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Numerical Approximation of MHD equations for real gases

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Abstract. We consider the MHD equations for real gases described by a Van der Waals equation of state. We present an explicit calculation of the spectral decomposition of the Jacobian of the fluxes and we propose a characteristic-based upwind numerical scheme to approximate the solution of the system of equations in the one dimensional case. We show a numerical example where we observe wave dynamics significantly stronger than the one obtained for the ideal MHD case.

1. Introduction

The magnetohydrodynamics (MHD) system of equations for real gases can be expressed as

$$\begin{aligned}
\rho_t + \nabla(\rho\mathbf{v}) &= 0 \\
(\rho\mathbf{v})_t + \nabla\Big(\rho\mathbf{v}\mathbf{v}^T + (P + \frac{1}{2}\mathbf{B}^2)I - \mathbf{B}\mathbf{B}^T\Big) &= 0 \\
\mathbf{B}_t - \nabla\times(\mathbf{v}\times\mathbf{B}) &= 0 \\
E_t + \nabla\Big((E + P^*)\mathbf{v} - (\mathbf{v}\times\mathbf{B})\times\mathbf{B}\Big) &= 0
\end{aligned}$$

where $\rho, \mathbf{v}, \mathbf{B}$ and E denote the mass density, the velocity field, the magnetic field and the total energy respectively. The energy is expressed as $E = \frac{1}{2}\rho q^2 + \frac{1}{2}B^2 + \rho\varepsilon$ where q^2 and B^2 are the squares of the magnitudes of the velocity field and the magnetic field respectively and ε the specific internal energy. $P^* = P + \frac{1}{2}B^2$ is the total pressure and $P = P(\rho, \varepsilon)$ the hydrodynamic pressure defined through a real gas equation of state (EOS).

The study of wave dynamics in real gases under severe regimes like the ones encountered in astrophysical scenarios is a field of increasing interest. The deviation of real gases from the ideal gas case is significant and therefore a more general analytic expression of the EOS permitting the development of specific features is necessary. Van der Waals EOS is a powerful and versatile mathematical model allowing strong complex wave dynamics including thermodynamic phase change (Landau & Lifschitz (1987); Thompson (1971); Menikof & Plohr (1989)). The behavior of shock waves in real gases described by the Euler equations ruled by a Van der Waals EOS (Thompson (1971); Thompson & Lambrakis (1973)) represents an initial step for the analysis of the wave dynamics arising in real plasmas.

In order to explore the complex dynamics of MHD equations for real gases we consider a numerical scheme that is designed considering full information of the wave structure of the system through the spectral decomposition of the Jacobians of the fluxes. We propose a complete system of eigenvectors and the corresponding eigenvalues of the Jacobian for the MHD fluxes in terms of the thermodynamic magnitudes of the Van der Waals EOS. We then design a characteristic-based numerical scheme following a similar approach as the one proposed in Serna (2009) for ideal MHD. We perform computations for a one dimensional shock tube problem showing a significantly stronger wave dynamics than the one obtained for the ideal MHD case.

2. Local characteristic approach for Van der Waals plasmas

We consider the hyperbolic system of equations for the MHD case in divergent form in one dimension

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = 0 \tag{1}$$

where $\mathbf{u}$ is the vector of conserved variables

$$\mathbf{u} \quad = \quad (\rho,\, \rho u,\, \rho v,\, \rho w,\, B_y,\, B_z,\, E)^T \tag{2}$$

and $\mathbf{f}(\mathbf{u})$ the flux vector represented as

$$\begin{aligned} \mathbf{f}(\mathbf{u}) \quad = \quad & (\rho u,\, \rho u^2 + P^* - B_x^2,\, \rho uv - B_x B_y,\, \rho uw - B_x B_z,\, uB_y - vB_x, \\ & uB_z - wB_x,\; u(E + P^*) - B_x(uB_x + vB_y + wB_z))^T \end{aligned} \tag{3}$$

where u, v, w represent the velocity field components and B_x, B_y, B_z the magnetic field ones. We assume B_x constant.

The pressure is defined from the expression of the Van der Waals EOS

$$P = \frac{R}{C_V}(\varepsilon + \eta_a \rho)\frac{\rho}{1 - \eta_b \rho} - \eta_a \rho^2 \tag{4}$$

where R is the gas constant, C_V is the specific heat at constant volume and $\eta_a > 0$ and $\eta_b > 0$ are positive constants accounting for the intermolecular forces and the molecule size respectively.

Hyperbolicity of a system of the form (1) of dimension m implies that the diagonalization of the Jacobian of the flux decouples the original hyperbolic system in m scalar conservation laws defining the so-called characteristic fields and the corresponding characteristic fluxes.

The eigenvalues of the Jacobian $\mathbf{f}'(\mathbf{u})$ are denoted as $\lambda_1(\mathbf{u}), \cdots, \lambda_m(\mathbf{u})$ counting each one as many times as its multiplicity. The complete system of right and left eigenvectors are defined as $R = \{\mathbf{r}_1(\mathbf{u}), \cdots, \mathbf{r}_m(\mathbf{u})\}$ and $L = \{\mathbf{l}_1(\mathbf{u}), \cdots, \mathbf{l}_m(\mathbf{u})\}$ diagonalizing $\mathbf{f}'(\mathbf{u})$ such that $\mathbf{r}_i \cdot \mathbf{l}_j = \delta_{ij}$ and

$$L(\mathbf{u})\, \mathbf{f}'(\mathbf{u})\, R(\mathbf{u}) = \Lambda = \mathrm{diag}(\lambda_1(\mathbf{u}), \cdots, \lambda_{\mathrm{m}}(\mathbf{u})) \tag{5}$$

Next we propose the spectral decomposition of the Van der Waals MHD equations. Let us define $(b_x, b_y, b_z) = (B_x, B_y, B_z)/\sqrt{\rho}$ and $b^2 = b_x^2 + b_y^2 + b_z^2$. The general expression of the square of the acoustic sound speed is given as

$$a^2 = P_\rho + \frac{P P_\varepsilon}{\rho^2} \tag{6}$$

where P_ρ represents the partial derivative of P with respect to ρ and P_ε the partial derivative of P with respect to ε.

In our case, considering P defined from the Van der Waals EOS (4) the expression for a^2 reads as

$$a^2 = \frac{R}{C_V}\frac{1}{1-\eta_b\rho}\left(\frac{1}{1-\eta_b\rho}(\varepsilon+\eta_a\rho)+\eta_a\rho+\frac{P}{\rho}\right)-2\eta_a\rho \tag{7}$$

The Alfven velocity $c_a = |b_x|$ and the fast and slow velocities are given by

$$c_{f,s} = \sqrt{\frac{1}{2}\left[(a^2+b^2) \pm \sqrt{(a^2+b^2)^2-4a^2b_x^2}\right]} \tag{8}$$

The seven characteristic velocities associated to the system are: $\lambda_1(\mathbf{u}) = u - c_f$, $\lambda_2(\mathbf{u}) = u - c_a$, $\lambda_3(\mathbf{u}) = u - c_s$, $\lambda_4(\mathbf{u}) = u$, $\lambda_5(\mathbf{u}) = u + c_s$, $\lambda_6(\mathbf{u}) = u + c_a$, $\lambda_7(\mathbf{u}) = u + c_f$.

We define $\mathrm{sgn}(t) = 1$ for $t \geq 0$ and $\mathrm{sgn}(t) = -1$ otherwise and set β_y and β_z values from the expressions

$$\beta_y = \begin{cases} \frac{B_y}{\sqrt{B_y^2+B_z^2}}; & B_y^2+B_z^2 \neq 0 \\ \mathrm{sgn(B_y)}\frac{1}{\sqrt{2}}; & \text{otherwise} \end{cases} \qquad \beta_z = \begin{cases} \frac{B_z}{\sqrt{B_y^2+B_z^2}}; & B_y^2+B_z^2 \neq 0 \\ \mathrm{sgn(B_z)}\frac{1}{\sqrt{2}}; & \text{otherwise} \end{cases}$$

The eigenvectors associated to λ_4, λ_2 and λ_6 are

$$\begin{aligned}
\mathbf{r}_4 &= \left(1, u, v, w, 0, 0, -\frac{1}{2}\Big(\frac{1}{\tau} - q^2 - \frac{a^2(1-\eta_b\rho)}{\kappa}\Big)\right)^T \\
\mathbf{l}_4 &= \tau\left(\frac{1}{\tau} + \frac{1}{2}\Big(\frac{a^2(1-\eta_b\rho)}{\kappa} - \frac{1}{\tau} - q^2\Big), u, v, w, B_x, B_y, B_z, -1\right) \\
\mathbf{r}_2 &= \left(0, 0, -\beta_z\mathrm{sgn(B_x)}, \beta_y\mathrm{sgn(B_x)}, -\frac{\beta_z}{\sqrt{\rho}}, \frac{\beta_y}{\sqrt{\rho}}, -\mathrm{sgn(B_x)}[\beta_z v - \beta_y w]\right)^T \\
\mathbf{r}_6 &= \left(0, 0, -\beta_z\mathrm{sgn(B_x)}, \beta_y\mathrm{sgn(B_x)}, \frac{\beta_z}{\sqrt{\rho}}, -\frac{\beta_y}{\sqrt{\rho}}, -\mathrm{sgn(B_x)}[\beta_z v - \beta_y w]\right)^T \\
\mathbf{l}_2 &= \left(\frac{1}{2}\mathrm{sgn(B_x)}[\beta_z v - \beta_y w], -\frac{\beta_z}{2}\mathrm{sgn(B_x)}, \frac{\beta_y}{2}\mathrm{sgn(B_x)}, -\beta_z\frac{\sqrt{\rho}}{2}, \beta_y\frac{\sqrt{\rho}}{2}, 0\right) \\
\mathbf{l}_6 &= \left(\frac{1}{2}\mathrm{sgn(B_x)}[\beta_z v - \beta_y w], -\frac{\beta_z}{2}\mathrm{sgn(B_x)}, \frac{\beta_y}{2}\mathrm{sgn(B_x)}, \beta_z\frac{\sqrt{\rho}}{2}, -\beta_y\frac{\sqrt{\rho}}{2}, 0\right)
\end{aligned}$$

where

$$\tau = \frac{\kappa\rho}{2\kappa\rho\varepsilon + 2\kappa P - a^2(1-\eta_b\rho)\rho} \qquad \text{and} \qquad \kappa = \frac{R}{C_V}$$

The eigenvectors associated to $\lambda_1, \lambda_3, \lambda_5$ and λ_7, can be expressed in an unified way for $k = 1, 3, 5, 7$ as

$$\mathbf{r}_k = \left(\alpha,\ \alpha(u+c),\ \alpha v - \overline{\alpha c}\,\mathrm{sgn(c^2-a^2)\,sgn(B_x)}\beta_y,\ \alpha w - \overline{\alpha\, c},\mathrm{sgn(c^2-a^2)}\right.$$

$$
\begin{aligned}
& \operatorname{sgn}(\mathrm{B_x})\beta_z,\ \bar{\alpha}\frac{\mathrm{a}}{\sqrt{\rho}}\ \operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\beta_y,\ \bar{\alpha}\frac{\mathrm{a}}{\sqrt{\rho}}\operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\beta_z, \\
& \alpha\Big(\frac{E+P}{\rho}-a^2+c^2+uc\Big)-\operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\overline{\alpha\,\mathrm{c}}\operatorname{sgn}(\mathrm{B_x})(\mathrm{v}\beta_y+\mathrm{w}\beta_z)\Big) \\
\mathbf{l}_k \;=\; & \frac{1}{2a^2}\Big(-\frac{\alpha\kappa}{2(1-\eta_b\rho)}\Big(\frac{1}{\tau}-q^2-\frac{a^2(1-\eta_b\rho)}{\kappa}\Big),-\frac{\alpha\kappa}{1-\eta_b\rho}u+\alpha c, \\
& \frac{-\alpha\kappa}{1-\eta_b\rho}v-\overline{\alpha c}\operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\operatorname{sgn}(\mathrm{B_x})\beta_y, \\
& \frac{-\alpha\kappa}{1-\eta_b\rho}w-\overline{\alpha c}\operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\operatorname{sgn}(\mathrm{B_x})\beta_z, \\
& \frac{-\alpha\kappa}{1-\eta_b\rho}B_y+\sqrt{\rho}\,a\bar{\alpha}\ \operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\beta_y, \\
& \frac{-\alpha\kappa}{1-\eta_b\rho}B_z+\sqrt{\rho}\,a\bar{\alpha}\operatorname{sgn}(\mathrm{c}^2-\mathrm{a}^2)\beta_z,\ \frac{\alpha\kappa}{1-\eta_b\rho}\Big)
\end{aligned}
$$

where c and $\bar{c}$ and α and $\bar{\alpha}$ are determined as:

- for $k = 1$ and $k = 7$, $c = \mp c_f$, $\bar{c} = \mp c_s$ and

$$
\alpha = \begin{cases} \alpha_f \cdot \operatorname{sgn}(\mathrm{B_y}); & a^2 < b_x^2 \\ \alpha_f; & \text{otherwise} \end{cases} \qquad \bar{\alpha} = \begin{cases} \alpha_s \cdot \operatorname{sgn}(\mathrm{B_y}); & a^2 < b_x^2 \\ \alpha_s; & \text{otherwise} \end{cases}
$$

- for $k = 3$ and $k = 5$, $c = \mp c_s$, $\bar{c} = \mp c_f$ and

$$
\alpha = \begin{cases} \alpha_s \cdot \operatorname{sgn}(\mathrm{B_y}); & a^2 > b_x^2 \\ \alpha_s; & \text{otherwise} \end{cases} \qquad \bar{\alpha} = \begin{cases} \alpha_f \cdot \operatorname{sgn}(\mathrm{B_y}); & a^2 > b_x^2 \\ \alpha_f; & \text{otherwise} \end{cases}
$$

α_f and α_s are defined from the following expressions,

$$
\alpha_f = \begin{cases} \frac{\sqrt{a^2-c_s^2}}{\sqrt{c_f^2-c_s^2}}; & B_y^2+B_z^2 \neq 0 \text{ or } B_x^2 \neq \rho a^2 \\ \frac{1}{\sqrt{2}}; & \text{otherwise} \end{cases} \quad \alpha_s = \begin{cases} \frac{\sqrt{c_f^2-a^2}}{\sqrt{c_f^2-c_s^2}} & B_y^2+B_z^2 \neq 0 \text{ or } B_x^2 \neq \rho a^2 \\ \frac{1}{\sqrt{2}}; & \text{otherwise} \end{cases}
$$

The proposed complete system of eigenvectors guarantees continuity with respect to the conserved variables as defended in Serna (2009).

3. High order numerical approximation

A scheme in conservation form for a system of conservation laws is written as

$$
\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \frac{\Delta t}{\Delta x}(\tilde{\mathbf{f}}_{j+\frac{1}{2}} - \tilde{\mathbf{f}}_{j-\frac{1}{2}}) \tag{9}
$$

where $\mathbf{u}_j^n \approx \mathbf{u}(x_j, t_n)$ is a numerical approximation of the solution in the computational cell $x_j = jh$, $t_n = n\Delta t$ where h and Δt are the spatial and time step sizes respectively and

$\tilde{\mathbf{f}}^n_{j+\frac{1}{2}}$ represents the numerical flux. We perform the local characteristic decomposition of the system decoupling the equations in linearly independent characteristic fields. We approximate the numerical fluxes at cell interfaces by means of two linearizations at each side of the interface following the interface splitting strategy used in the Marquina flux formula (Donat & Marquina (1996)). Numerical schemes based in one linearization might be convenient when exact formulas to satisfy Rankine-Hugoniot relations are available (Roe (1981)). That is the case for ideal gas dynamics and the case for adiabatic exponent $\gamma = 2$ in ideal MHD (Brio & Wu (1988)). In the case of non-ideal gases and plasmas Marquina's flux splitting procedure allows to satisfy approximately Rankine-Hugoniot relations at interfaces. The procedure avoids arbitrary averaging and therefore thermodynamic inconsistencies at intermediate states.

To compute $\tilde{\mathbf{f}}$ in terms of two linearizations at each interface we use the first order flux splitting formula

$$\tilde{\mathbf{f}}_{j+\frac{1}{2}} = \tilde{\mathbf{f}}(\mathbf{u}^n_j, \mathbf{u}^n_{j+1}) = \sum_{p=1}^{7} \left[\psi^p_+ \mathbf{r}_p(\mathbf{u}^n_j) + \psi^p_- \mathbf{r}_p(\mathbf{u}^n_{j+1}) \right] \tag{10}$$

where ψ^p_+ and ψ^p_- represent the lateral numerical characteristic fluxes. These are computed at the interface following the entropy-fix upwind procedure proposed in Serna (2009) from the local characteristic fluxes and variables

$$\begin{aligned} \phi^p_j &= \mathbf{f}(\mathbf{u}^n_j) \cdot \mathbf{l}_p(\mathbf{u}^n_j) \qquad \phi^p_{j+1} = \mathbf{f}(\mathbf{u}^n_{j+1}) \cdot \mathbf{l}_p(\mathbf{u}^n_{j+1}) \\ w^p_j &= \mathbf{u}^n_j \cdot \mathbf{l}_p(\mathbf{u}^n_j) \qquad w^p_{j+1} = \mathbf{u}^n_{j+1} \cdot \mathbf{l}_p(\mathbf{u}^n_{j+1}) \end{aligned}$$

for $p = 1, 2, \cdots, 7$. Due to page limitation we will not detail the procedure to calculate the lateral numerical characteristic fluxes. We refer the reader to the extended description presented in Serna (2009).

Third order accuracy in space is achieved by applying a reconstruction function on local characteristic fluxes and variables. This is performed evaluating at the interface the reconstruction function that is determined via primitive function and satisfies the conservation property (Shu & Osher (1989)). We use a third order accurate piecewise hyperbolic reconstruction procedure as used in Serna (2009). For the integration in time we use a third order Runge-Kutta time stepping procedure.

3.1. Brio-Wu shock tube problem

We perform a numerical experiment consisting of the approximation of the solution of the one dimensional Brio-Wu (Brio & Wu (1988)) shock tube Riemann problem for the Helium Van der Waals EOS with parameters $\eta_a = 0.03412$, $\eta_b = 0.23$, $R = 0.0821$ and $C_V = 20.81$.

The two initial constant states, u_L and u_R are

$$(\rho, u, v, w, B_y, B_z, P) = \begin{cases} (1, 0, 0, 0, 1, 0, 1); & x \leq 0 \\ (0.125, 0, 0, 0, -1, 0, 0.1); & x > 0 \end{cases}$$

and $B_x = 0.75$ constant at both sides. We solve the one-dimensional MHD system for $x \in [-1, 1]$ with $N = 800$ equally spaced grid points. We evolve the numerical scheme using a CFL number of $C = 0.5$ such that $\Delta t = C \frac{\Delta x}{\max(|u| + c_f)}$ and compute the approximate solution at $t = 0.2$.

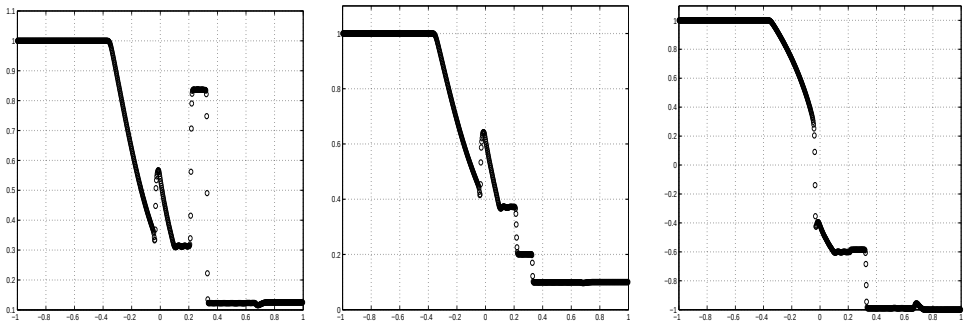

Figure 1. Brio-Wu Riemann MHD problem for Van der Waals equation of state for Helium : (left) density, (middle) pressure, (right) y-component of magnetic field at time $t = 0.2$

This example was proposed in Brio & Wu (1988) for ideal MHD gases to show the formation of a compound wave. In Figure 1 we display the density, pressure and y-component of the magnetic field profiles at time $t = 0.2$. We observe stronger dynamics than the one for the ideal MHD case as shown in Brio & Wu (1988). We obtain two fast rarefaction waves and a slow compound wave interacting with the tail of the left rarefaction. The right hand slow shock wave shows a blast wave structure with a significant increment of the density.

4. Conclusion

With the aim of studying the wave dynamics of the MHD equations under a real gas described by a Van der Waals type equation of state, we use a characteristic based numerical scheme to approximate the numerical solution of the system of equations. We propose a complete system of eigenvectors for the MHD equations for the Van der Waals equation of state. We present a numerical experiment in one dimension that shows stronger dynamics than the ones for the ideal MHD case. This results represent an initial step for an extended study in progress of different problems in multidimensions.

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