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A non-linear residual distribution scheme for real-gas computations

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ABSTRACT

This paper deals with a high-order accurate Residual Distribution scheme for the numerical solution of dense gas flows on unstructured grids. Dense gas-dynamics studies the flow of gases in the thermodynamic region above the upper saturation curve, close to the liquid–vapor critical point. In such conditions, some fluids may exhibit negative values of the fundamental derivative of gas-dynamics, leading to non-classical gas-dynamic behaviors, such as rarefaction shock waves, mixed shock/fan waves, and shock splitting. Due to the complexity in performing reliable experimental studies for non-classical gas-dynamics, accurate numerical simulations of dense gas flows are of paramount importance. In this work, advantages in using high-order methods are highlighted, in terms of number of degrees of freedom and computational time used, for computing the numerical solution with a greater accuracy compared to lower-order methods, even for shocked flows. Several numerical experiments are also performed to assess the influence of the thermodynamic models on the problem solution.

1. Introduction

In numerical simulations of compressible flows for standard aerodynamic applications the ideal gas model, despite its simplicity, represents an acceptable approximation. However, the ideal gas approximation cannot be considered accurate when pressures and temperatures are of the order of magnitude of their liquid–vapor saturation curve. This thermodynamic region is generally called dense gas region, in contrast to the dilute gas region where the use of the ideal gas model can be retained valid.

Fluids in dense regime may display so-called non-classical gas-dynamics phenomena. In these cases, dense gases may have significantly different properties with respect to dilute gases, from a quantitative and qualitative point of view. For example, for some molecularly complex fluids and for some specific conditions near the saturation curve, the speed of sound can increase with a decreasing density, differently from what happens in the ideal gas model [1].

The dynamics of dense gases is governed by a thermodynamic parameter known as the fundamental derivative of gasdynamics [2]

$$\Gamma = 1 + \frac{\rho}{c}\left(\frac{\partial c}{\partial \rho}\right)_s, \tag{1}$$

where ρ is the density, c is the speed of sound and s is the entropy. For ideal gases $\Gamma = (\gamma+1)/2 > 1$. For some complex fluids and some particular conditions of pressure and temperature, Γ may be lower that one, implying that $(\partial c/\partial \rho)_s < 0$. This means that the behavior of the speed of sound upon isentropic perturbations is reversed with respect to classical fluids. For some classes of highly complex heavy fluids, such as for example heavy hydrocarbons, perfluorocarbons, and siloxanes [3], Γ may have negative values in a subset of the dense gas region next to the saturation curve. Such fluids are usually referred to as Bethe–Zel'dovich–Thompson (BZT) fluids, from the researchers who first postulated their existence; the thermodynamic region characterized by negative values of Γ is called the inversion zone. It has been theoretically shown that, for $\Gamma < 0$, compression waves are smoothed out. As a consequence, compression shocks within the inversion zone violate the entropy inequality, and are therefore inadmissible; conversely, rarefaction shocks are allowed [1,2,4,5].

The interest in BZT fluids is motivated by the potential benefits in the use of such class of fluids in energy applications. For instance, in turbo-machinery flows, the shock formation and the consequent loss of energy could be ideally suppressed if the turbine expansion could happen within the inversion zone. The complexity of performing reliable experimental studies for non-classical gasdynamics, makes numerical simulation of dense gas flows an active research field.

In [6], an unstructured implicit Finite Volume (FV) solver, based on approximate Riemann solver, is used for the simulation of two

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dimensional dense gas flows with the Peng–Robinson–Strijeck–Vera cubic equation of state [7], and with the Span–Wagner multi-parameter equation of state [8] in [9]. In [10–12], a centered solver is used for simulations with the van der Waals and the Martin–Hou [13] equation of state. Two-dimensional flows exhibiting non-classical effects through turbine cascades were simulated in [14,15] with the Martin–Hou [13] equation of state and in [16] with the Martin–Hou, Peng–Robinson–Strijeck–Vera and the Span–Wagner equations of state. The McCormack scheme was used in [14], a second-order time–space accurate flux-limited method was adopted in [15], while in [16] both structured and unstructured cell-centered Finite Volume (FV) discretization has been used. Numerical simulations of three-dimensional flows of dense gases were performed in [17,18] for a shock tube configuration and in [19] for flows over finite wings.

The majority of the CFD tools presented are based on second-order FV methods. When complex applications are considered, the accuracy of these methods is degraded, ranging between first and second-order due to the irregular and highly stretched meshes. This work has been motivated by the need to increase the predictive accuracy of simulations of complex flows over complex geometries or (in case of the same accuracy) to alleviate the computational cost compared to existing numerical schemes. In this respect, high-order methods seem to be potentially superior to classical FV schemes, which require extremely fine grids to compute the solution with a sufficiently small level of error, hence with high computational time and memory usage. When complex fluid dynamics phenomena are considered, high fidelity solutions are required to separate numerical discretization errors from modeling errors, making possible to check the deficits of physical modeling, since very few experimental data are available.

In this work, the high-order Residual Distribution (RD) approach [20] for the discretization of the steady Euler equations is extended for the first time in literature to take into account complex thermodynamic models. The RD method based on the continuous formulation of the problem, introduces less degrees of freedom (DoFs) than other high-order schemes based on the discontinuous approximation of the solution, like Discontinuous Galerkin methods [21] for example. In addition, with the possibility to construct non-linear RD schemes, the discretization of continuous and discontinuous solutions within the same numerical scheme is straightforward, without the necessity to add artificial viscosity or empirical shock capturing procedures. Furthermore, differently from ENO/WENO schemes [22,23], which require large stencils for the solution reconstruction, RD methods are compact and hence more efficient.

The present paper is structured as follows. In Section 2, the governing equations are introduced, together with thermodynamic models for ideal and dense gases. In Section 3, the description of a non-linear RD scheme for the solution of advection problems is presented. In addition, the procedure to impose boundary conditions and the construction of an efficient implicit solver are shown. Section 4 presents numerical results for two and three dimensional problems. In particular, the accuracy and the efficiency of the solver are assessed in terms of number of DoFs and CPU time to reach the desired level of accuracy in the numerical discretization. The effects of the thermodynamic models [24] on the fluid-dynamic behavior are also investigated. Finally, in Section 5, conclusion are drawn.

2. Physical model

2.1. Governing equations

In the general case of three spatial dimensions, the dynamics of compressible flows, when viscous and thermal effect are neglected, is governed by the following set of non-linear equations, written in conservative form,

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{m} = 0 \\ \frac{\partial \boldsymbol{m}}{\partial t} + \nabla \cdot \left(\frac{\boldsymbol{m} \otimes \boldsymbol{m}}{\rho} + P\mathbb{I} \right) = \mathbf{0} \\ \frac{\partial E^t}{\partial t} + \nabla \cdot \left(\left(E^t + P\right) \frac{\boldsymbol{m}}{\rho} \right) = 0 \end{cases} \tag{2}$$

where ρ is the density, P is the pressure, $\mathbb{I} \in \mathbb{R}^3$ is the identity tensor, the momentum vector $\boldsymbol{m} = \rho \boldsymbol{v}$, with $\boldsymbol{v}$ the velocity vector, and E^t is the total energy per unit volume defined as

$$E^t = \rho e + \frac{\|\boldsymbol{m}\|^2}{2\rho} = \rho e^t, \tag{3}$$

with e the specific (*i.e.,* per unit mass) internal energy and e^t the specific total energy.

It is common practice to introduce the vector u of the conservative variables and the advective flux function $\mathbf{f}^a(\mathrm{u})$

$$\mathrm{u} = \begin{pmatrix} \rho \\ \boldsymbol{m} \\ E^t \end{pmatrix} \quad \text{and} \quad \mathbf{f}^a(\mathrm{u}) = \begin{pmatrix} \boldsymbol{m} \\ \frac{\boldsymbol{m} \otimes \boldsymbol{m}}{\rho} + P\mathbb{I} \\ \left(E^t + P\right) \frac{\boldsymbol{m}}{\rho} \end{pmatrix}, \tag{4}$$

such that the system (2) can be recasted in the following vector form

$$\frac{\partial \mathrm{u}}{\partial t} + \nabla \cdot \mathbf{f}^a(\mathrm{u}) = \mathbf{0}. \tag{5}$$

The system (5) is completed with thermodynamic relations for the variables P and e by the means of the following equations of state

$$\begin{aligned} P &= P(\rho(\mathrm{u}), T(\mathrm{u})), \\ e &= e(\rho(\mathrm{u}), T(\mathrm{u})), \end{aligned} \tag{6}$$

with T the absolute temperature.

It is worth noting that the Jacobian matrix of the advective flux function and the relative eigen-structure are functions of some thermodynamic relations, thus the Jacobian matrix and its eigenvectors should be computed for a generic gas, to avoid model-dependent implementations, see Appendix A.

2.2. Thermodynamic models

In this work, three thermodynamic models are considered. The first one is the classical model for the polytropic ideal gas. The other two models are sufficiently accurate to describe dense gas effects: the Peng–Robinson–Stryjek–Vera (PRSV) [7] and the Span–Wagner (SW) [8] models.

2.2.1. Polytropic ideal gas

In the case of the polytropic ideal gas, it is possible to formulate the pressure as a function of the specific variables e and ρ as follows

$$P(e, \rho) = (\gamma - 1)\rho e, \tag{7}$$

where $\gamma = c_p/c_v$ is the specific heat ratio, and $\mathcal{R}$ is the gas constant. Here it is always taken $\gamma = 1.4$.

Since in the Euler equations the actual unknown is the total energy per unit volume (E^t) and not the specif energy (e), it is convenient to rewrite the previous relation as

$$P = P(\mathrm{u}) = (\gamma - 1)\left(E^t - \frac{\|\boldsymbol{m}\|^2}{2\rho} \right), \tag{8}$$

where, with a slight abuse of notation, the same symbol has been used to indicate the pressure as function of the ρ and e and as function of the conservative variables.