) the Hall term and the gradient of the electron pressure are neglected in the induction equation to avoid the stiffness due to Whistler waves. BATSRUS can include resistivity as well as the Hall term (Toth, Ma, & Gombosi 2008), but we will not use these features in this study.
The electron pressure can either be assumed to be some fraction of the total ion pressure \( p_e = \alpha \sum \rho_i \) or we can solve the electron pressure equation
\[
\frac{\partial p_e}{\partial t} + \nabla \cdot (p_e \vec{u}_e) = -(\gamma - 1) p_e \nabla \cdot \vec{u}_e + S_{p_e}
\] (5)
where the source term may include the electron heat conduction.

We have also implemented the option of solving for the hydrodynamic energy density
\[ e_s = \rho_s \vec{u}_s^2 / 2 + p_s / (\gamma - 1) \]
as
\[
\frac{\partial e_s}{\partial t} + \nabla \cdot [(e_s + p_s) \vec{u}_s] = \vec{u}_s \cdot \left[ n_s q_s (\vec{u}_s - \vec{u}_+) \times \vec{B} + \frac{n_s q_s}{n_e e} (\vec{J} \times \vec{B} - \nabla p_e) \right] + S_{e_s}
\] (6)
instead of solving for the ion pressure \( p_s \).

The source terms \( S_{\rho_s}, S_{\rho_s\vec{u}_s}, S_{p_s}, S_{p_e}, \) and \( S_{e_s} \) represent the mass, momentum, pressure or energy sources, respectively. They may contain charge exchange, recombination, photo-ionization, chemistry, ion-ion collisions, etc.

### 2.1. Boris correction

It is a usual practice in magnetospheric MHD codes to use a semi-relativistic correction with the actual or an artificially reduced speed of light (see Gombosi et al. 2001 and references therein). This so-called Boris correction (Boris 1970) limits the Alfvén speed to the speed of light as demanded by the theory of relativity. The artificial light speed reduction is done to further reduce the Alfvén speed so that the equations are less stiff.

This idea can be extended to the multi-fluid MHD equations too. In semi-relativistic multi-ion MHD the momentum \( \vec{m}_s \) of fluid \( s \) is modified by the momentum of the electro-magnetic field to
\[
\vec{m}_s = \rho_s \vec{u}_s + \frac{n_s q_s}{n_e e} \frac{\vec{E} \times \vec{B}}{c^2}
\] (7)
To arrive at a simple, but still reasonable formula, in the semi-relativistic term we approximate \( \vec{E} \approx -\vec{u}_s \times \vec{B} \) so that
\[
\vec{m}_s = \rho_s \vec{u}_s \left[ I + \frac{V_{A,s}^2}{c^2} (\vec{b} \vec{b} - I) \right]
\] (8)
where \( \vec{b} = \vec{B} / B \) is the unit vector of the magnetic field direction and we introduced the species Alfvén speed as
\[
V_{A,s}^2 = \frac{n_s q_s}{n_e e} \frac{B^2}{\rho_s} = \frac{\mu}{\rho_s} \frac{B^2}{\rho}
\] (9)
where \( \mu_s = \rho_s / (n_s q_s) \) is the ion mass per charge for fluid \( s \) and \( \mu = \rho / (n_e e) \) is the average ion mass per charge. We can now use the simplest form of the Boris modification (see Gombosi et al. 2001) by changing the number densities on the right hand sides of the momentum and energy equations as
\[
n_s' = \frac{n_s}{1 + V_{A,s}^2 / c^2}
\] (10)
where \( c' \) is the actual or modified (lowered) speed of light. The lowered speed of light allows larger explicit time steps and it reduces the numerical diffusion.
2.2. Two-stream instability

Two-stream instabilities physically restrict the relative velocities of the ions parallel to the magnetic field line. This sub-grid process is difficult to directly include into our model. We therefore mimic its effect by including a nonlinear artificial friction term to limit the relative velocities to realistic values, rather than directly simulate the instability. In particular we used the following source term in the momentum equation:

$$S_{\text{friction}}^{\rho u_s} = \frac{1}{\tau_c} \sum_{q \neq s} \min(\rho_s, \rho_q) \left( \frac{|u_s - u_q|}{u_c} \right)^{\alpha_c}$$

(11)

where $q$ indexes all the other fluids, $\tau_c$ is the cut-off time scale, $u_c$ is the cut-off velocity and $\alpha_c$ is the cut-off exponent. The larger the exponent, the sharper the cut-off is for velocity differences nearing or exceeding $u_c$. We take the minimum of the two densities instead of their product so that the friction term is equally effective in regions of low and high densities.

While this is a rather ad-hoc formula, it achieves some control over the velocity differences. Without the friction term the velocity differences may grow to unrealistically high values. Currently we set $\tau_c$, $u_c$ and $\alpha_c$ as input parameters for the run, and hold them constant. In the future we will explore more physics based parameter settings and friction formulas.

3. Numerical Schemes

Here we address some of the numerical challenges in discretizing the multi-ion MHD equations.

3.1. Stability

The momentum equation is discretized in a point-implicit manner

$$\left( \rho_s u_s \right)^{n+1} = \left( \rho_s u_s \right)^n - \Delta t \nabla \cdot \left( \rho_s u_s u_s + I \rho_s \right)^n$$

$$+ \Delta t \left[ \frac{q_s}{M_s} \left( \rho_s u_s - \rho_s u_+ \right)^{n+1} \times B^n + \frac{n_s}{n_+} \frac{q_s}{n_e} \left( J^n \times B^n - \nabla p_e^n \right) \right]$$

$$+ \Delta t S_{\text{friction}}^{\rho u_s, n+1} + \Delta t S_{\text{other}}^{\rho u_s}$$

(12)

where $M_s$ is the atomic/molecular mass of species $s$. Notice that the term $\rho_s u_s - \rho_s u_+$ and the friction source term $S_{\text{friction}}^{\rho u_s}$ are evaluated at time level $n+1$ instead of $n$. Only the momenta are treated implicitly, so we have to invert a $3N$ by $3N$ matrix, where $N$ is the number of fluids. The matrix elements are calculated analytically for sake of efficiency and accuracy. If there are other stiff source terms, e.g. due to chemical reaction, we also include them into the point-implicit scheme.

3.2. Conservation

Shock capturing schemes require a conservative discretization to provide the proper weak solution. Unfortunately the multi-ion MHD equations cannot be
written in conservation form, therefore a conservative discretization is not possible. The multi-ion equations are conservative in the hydrodynamic limit, i.e. when the magnetic energy density is small relative to the kinetic and thermal energy densities, and the electron pressure gradient is also small relative to other terms. In that case the shock solutions should be well approximated.

In some applications shock waves are only present in regions dominated by a single ion fluid. For example the bow shock around the Earth is dominated by hydrogen. We have implemented the option of switching to the single fluid MHD equations in a region determined by physical and/or geometrical parameters.

Finally one can also solve for the total mass density $\rho$ and the total momentum $\rho u$ in addition to the multi-ion MHD equations, so that the total mass and momentum conservation can be enforced. The equation for total density conservation is simply the sum of the separate fluid mass conservation equations, so using the total sum is only different in the numerical discretization. The total momentum equation, on the other hand, can be written in a fully conservative form

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \left[ \sum_s (\rho_s u_s u_s) + I(p + p_e + B^2/2) - BB \right] = S_{\rho u} \quad (13)$$

Note that the total momentum diad $\rho uu$ is replaced by the sum of the ion fluid diads. After each time step one can replace the intermediate individual ion momenta $(\rho_s u_s)^*$ with the appropriate fraction of the total momentum, i.e.

$$(\rho_s u_s)^{n+1} = (\rho_s u_s)^* \frac{(\rho u)^{n+1}}{\sum_q (\rho_q u_q)^*} \quad (14)$$

This scheme can be applied as long as the total momentum is not (close to) zero.

3.3. Positivity

Another difficulty in modeling multi-ion MHD is maintaining the positivity of the density and pressure of all ion fluids. Some regions may be completely devoid of some of the ions. In such regions we initialize the particular ion density to a small fraction ($\approx 10^{-4}$) of the total ion density, while velocity and temperature are set to the same value as for the total ion fluid. This is a physically meaningful state that can interact properly with the truly multifluid regions. We follow the same procedure for inflow type boundary conditions. In principle one can repeat this procedure after every time step in the whole computational domain, but so far our applications worked without such a continuous positivity fixing.

4. Application

The multi-fluid MHD code has been successfully applied to the Earth’s magnetosphere (see Glocer et al. 2009b). Here we show some preliminary results for the interaction of the solar wind with the Mars ionosphere. The solar wind flows from the $+X$ direction carrying a magnetic field pointing in the $Y$ direction. In this idealized simulation the ionosphere model is also symmetric with respect to the $Y$ and $Z$ directions. We use a 3D spherical grid with 2 levels of mesh refinement near the surface of Mars.
Figure 1. Comparison of single-fluid (left) and multi-fluid MHD (right) results.

Figure 1 compares the density of the O$^+$ ions in the $X-Z$ plane for the steady state solutions obtained by the multi-species but single-fluid and the truly multifluid MHD codes. In multi-fluid MHD the hot O$^+$ ions (generated by charge exchange from the neutral oxygen) can move upstream and across the dominant H$^+$ ions of the solar wind. The outflow is asymmetric due to the multi-fluid terms in the momentum equation unlike in the single-fluid case.

References