Journal of Computational Physics 313 (2016) 687–712

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A mathematical and numerical framework for the analysis of compressible thermal convection in gases at very high temperatures

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ARTICLE INFO

Article history:
Received 16 November 2015
Received in revised form 23 February 2016
Accepted 24 February 2016
Available online 27 February 2016

Keywords:
Buoyancy convection
High temperature
Projection method
Non-Boussinesq effects
Molecular degree of freedom excitation

ABSTRACT

The relevance of non-equilibrium phenomena, nonlinear behavior, gravitational effects and fluid compressibility in a wide range of problems related to high-temperature gas-dynamics, especially in thermal, mechanical and nuclear engineering, calls for a concerted approach using the tools of the kinetic theory of gases, statistical physics, quantum mechanics, thermodynamics and mathematical modeling in synergy with advanced numerical strategies for the solution of the Navier–Stokes equations. The reason behind such a need is that in many instances of relevance in this field one witnesses a departure from canonical models and the resulting inadequacy of standard CFD approaches, especially those traditionally used to deal with thermal (buoyancy) convection problems. Starting from microscopic considerations and typical concepts of molecular dynamics, passing through the Boltzmann equation and its known solutions, we show how it is possible to remove past assumptions and elaborate an algorithm capable of targeting the broadest range of applications. Moving beyond the Boussinesq approximation, the Sutherland law and the principle of energy equipartition, the resulting method allows most of the fluid properties (density, viscosity, thermal conductivity, heat capacity and diffusivity, etc.) to be derived in a rational and natural way while keeping empirical contamination to the minimum. Special attention is deserved as well to the well-known pressure issue. With the application of the socalled multiple pressure variables concept and a projection-like numerical approach, difficulties with such a term in the momentum equation are circumvented by allowing the hydrodynamic pressure to decouple from its thermodynamic counterpart. The final result is a flexible and modular framework that on the one hand is able to account for all the molecule (translational, rotational and vibrational) degrees of freedom and their effective excitation, and on the other hand can guarantee adequate interplay between molecular and macroscopic-level entities and processes. Performances are demonstrated by computing some incompressible and compressible benchmark test cases for thermal (gravitational) convection, which are then extended to the high-temperature regime taking advantage of the newly developed features.

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http://dx.doi.org/10.1016/j.jcp.2016.02.062
0021-9991/

1. Introduction

Variable density flows occurring at low Mach number are encountered in several physical phenomena. Applications involving such flows abound in the fields of thermal, mechanical, chemical, civil and nuclear engineering. Many industrial (and also nonindustrial) applications in heat transfer have directly or indirectly engaged with research in these fields.

As an example, the "natural" motion of gases in enclosures with different aspect ratios is relevant to various engineering areas such as heat transfer from electronic packaging (Sun and Jaluria [1]), furnace engineering (Baltasar et al. [2]), the production of semiconductor and optoelectronics materials (where the processing itself requires that the high-temperature melt is in contact with a gas, e.g., the Bridgman, CZ and Floating Zone methods, Lappa and Savino [3]; Lappa [4] and references therein).

Low-Mach-number natural flows of compressible gases play a key role in numerous other technological contexts, such as the cooling of high-power devices, solar energy and nuclear power plants (von Backström and Gannon [5]; Elmo and Cioni [6]; Hu et al. [7]; Martineau et al. [8]). Other relevant examples include (but are not limited to) plumes from urban mass fires, the release in the atmosphere of smokes from industrial stacks (McGrattan et al. [9]), plumes resulting from nuclear explosions and pyroclastic flows from volcanic eruptions (Valentine and Wohletz [10]).

In spite of considerable research and efforts on such topics, a clear and urgent need does exist to develop new strategies to attack these problems.

First of all, the vast majority of natural convection calculations that have been reported in the literature have been performed after invoking the Oberbeck–Boussinesq (OB) approximation (see, e.g., Lappa [11,12]). This approximation relies on a first-order Taylor series to approximate the density variations according to the difference between local temperature and a reference temperature. More precisely, it ignores the temperature dependence *of all fluid properties*, except for the temperature-induced density variation that is retained in the buoyant force driving the flow. This philosophy is highly effective if density variations are low. Nevertheless, neglecting the importance of density variations in thermal flows of gravitational nature with strong temperature differences can cause a considerable departure from the correct prediction of fluid flow behavior (non-Oberbeck–Boussinesq (NOB) effects inevitably arise).

For large temperature differences, the Boussinesq assumption breaks down (Gray and Giorgini [13]) and, in order to capture NOB effects, one needs to resort to a compressible flow model, or since the Mach number remains small, to a low Mach number approximation model.

2. A review of existing algorithms

As explained in Munz et al. [14] and Beccantini et al. [15], the main difficulty in constructing numerical methods for low-speed compressible flows is the fact that, in the transition from compressible to incompressible flows, the governing equations *change nature*. The popular Euler equations for compressible flows are hyperbolic in nature, but they become hyperbolic–elliptic as the characteristic flow speed becomes zero compared with the sound speed (i.e. in the limit as the Mach number tends to zero).

The strategies elaborated over the years to deal with such a complex issue can be roughly divided into two main categories: the socalled density-based solvers and the pressure-based methods, which in turn have given rise to two lines of inquiry running in parallel in the literature.

The first category consists of variants of methods originally conceived to deal with the compressible Navier–Stokes equations. It is well known that such methods in their original fully-compressible formulation cannot be used to compute flows at low Mach regime without major modification. The reason is the existence of a large disparity between the eigenvalues of the Euler equations (Turkel [16]). In the last two decades, different techniques have been developed to extend these solvers to the quasi-incompressible regime, based on the modification of the time-dependent properties of the governing equations (to cluster the otherwise poorly distributed eigenvalues of the Euler equations) or on alternate forms of the related integration strategies (Volpe [17]; Guillard and Viozat [18]; Mary et al. [19]; Paillere et al. [20]; Vierendeels et al. [21]; Parchevsky [22]; Martineau et al. [8]; Könözsy and Drikakis [23]). The resulting solvers often allow the simulation of flows ranging from supersonic to low Mach number regime, including aeroacoustics and natural thermal flows.

The second category includes techniques derived from standard methods for incompressible flows (see, e.g., the excellent methods by Kothe et al. [24]) properly extended to the compressible regime. The main distinguishing mark of this approach is the selection of pressure as a dependent variable in preference to density, such a choice being motivated by the significant changes experienced by pressure at low Mach numbers as opposed to variations in density (which become very small, Moukalled and Darwish [25]).

These techniques are known under several names: *projection method, fractional-step method or pressure-correction method* (also simply referred to as *primitive-variables methods*). This approach was originally introduced by Harlow and Welch [26] and Welch et al. [27] as the MAC method, and successively modified in the projection method developed independently by Chorin [28] and Temam [29,30]. Despite some minor differences, basically, a common feature of all these methods is that they are conceived to "turn around" the coupling between the pressure and the velocity that is implied by the incompressibility constraint. Related variants for compressible flows have been elaborated by extending the related principles to non-divergence free velocity flows (basically, from a purely mathematical point of view, they rely on the Ladyzhenskaya