Numerical Simulation of Dense Gases over simple geometries using novel and robust central solvers

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Abstract
Non-classical non-linear waves exist in dense gases at high pressure in the region close to a thermodynamical critical point. These waves behave precisely opposite to the classical non-linear waves (shocks and expansion fans) and do not violate entropy conditions. More complex EOS other than the ideal or perfect gas equation of state (EOS) is used in describing dense gases. Algorithm development with non-ideal/real gas EOS and application to dense gases is gaining importance from a numerical perspective. Algorithms designed for perfect gas EOS can not be extended directly to arbitrary real gas EOS with known EOS formulation. Most of the algorithms designed with prefect gas EOS are modified significantly when applied to real gas EOS with the known formulation. These algorithms can become complicated and some times impossible based on the EOS under consideration. The objective of the present work is to develop central solvers with smart diffusion capabilities independent of the eigenstructure and extendable to any arbitrary EOS. Euler equations with van der Waals EOS along with algorithms like MOVERS, MOVERS+, and RICCA are used to simulate dense gasses over simple geometries. Various 1D and 2D benchmark test cases are validated using these algorithms, and the results compared with the data obtained from the literature.

Keywords: Non-classical waves, Dense gases, Fundamental Derivative, van

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1. Introduction

Occurrence of classical non-linear waves like shocks, expansion fans are common phenomenon that are observed in high speed flow of a compressible gas. Most of the experiments and numerical simulations are carried out assuming gas to follow perfect/ideal gas equation of state. In this context, expansion shock and compression fans are not valid solutions as they violate the entropy condition.

The behaviour of high-speed flow in the dense regime (i.e., at conditions close to thermodynamic critical point) is gaining attention from both application as well as numerical perspective. In the dense gas region, perfect gas EOS is not valid and real gas effects play a crucial role in predicting the dynamic behaviour of the gases.

Dense gases are usually ‘single-phase vapours whose thermodynamic state is close to saturation conditions or thermodynamical critical point’. These gases exhibit non-classical behaviour (i.e., occurrences of non-classical waves). Non-classical waves are the waves where expansion shocks and mixed compression-expansion fans occur without violating the entropy conditions (or the second law of thermodynamics) as shown in figure [1].

Examples of dense gases are BZT (Bethe-Zel’dovich-Thompson) fluids, refrigerants, hydrocarbons, perfluorocarbons or siloxanes, and heavy polyatomic fluids which are commonly used in engineering applications as heat transfer fluids. These fluids have many practical applications, for example in energy-conversion cycles operating on low-temperature heat sources, such as Organic Rankine Cycle (OCR) [2] and heavy gas wind tunnels [4].

The non classical wave behaviour in dense gases can be justified through the second law of thermodynamics and shock theory. The relationship between the entropy change Δs and the specific volume v across a weak shock is given by [1] (1)

$$\Delta s = - \left( \frac{\partial^2 p}{\partial v^2} \right) \frac{(\Delta v)^3}{12T}. \quad (1)$$
The nonlinear dynamics of dense gases are governed by an important property called the \textit{fundamental derivative}, $\Gamma$, of gas dynamics \cite{39} as given by

$$\Gamma = \frac{v^3}{2a^2} \left( \frac{\partial^2 p}{\partial v^2} \right)_s. \tag{2}$$

From (2) it can be observed that the curvature of an isentrope is given by $\left( \frac{\partial^2 p}{\partial v^2} \right)_s$ which becomes zero at critical points. In the case of dilute or perfect gases away from the critical point as shown in figure(1), the curvature of the isentrope is always positive $\left( \frac{\partial^2 p}{\partial v^2} \right)_s > 0$ which enforces $\Delta v < 0$ satisfying $\Delta s > 0$. For dense gases it is possible that the curvature of isentrope can be negative given by $\left( \frac{\partial^2 p}{\partial v^2} \right)_s < 0$ and in order to have $\Delta s > 0$, $\Delta v > 0$ must be satisfied. This is the reason why the expansion wave steepens and compression wave spreads without violating the entropy.

The Fundamental derivative (2) can also be interpreted as the rate of change of speed of sound w.r.t. density as given in (3) for an isentropic process.

$$\Gamma = 1 + \frac{\rho}{a} \frac{\partial a}{\partial \rho} \tag{3}$$

It can be observed from (3) that for a perfect gas EOS in an isentropic
process \((p \propto \rho^\gamma)\) and with \(a = \sqrt{\left(\frac{\gamma p}{\rho}\right)}\) the fundamental derivative becomes \(\Gamma = \frac{1+\gamma}{2}\). For perfect gas EOS, \(\gamma > 1\), and therefore \(\Gamma > 1\) is always true. For Dense gases the value of fundamental derivative can be \(\Gamma > 0\) or \(\Gamma < 0\) which depends upon the EOS being considered. The existence of non-classical non-linear waves fundamentally depends on the sign of this fundamental derivative.

Initially, shock tube studies were confined to gases that produce classical wave fields (regular shocks and expansion waves) where entropy conditions are satisfied by both shock and expansion fans. Any violation of entropy conditions are not considered as physical, but Borisov et al. were the first to demonstrate the non-classical behaviour of gas in a shock tube. As per the literature, this was the first instance where a shock tube experiment was used to investigate the nonclassical behaviour. Since then several others authored and explored nonclassical dense gas dynamics, with particular attention to the creation and evolution of expansion shocks in the region of negative nonlinearity (3, 6, 7, 8, 9, 10, 11, 12, 31). They have demonstrated that in dense gases expansion shocks and smooth variations in the regions of shocks are physically possible without violating the entropy.

Cinnella proposed a simplification of Roe’s scheme to solve for dense gases. Though this simplification does not satisfy the usual Roe’s conditions for the approximate Riemann solver exactly, it reduces the complexity and computational cost. Higher order extension of the schemes are carried out using MUSCL method.

Congedo et al. studied the dense gas behaviour in turbo-machinery. In this work HLL scheme has been used in evaluating fluxes at the interfaces and MUSCL type reconstruction is used for higher order accuracy. The gradients at cell centers are evaluated using least squares formula.

Argrow has published numerical simulation of dense gas flows using a TVD Predictor-Corrector scheme for 1D Euler equations with van der Waals EOS.

Brown and Argrow have used a predictor-corrector, TVD (PCTVD) scheme based on the Davis-Roe flux limited method to simulate the flow of non-classical dense gas over simple geometries. They have used van der Waals EOS which is a representative equation for heavy fluorocarbons with high specific heat and conditions near thermodynamic critical point. Comparisons have been made with equivalent perfect gas EOS.

In the present work, algorithms having controllable numerical diffusion
and independent of the eigenstructure are utilised in resolving the non-classical waves on simple geometries. A recently developed central solver with controlled numerical diffusion named MOVERS [27] along with the two new algorithms MOVERS+ and RICCA [32] are used to solve Euler equations with van der Waals EOS. This paper is arranged as follows, section 2 reviews the governing equations and the numerical method used in solving them. In sections 3 & 4.2, the basic idea of the algorithms are described in detail. The results obtained for benchmark test cases in 1D and 2D are presented in section 5.

2. Governing equations and Numerical Models

The basic governing equations considered for this study are compressible inviscid Euler equations. These equations are expressed in conservative form as

\[
\frac{dU}{dt} = -R, \quad R = \frac{1}{\Omega} \left[ \sum_{i=1}^{N} F_c \, dS \right],
\]

\[
U = [\rho, \rho u, \rho v, \rho E_t]^T, \quad F_c = [\rho V_n, \rho u V_n + p\hat{n}, \rho v V_n + p\hat{n}, (\rho E_t + p) V_n]^T
\]

where \( U \) is conserved variable vector, \( F_c \) is convective flux vector of a control volume as shown in figure (2), \( R \) represents net flux or residue from a given control volume, \( \Omega \) is the volume of control volume with \( N \) faces, \( V_n \) is the normal velocity \( V_n = \vec{V} \cdot \hat{n} = u_n x + v_n y \) on the control surfaces and \( E_t = e + \frac{u^2 + v^2}{2} \) is the total energy per unit mass. These basic equations are not closed and requires an EOS of the form \( p = p(\rho, e) \) for closure. The simplest EOS which represent dense gas is van der Waals EOS given by

\[
(p + a \rho^2) \left( \frac{1}{\rho} - b \right) = RT,
\]

\[
a = 0.138 \times 10^{-3}, \quad b = 3.258 \times 10^{-5}.
\]
factor $Z_c = \frac{p}{\rho RT} = \frac{3}{8}$ resulting in

$$(\bar{\rho} + a\bar{\rho}^2) (b - \bar{\rho}) = 8\bar{R}\bar{T},$$

$$a = 3, \quad b = 3. \tag{7, 8}$$

These governing equations are solved using a cell entered finite volume method with cell integral averages defined as \([9]\). The finite volume update formula for Euler equations is given by \([10]\) with interface flux evaluated as in \([11]\).

\[
U = \frac{1}{\Omega} \int \Omega \, U \, d\Omega. \tag{9}
\]

\[
U^n_{j+1} = U^n_j - \frac{\Delta t}{\Delta x} \left[ F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}} \right] \tag{10}
\]

\[
F_{j\pm\frac{1}{2}} = F_I (U_L, U_R) = \frac{1}{2} [F(U_L) + F(U_R)] - \Delta F_{num} \tag{11}
\]

where the first term on the right hand side is an average flux from the left (L) and the right (R) states and $\Delta F_{num}$ is a flux difference representing numerical diffusion. The numerical diffusion flux can be written as \([12]\)

\[
\Delta F_{num} = \frac{|\alpha|}{2} (U_R - U_L) \tag{12}
\]
where $\alpha$ coefficient of numerical diffusion. Most of the numerical methods differ in the way this coefficient is determined. In the present work, $\alpha$, is obtained by algorithms like MOVERS [27], RICCA and MOVERS+ [32]. The details of these algorithms are explained in the following sections.

2.1. Why do we need algorithm independent of EOS?

In this section we present the analysis on, why is an algorithm required to be independent of EOS?. Let us consider the governing equations (4) in 1D with general EOS of the form $p = p (\rho, e)$. In nonconservative form these equations can be written as (13) where $A(U)$ is the flux Jacobian matrix (14).

$$\frac{\partial U}{\partial t} + A(U) \frac{\partial U}{\partial x} = 0 \quad (13)$$

$$A(U) = \frac{\partial F}{\partial U} \quad (14)$$

For 1D Euler equations flux Jacobian matrix is given by (15) with total enthalpy $H = E_t + \frac{\rho}{\rho}$

$$A(U) = \frac{\partial F(U)}{\partial U} = \begin{bmatrix} 0 & 1 & 0 \\ (a^2 - u^2) - \frac{\partial p}{\partial e} (H - u^2) & 2u - \frac{u}{\rho} \frac{\partial p}{\partial e} & 0 \\ (a^2 - H) u - \frac{u}{\rho} \frac{\partial p}{\partial e} (H - u^2) & H - \frac{u^2}{\rho} \frac{\partial p}{\partial e} & u + \frac{u}{\rho} \frac{\partial p}{\partial e} \end{bmatrix} \quad (15)$$

It can be observed that the flux Jacobian matrix with general EOS is a function of $\frac{\partial p}{\partial e}$. The eigenvalues for the flux Jacobian matrix are

$$\lambda_1 = u - a; \quad \lambda_2 = u; \quad \lambda_3 = u + a \quad (16)$$

with the corresponding eigenvectors being

$$R^1 = \begin{bmatrix} 1 \\ u - a \\ H - ua \end{bmatrix}; \quad R^2 = \begin{bmatrix} 1 \\ u \\ H - \frac{\rho u^2}{(\rho u)} \end{bmatrix}; \quad R^3 = \begin{bmatrix} 1 \\ u + a \\ H + ua \end{bmatrix}; \quad (17)$$
The acoustic speed or sound speed, \( a \), with general EOS is given by (18) or alternatively by (19)

\[
a = \sqrt{\frac{p}{\rho^2}} \frac{\partial p}{\partial e} + \frac{\partial p}{\partial \rho}
\]

\[
a = -\frac{C_p}{C_v} \frac{\partial T}{\partial \rho}
\]

It can be observed that, speed of sound "a" (18), is a function of the derivatives \( \left( \frac{\partial p}{\partial e} \text{ & } \frac{\partial p}{\partial \rho} \right) \) and is strongly related to the formulation of EOS. If an analytic expression for EOS exists then the derivatives can be found and hence the eigenstructure of the hyperbolic system. The complications of estimating the eigenstructure depends on the nature of the EOS. Hence, if the numerical schemes depend upon the eigenstructure of the flux Jacobian matrix, for example as in Roe scheme, then the development of the numerical method for real gases becomes complicated or some times even impossible. Most of the upwind schemes like those of Steger-Warming, van Leer, require the complete knowledge of eigenstructure of the flux Jacobian matrix, evaluation of which might become complicated based on the nature of EOS. Thus substantial modifications are to be carried out for the upwind schemes when applied to real gases.

The numerical schemes explained in the following sections, MOVERS, MOVERS+ and RICCA, do not depend strongly on the eigenstructure of the underlying hyperbolic system, especially on the eigenvectors. Out of these three schemes the first one requires an estimate of the maximum and minimum of the eigenvalues but no eigenvector information is needed. The other two do not even require the knowledge of the eigenvalues. Thus application of these central solvers to real gases is simple and requires no modification at all and hence can be extended to any sort of EOS [32].

3. Riemann Invariant based Contact-discontinuity Capturing Algorithm (RICCA)

In this section a novel scheme is presented which is based on Generalized Riemann Invariants (GRIs). When the concept of GRI is utilized in the discretization process it leads to a scheme which captures steady contact discontinuities exactly.
3.1. Generalised Riemann Invariants (GRI)

The concept of GRI is briefly introduced here (for a more detailed explanation see [26, 40, 36]). Consider a general quasi-linear hyperbolic system as given by (20).

\[
\frac{\partial U}{\partial t} + A(U) \frac{\partial U}{\partial x} = 0, \tag{20}
\]

\[
U = [U_1, U_2, \ldots, U_m]^T, \tag{21}
\]

where \( U \) represents the conserved variable vector of the hyperbolic system. Of the \( m \) waves associated with the system (20) for the \( i^{th} \) characteristic field associated with eigenvalue \( \lambda_i \), corresponding right eigenvector is given by

\[
R_i = [r_{i1}, r_{i2}, \ldots, r_{im}]^T \tag{22}
\]

The Generalised Riemann Invariants are relations that hold true across expansion waves and contact-discontinuities. This can be mathematically written as

\[
\frac{dU_1}{r_{11}} = \frac{dU_2}{r_{21}} = \ldots = \frac{dU_m}{r_{m1}} \tag{23}
\]

These equations relate ratios of \( dU_j \) to the respective component \( r_{ij} \) of the right eigenvector \( R_i \), corresponding to an eigenvalue \( \lambda_i \). Here, the above relations (GRIs) are utilized in developing a new algorithm which can exactly resolve contact-discontinuities and the algorithm is expected to be accurate enough for flow simulations. This idea avoids Riemann solvers, field-by-field decompositions and complicated flux splittings and yet accurate enough to resolve all the flow features appropriately [32].

3.2. Riemann Invariant based Contact-discontinuity Capturing Algorithm (RICCA)

The modelling of the numerical diffusion is carried out as follows. Consider an interface of a control volume, as shown in figure (3), across which the flow is assumed to be 1D and diffusion flux is to be evaluated. Evaluating the flux difference as given in (24).

\[
\Delta F_{\text{num}} = \left( \frac{\Delta F}{\Delta U} \right)_{\text{num}} \Delta U = \alpha_{\text{num}} \Delta U = \alpha_I \Delta U \tag{24}
\]

The coefficient of numerical diffusion, \( \alpha_{\text{num}} \), is modeled using a diagonal
Various numerical schemes differ in the way the wave speed or the coefficient of numerical diffusion is determined. The basic idea of the present work is to use Generalized Riemann Invariant (GRI) across the interface to determine the coefficient of diffusion, $\alpha_I$. When a GRI (23) is applied to a contact discontinuity we obtain (26)

$$
\alpha_1 = \alpha_2 = \alpha_3 = \alpha_I = |u|
$$

which for any arbitrary interface as given in figure (3) can be given by (27)

$$
\alpha_I = |V_n| = |V_{nL}| = |V_{nR}| = \frac{|V_{nL}| + |V_{nR}|}{2} = max(|V_{nL}|, |V_{nR}|)
$$

Numerical experimentation has revealed that, this numerical diffusion evaluated by (27), though adequate in capturing the contact-discontinuities exactly, is not sufficient enough for the case of shocks being located at the cell interface. So in order to generalize the diffusion for any case, the Riemann Invariant based Contact-discontinuity Capturing Algorithm (RICCA)
is designed with the following coefficient of numerical diffusion:

$$\alpha = \begin{cases} 
\frac{|V_{nL}| + |V_{nR}|}{2}, & \text{if } |\Delta F| < \delta \text{ and } |\Delta U| < \delta \\
\max(|V_{nL}|, |V_{nR}|) + \text{sign}(|\Delta p_I|)a_1, & \text{otherwise}
\end{cases}$$

(28)

where $\delta$ is a small number and $a_1 = \sqrt{\gamma p_I \rho_I}$ is the speed of sound evaluated with the values at the interface given by

$$p_I = \frac{p_L + p_R}{2},$$

(29)

$$\rho_I = \frac{\rho_L + \rho_R}{2},$$

(30)

$$\Delta p_I = (p_R - p_L).$$

(31)

This design of the coefficient of numerical diffusion therefore does not require any entropy fix.

Features of the new central scheme RICCA are:

- It can capture steady grid-aligned contact-discontinuities exactly,

- It has sufficient numerical diffusion near shocks so as to avoid shock instabilities, and

- It does not need entropy fix at sonic points.

- It is not tied down to the eigen-structure and hence can be easily extended to any general equation of state, without modification.

4. MOVERS and MOVERS+

The second of the two new algorithms presented in this paper is based on substantial modification of a central Rankine-Hugoniot solver developed by Jaisankar & Raghurama Rao [27], called as MOVERS (Method of Optimal Viscosity for Enhanced Resolution of Shocks). This is first briefly reviewed in the following subsection, before introducing the new scheme, named as MOVERS+. 
4.1. MOVERS

MOVERS [27] is a central scheme which can capture grid aligned steady shocks and contact discontinuities exactly, with controlled numerical diffusion. As it is a central scheme, it avoids all the complications of Riemann solvers and is not tied to the eigen-structure of the underlying hyperbolic systems. The accurate discontinuity capturing is achieved by enforcing the Rankine-Hugoniot jump condition directly in the discretization process. The basic idea of this algorithm is briefly explained in the following.

Consider the Rankine-Hugoniot conditions, given by (32)

\[
\Delta F = s \Delta U, \quad \Delta (\cdot) = (\cdot)_R - (\cdot)_L
\]

where \( s \) is the speed of the discontinuity, \( F \) is flux vector and \( U \) is the conserved variable vector. First, the speed of the discontinuity is split into a positive part (corresponding to a right-moving discontinuity) and a negative part (corresponding to a left-moving discontinuity), as shown in figure (4) and as given in (33)

\[
s_i = s_i^+ + s_i^-
\]

\[
s_i^\pm = s_i \pm |s_i|/2.
\]

Using the above wave speed splitting, the RH condition at the interface is
split into two parts as

\[
\begin{align*}
F_R - F_I &= s^+_I \Delta U, \\
F_I - F_L &= s^-_I \Delta U
\end{align*}
\]  

(35)

These split RH conditions (35) lead to the cell-interface flux as

\[
F_I = \frac{F_L + F_R}{2} - \frac{|s_I|}{2} \Delta U
\]

(36)

Comparing this cell-interface flux with the general expression (12), the numerical diffusive flux can be obtained as

\[
d_I = \frac{|s_I|}{2} \Delta U
\]

(37)

It can be observed from (32) that \(\Delta F\) and \(\Delta U\) are \(n \times 1\) vectors and thus a suitable choice for \(s\) is an \(n \times n\) matrix. One of the simplest assumptions for the matrix \(s\) that can be conceived is a diagonal matrix with \(n\) diagonal elements. Using this strategy the relation for obtaining the coefficient of numerical diffusion can be written as in (38).

\[
\Delta F_i = s_i \Delta U_i, \quad i = 1, 2, \cdots n
\]

(38)

Thus the coefficient of numerical diffusion can be obtained as (39)

\[
\alpha_{I,i} = |s_i| = \left| \frac{\Delta F_i}{\Delta U_i} \right|, \quad i = 1, 2, 3
\]

(39)

As \(\Delta F_i = 0\) for stationary discontinuities, the numerical diffusion then vanishes, leading to exact capturing of grid-aligned discontinuities. It can be observed from (39) that the coefficient \(\alpha_I\) can go out of bounds when the denominator becomes small.

\[
\Delta U \to 0, \quad \alpha_I \to \infty.
\]

(40)

In order to introduce boundedness and stabilize the numerical scheme, \(\alpha_I\) is to be restricted to a physically feasible range of eigenvalues of the flux Jacobian matrix. This process, termed as wave speed correction, (41) is incorporated such that the coefficient of numerical diffusion lies within the
eigenspectrum of the flux Jacobian i.e., $\alpha_I \in [\lambda_{\text{max}}, \lambda_{\text{min}}]$. 

$$|\alpha_I| = \begin{cases} \\ \\ 
\lambda_{\text{max}}, & \text{if } |\alpha_I| > \lambda_{\text{max}} \\
\lambda_{\text{min}}, & \text{if } |\alpha_I| < \lambda_{\text{min}} \\
|\alpha_I|, & \text{otherwise} \end{cases}$$ \hspace{1cm} (41)

$$F_I = \frac{1}{2} [F_L + F_R] - \frac{|\alpha_I|}{2} [U_R - U_L].$$ \hspace{1cm} (42)

Hence the final numerical flux at the cell-interface in MOVERS is given by (39), (41) and (42). This method is independent of eigen-structure of the underlying hyperbolic systems, is simple and can capture grid-aligned stationary discontinuities exactly. Two variations of MOVERS are introduced in [27]: (i) an $n$-wave based coefficient of numerical diffusion, corresponding to $n$ number of conservation laws (MOVERS-$n$) and (ii) a scalar diffusion, corresponding to the energy equation (as it contains the maximum of information), referred to as MOVERS-1. The robustness of the basic scheme has been improvised through its variants by Maruthi N.H. [30] and extended to other hyperbolic systems for magnetohydrodynamics and shallow water flows. The simplicity and accuracy of MOVERS makes this scheme a well-suited base-line solver for further research, apart from its independency of the eigenstructure. In this work this algorithm is chosen as the foundation to devise a new and efficient algorithm, named as MOVERS+. First, the wave-speed correction mechanism is removed by a reformulation of the basic Rankine-Hugoniot solver. Further, exact shock capturing is deliberately given up for enhancing robustness but exact contact discontinuity capturing is retained for preserving accuracy.

4.2. A new central solver: MOVERS+

MOVERS [27] requires wave speed correction in order to restrict the coefficient of diffusion to within the eigenspectrum. To avoid wave speed correction, a simpler strategy is proposed in this section which is described
where the relation \( \frac{1}{\text{Sign}(\cdot)} = \text{Sign}(\cdot) \) is used. This form of \( d_I \) will eliminate the need of wave speed correction for MOVERS. Numerical experimentation has revealed that this numerical scheme has very low diffusion and captures steady discontinuities exactly but encounters problems in smooth regions due to lack of sufficient numerical diffusion. Therefore, using a shock sensor \( (47) \), an additional numerical diffusion is introduced. This additional diffusion is based on the fluid velocity, which is demonstrated to be sufficient to avoid unphysical expansions in smooth regions \( (41) \). The coefficient of numerical diffusion for MOVERS+ is given by

\[
|d_I|_j = \Phi \text{Sign}(\Delta U_j) |\Delta F_j| + \left( \frac{|V_{nL}| + |V_{nR}|}{2} \right) \Delta U_j, \quad j = 1, 2, 3
\]  

where the \( \Phi \) is the shock sensor defined by

\[
\Phi = \frac{|\Delta p|}{2p_I} \quad \text{with} \quad p_I = \frac{p_L + p_R}{2} \quad (47)
\]

The features of this modified algorithm, MOVERS+, are as follows.

• It can capture steady grid-aligned contact discontinuities exactly and provides low diffusion otherwise.

• It has sufficient numerical diffusion near shocks so as to avoid shock instabilities (deliberately giving up exact shock capturing of MOVERS for gain in robustness).

• It does not need entropy fix for smooth regions or in expansion regions.

• It does not require any wave speed correction, unlike in MOVERS.
• It is a simple central solver and is not based on Riemann solvers, field-by-field decompositions or complicated flux splittings, thus making it a suitable candidate for further extensions.

It can be observed that the above numerical schemes do not depend on the EOS and on the eigenstructure of the underlying hyperbolic systems. If the information of the properties in the cell or the control volume are known then they can be utilised directly. Hence these algorithms can be extended to any form of EOS.

5. Test cases and results for dense gas

To test the capabilities of the algorithms mentioned in the previous sections some interesting 1D and 2D test cases are carefully chosen where the physics of the problem is utmost important and the non-classical behaviour of the gases is clearly predominant. Numerical simulations are carried out with MOVERS-1, MOVERS-n, MOVERS+ and RICCA in 1D and 2D results of MOVERS+ and RICCA are presented in this section.

5.1. 1D dense gas test cases

In this section numerical simulations for 1D dense gases are presented. These test cases are taken from [1, 13] and use van der Waals EOS for simulations. Three test cases are considered to study the non-classical wave phenomena and are chosen such that the flow field contains some regions of negative fundamental derivative ($\Gamma < 0$). Initial conditions used for shock tube test case are described in table (1) and results are compared with the reference data obtained from [1].

<table>
<thead>
<tr>
<th>Test case</th>
<th>$\delta$</th>
<th>$\rho_L$</th>
<th>$p_L$</th>
<th>$\rho_R$</th>
<th>$p_R$</th>
<th>Time</th>
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<td>1</td>
<td>0.0125</td>
<td>1.818</td>
<td>3.0</td>
<td>0.275</td>
<td>0.575</td>
<td>0.1807</td>
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<td>1.090</td>
<td>0.562</td>
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<td>0.4801</td>
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<tr>
<td>3</td>
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<td>0.879</td>
<td>1.090</td>
<td>3.630</td>
<td>0.575</td>
<td>0.2917</td>
</tr>
</tbody>
</table>

Table 1: Test cases for simulation of dense gas flows

Test case 1 in table (1) represents a Riemann problem where initially both the left and the right states lie within ($\Gamma > 0$) region. The solution has a left moving rarefaction fan, a contact-discontinuity in the middle and a right moving shock wave. Initially the rarefaction fan is in ($\Gamma > 0$) region.
However, as the flow evolves $\Gamma$ changes its sign to $(\Gamma < 0)$ and rarefaction fan steepens into a rarefaction shock. Figure (5) refer to the numerical simulation of this test case using RICCA, MOVERS-1, MOVERS-n and MOVERS+. It can be observed that all the numerical methods are resolving the fundamental features accurately. It can also be seen that MOVERS-1 and RICCA though diffusive in nature can be utilised in accurately predicting the flow features. Further no oscillations are observed.

![Graphs](image)

Figure 5: Dense gas test case 1 with MOVERS-n, MOVERS-1, MOVERS+ and RICCA

Test case 2 in the table (1) has both left and right states lying in the $\Gamma < 0$ region. The fundamental derivative remains negative everywhere and the flow behaviour is exactly opposite with respect to classical Riemann problem. Specifically, the solution presents a left running rarefaction shock, a middle contact discontinuity, and a right running compression fan. Except for the fact that $\Gamma$ is negative in the entire domain for this test case, the non-linear waves are similar to those in the classical Riemann problem. Figures (6) refer to the numerical simulation of this test case using RICCA, MOVERS-1, MOVERS-n and MOVERS+.

Test case 3 is an example of flow evolution with two states corresponding to $(\Gamma < 0)$ and $(\Gamma > 0)$. The fundamental derivative changes its sign from left to right and a mixed rarefaction wave forms at the crossing of the transition line. The compression wave lies entirely within the classical zone and hence a classical shock wave appears in this region. Figures (7) refer to the numerical simulation of test case 3 using RICCA, MOVERS-1, MOVERS-n.
Figure 6: Dense gas test case 2 with MOVERS-n, MOVERS-1, MOVERS+ and RICCA

and MOVERS+. From the above three test cases it can be inferred that

all the numerical algorithms are capable of capturing the non-classical wave phenomena with reasonable accuracy without any modification to the basic algorithm.
5.2. 2D dense gas test cases and results

To analyse the non-classical behaviour of dense gases in 2D both steady state and transient test cases on simple geometries are considered. To distinguish between classical and non-classical waves both perfect gas EOS and van der Waals EOS are used for comparison. Algorithms RICCA and MOVERS+ are used in these simulations and their ability to capture the non-classical phenomena is thoroughly explored and only second order accurate solutions are presented. Initial conditions for the transient test cases are given in table 2 and for steady state cases in table 3. Transient conditions for test cases using perfect gas EOS are indicated as TPG1 and TPG2 similarly transient cases for dense gases are indicated as TDG1 and TDG2, where 1 and 2 refer to pre-shock and post-shock conditions. Steady state conditions for the dense gases are represented as DGS1, DGS2 and DGS3.

<table>
<thead>
<tr>
<th>Case</th>
<th>$p_2$</th>
<th>$\rho_2$</th>
<th>$u_2$</th>
<th>$p_1$</th>
<th>$\rho_1$</th>
<th>$u_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TPG1</td>
<td>1.64</td>
<td>1.34</td>
<td>0.40</td>
<td>1.00</td>
<td>1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>TPG2</td>
<td>12.164</td>
<td>3.06</td>
<td>2.74</td>
<td>1.00</td>
<td>1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>TDG1</td>
<td>0.98</td>
<td>0.80</td>
<td>0.14</td>
<td>0.56</td>
<td>1.79</td>
<td>0.0</td>
</tr>
<tr>
<td>TDG2</td>
<td>0.98</td>
<td>0.62</td>
<td>-0.14</td>
<td>1.09</td>
<td>0.88</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 2: Free Stream conditions for transient test cases for simulation of perfect gas and dense gas flows

<table>
<thead>
<tr>
<th>test case</th>
<th>$\delta$</th>
<th>$p$</th>
<th>$\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DGS1</td>
<td>0.0125</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>DGS2</td>
<td>0.0125</td>
<td>0.88</td>
<td>1.09</td>
</tr>
<tr>
<td>DGS3</td>
<td>0.0125</td>
<td>0.62</td>
<td>0.98</td>
</tr>
</tbody>
</table>

Table 3: Free stream conditions for steady state test cases for simulation of dense gas flows

The following steady state test cases are considered.

- Supersonic flow over a forward facing step
- Supersoinc flow over a circular arc.
- Supersonic flow over a smoothly varying expansion ramp
5.2.1. *Supersonic flow over a forward facing step*

A steady supersonic flow of perfect gas and dense gas over a forward facing step is considered here. The computational domain consists of \([0, 2] \times [0, 1]\) with a step height of 0.2m placed at \(x = 0.75\). The left boundary is considered as supersonic inlet, right boundary as supersonic exit, top and bottom boundaries as inviscid walls. For perfect gas EOS the value of \(\gamma\) is taken as \(\frac{5}{3}\) and for van der Waals gas the value of gamma considered is \(\frac{7}{5}\) representing dense gas. For perfect gas the incoming supersonic flow \((M = 3.0)\) encounters a forward facing step. A detached bow shock is formed because of the step and terminates into an oblique shock reflection on the upper boundary. The reflected oblique shock exits out of the boundary as shown in Figure (8b). An expansion fan centred at the corner of the step evolves and interacts with the reflected shock. It can be observed that the fundamental derivative does not change its sign as evident from Figure (8a) and the flow features are captured well. Next we consider a supersonic flow

\[\text{(a) Density contours overlapped with FD} \quad \text{(b) Density Contours}\]

of a dense gas with \(M = 1.5\) encountering the same forward step for the test conditions as shown in the table [2]. Similar to the perfect gas case, a detached bow shock terminates into a Mach reflection compressing the flow into the \(\Gamma > 0\) region. The wave centred on the corner of the step takes the form of a physical expansion shock. The flow features obtained are compared to the case as in [1]. It can be seen from the figure [9] that the Mach stem and the reflected shock are well resolved using the numerical schemes.

5.2.2. *Supersonic flow over a circular arc*

The second test case considered is flow over a circular arc of radius \(r = 0.15\), with computational domain \([0, 1] \times [0, 1]\). A total of 200 \(\times\) 200 control volumes are used for simulation. Consider the flow of a perfect gas case with \(M_\infty = 3.0\) over this circular bump as shown in figure [12]. The shock is attached to the leading edge of the arc and followed by expansion fan on
the curved surface till it encounters a trailing edge shock. It can also be observed from the figure that the fundamental derivative doesn’t change its sign across the curved surface. Next we consider the flow of a dense gas on the circular arc with Mach number $M = 1.5$. The flow detaches from the leading edge forming a bow shock. Further the fundamental derivative changes its sign $\Gamma > 0$ across the shock and the flow behind the leading-edge forms an expansion shock which expands the flow through $\Gamma < 0$ region as explained in [1]. It can be seen from the figures (11, 12) that both the numerical schemes capture the flow features well without any deviation.
5.2.3. Supersonic flow over a smoothly varying expansion ramp

In this test case a Mach 2 flow over a smooth expansion ramp with 20° inclination is considered. Since the incoming flow is supersonic, it is expected to have a smooth transition and according to the principles of gas dynamics, an expansion fan should evolve from the surface if the flow is for a perfect gas as shown in figure (13). In the case of dense gas, starting from the leading edge an expansion shock is observed as the fundamental derivative transition takes from positive to negative as shown in figure (14).

5.2.4. Transient test cases

TPG1 is a typical case of a weak shock interacting with a large deflecting wedge resulting in a single Mach reflection using perfect gas EOS as shown in figure (15). As the shock wave moving with a constant velocity approaches a solid wedge, the flow generated by the shock impinges on the wedge thus generating a second reflected shock, which ensures that the velocity of the flow is parallel to the wedge surface. From the frame of the reflection point, this flow is locally steady, and the flow is referred to as pseudo-steady. When the angle between the wedge and the primary shock is sufficiently large, a single reflected shock is not able to turn the flow to a direction parallel to the wall and a transition to Mach reflection occurs. Mach reflection consists of three shocks, namely the incident shock, the reflected shock, and a Mach stem, as well as a slip line.
The second transient test case is a moving shock wave refracting over a backward facing step. In the case of perfect gas, it is observed that an expansion fan evolves from the corner, together with an evolving shock and a contact discontinuity present in between them [32]. The flow structure in the case of dense gas with TDG2 conditions is quite different from that of a perfect gas. Instead of an expansion fan at the corner an expansion shock evolves as shown in figure(22) this is because the fundamental derivative $\Gamma$ changes its sign from positive to negative $\Gamma < 0$, further the compression shock continues to move with $M = 1.23$ as shown in figure [22].

6. Conclusions

Numerical simulations are carried out for dense gas using Euler equations with van der Waals EOS to resolve non-linear non classical waves. Various benchmark test cases in 1D are carried out using MOVERS-n, MOVERS-1,MOVERS+ and RICCA. These test cases demonstrate behaviour of the non-classical waves based on the sign of $\Gamma$. All the four numerical schemes could resolve these waves reasonably well. Further study of wave struc-
tured and flow features over simple geometries in 2D are carried out using MOVERS+ and RICCA as these two schemes are more robust than MOVERS. Both steady and unsteady test cases are considered in testing the capability of these algorithms. It is observed that the wave fields of dense gas are significantly different from those corresponding to the perfect gas. The ability of these algorithms in resolving the flow features with real gas EOS is clearly demonstrated. It can be concluded that these algorithms can be used with any real gas EOS without any modifications to general hyperbolic systems.

7. References

References


(a) Perfect gas EOS  
(b) van Der Waals EOS

Figure 17: Density contours overlapped with fundamental derivative

(a) Perfect gas EOS  
(b) van Der Waals EOS

Figure 18: Transient flow over compression ramp using RICCA with TP1 Conditions


Figure 19: Density contours overlapped with fundamental derivative

(a) Perfect gas EOS  
(b) van Der Waals EOS

Figure 20: Transient flow over compression ramp using MOVERS+ scheme with TP1 Conditions

(a) MOVERS+  
(b) RICCA

Figure 21: Density contours overlapped with fundamental derivative

(a) MOVERS+  
(b) RICCA

Figure 22: Shock Diffraction Test case using van Der Waals EOS


