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Roe-type schemes for dense gas flow computations

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Abstract

Dense gas dynamics studies the dynamic behavior of gases in the thermodynamic region close to the liquid–vapor critical point, where the perfect gas law is no longer valid, and has to be replaced by more complex equations of state. In such a region, some fluids, known as the Bethe–Zel'dovich–Thompson fluids, can exhibit non-classical nonlinearities, such as expansion shocks, and mixed shock-fan waves. In the present work, the problem of choosing a suitable numerical scheme for dense gas flow computations is addressed. In particular, some extensions of classical Roe's scheme to real gas flows are reviewed and their performances are evaluated for flow problems involving non-classical nonlinearities. A simplification to Roe's linearization procedure is proposed, which does not satisfy the U-property exactly, but significantly reduces complexity and computational costs. Such simplification introduces an additional error $O(\delta x^2)$, with δx the mesh size, with respect to the first-order accurate Roe's scheme, and $O(\delta x^6)$ with respect to its higher-order MUSCL extensions. Numerical experiments, concerning a one-dimensional dense gas shock tube, supersonic flow of a BZT gas past a forward-facing step, and transonic dense gas flow through a turbine cascade, show a negligible influence of the adopted linearization procedure on the solution accuracy, whereas it significantly affects computational efficiency.

1. Introduction

The assumption that the fluid behaves like a perfect gas is the basis of classical gas dynamics, and is used in most compressible flow analyses in the engineering sciences. Dense gas dynamics, on the other hand, studies the dynamic behavior of gases in the dense regime, i.e. at thermodynamic conditions close to the liquid–vapor coexistence curve, where the perfect gas law is invalid. The computation of dense gas flows has received increased attention in the last decade, motivated by the fact that some very common fluids employed in engineering applications, mainly heavy polyatomic fluids, can exhibit unusual gas dynamic behavior in the dense gas regime at transonic and supersonic speeds. The most impressive differences occur for the so-called Bethe–Zel'dovich–Thompson (BZT) fluids, for which compression shocks violate the entropy inequality over a certain range of temperatures and pressures, and are therefore inadmissible.

The dynamics of dense gases is governed by the key parameter [1]:

$$\Gamma := \frac{v^3}{2a^2}\left(\frac{\partial^2 p}{\partial v^2}\right)_s, \tag{1}$$

here presented in its non-dimensional form. In Eq. (1), v is the fluid specific volume, p is the pressure, a the sound speed, and s the entropy. Γ is commonly referred-to as *the fundamental derivative of gas dynamics* [1]. Remembering that the square of the sound speed a is given by

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

Γ can be interpreted as a measure of the rate of change of the sound speed with density due to isentropic perturbations. The sign of Γ is entirely determined by the sign of the second derivative $\left(\frac{\partial^2 p}{\partial v^2}\right)_s$, i.e. the concavity of the

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constant-entropy lines (isentropes) in the p–v plane. Now, the relationship between the entropy change and the specific volume change through a weak shock wave can be written as [2]:

$$\Delta s = -\frac{a^2\Gamma}{v^3}\frac{(\Delta v)^3}{6T} + O(\Delta v^4), \tag{2}$$

where Δ represents a change in a given fluid property through the shock, and T is the absolute temperature. For perfect gases, Γ is just equal to $\frac{\gamma+1}{2}$, where γ is the specific heat ratio. As γ is necessarily greater than one, for thermodynamic stability reasons, than $\Gamma > 1$ also. As a result, a negative change in the specific volume through the shock, i.e. a compression, is required in order to satisfy the second law of thermodynamics. For dense gases, the perfect gas law no longer holds, and more complicated equations of state have to be considered. In this case, the isotherms are no longer concave-up hyperbolas in the p–v plane, but more complicated curves that exhibit negative concavity in the neighborhood of the liquid–vapor coexistence curve, in order to satisfy the thermodynamic conditions of zero slope and zero curvature at the critical point. It is well known that the isentropes tend to coincide with the isotherms as the specific heats tend to infinity; therefore, any fluid with sufficiently large specific heats will necessarily have concave-down isentropes in the dense-gas region of the p–v plane, which immediately implies $\Gamma < 0$ in the same region. The *Bethe–Zel'dovich–Thompson fluids* (from the names of the researchers who for the first time postulated their existence) are precisely defined as fluids which exhibit a region of negative Γ above the saturation curve in the vapor phase. The thermodynamic region where $\Gamma < 0$ is called the *inversion zone* and the curve $\Gamma = 0$ the *transition line*. If Γ is negative, from Eq. (2) we conclude that the specific volume must increase through a shock wave in order to have a corresponding increase of the entropy. This indicates that only expansion shocks will be admissible in these regions, whereas discontinuous compression waves will always spread into fans if inserted within the flow. BZT properties are typically encountered in heavy fluids characterized by large c_v/R ratios (e.g. [3]), where c_v is the constant volume specific heat and R the gas constant. In Fig. 1, the p–v diagram for a van der Waals gas with $\gamma = 1.0125$ is shown, representative of a typical heavy fluorocarbon.

The disintegration of compression shocks and other non-classical effects typical of BZT fluids could find application in technology. Particularly, attractive seems the possibility of reducing losses due to shock waves and boundary layer separation in turbomachines and nozzles.

In the past, several numerical methods have been proposed for the computation of the so-called "real gas flows". Such methods are typically extensions of schemes previously developed for perfect gas problems.

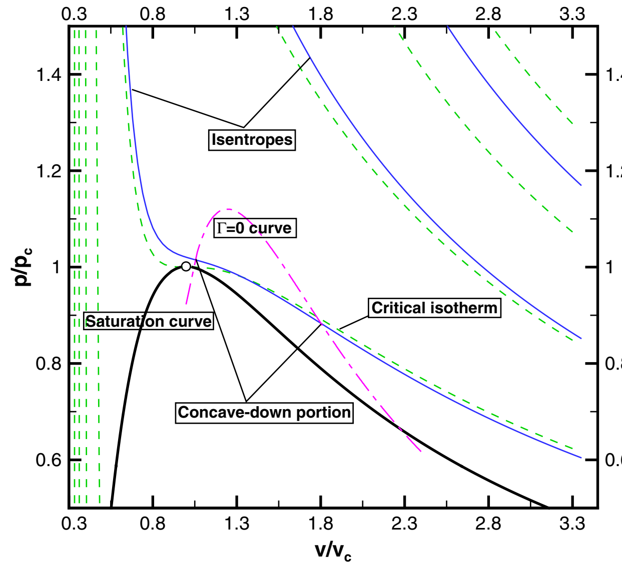

Fig. 1. p–v diagram for a van der Waals gas with $\gamma = 1.0125$. The variables are normalized with their critical values.

Roe's method being may be the most widely used in perfect gas CFD codes, it is also the one for which more real-gas extensions have been proposed. In fact, it is well known that the linearization procedure of Roe's scheme is not uniquely determined when a real gas equation of state is taken into account. Some examples of real-gas generalizations of Roe's scheme are given by Refs. [4–8]. In practice, however, no dramatic evidence of the numerical superiority of one formulation over another has been provided, even for very severe applications such as hypersonic flows, characterized by strong shock waves, chemical reactions, ionization and so on, see for example [4,9]. This has even driven some researchers to adopt, in the current use, approximate averages which do not satisfy the U-property, but work fairly fine in practice. An approximate Roe-type scheme has been proposed, for example, in [10,11]. Dense gas flows, on the other hand, can be characterized by quite "exotic" waves, such as shock/fan combinations, expansion shocks, etc.; however, flow discontinuities are generally very weak for a large range of temperatures and pressures. Thus, it seems reasonable to suppose that, for dense gas problems, the choice of a particular Roe linearization would have a quite small influence on the quality of the numerical results. On the contrary, the complexity of the particular formulation does affect computational costs significantly, especially when complicated equations of state are taken into account.

The aim of the present work is to provide a theoretical justification for the limited influence of the chosen Roe linearization on the solution accuracy, and to the fact that even "approximate" averages give substantially correct results. To do that, an "extreme" case is considered: a simplified procedure is introduced, which reduces