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Numerical Simulation of Wall-Bounded Flows with Thermally Perfect Gases

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Abstract. The present study addresses the numerical simulation of wall-bounded flows with thermally perfect gases using structure-preserving spatial discretizations. The supersonic turbulent boundary layer and channel flow are chosen as numerical flow cases to highlight the differences with respect to the widely used calorically perfect gas model when relatively high temperature ranges are present. Specifically, we compare literature results obtained for air flows with the ones carried out for carbon-dioxide, which is likely to be treated as a thermally perfect gas in high-temperature cases. Results show non-negligible physical differences with the reference cases, and the numerical treatment of the convective terms of the integrated equations is taken into account as well.

Introduction

Supersonic wall-bounded flows are among the most extensively studied physical configurations and encompass a wide range of applications, including the aerodynamics of supersonic and hypersonic vehicles, aerospace propulsion and aerothermal heating and heat transfer. In most applications, when the working fluid is air, it is well known that the calorically perfect (CP) hypotheses hold, up to negligible differences, in a wide range of Mach numbers, even when strongly diabatic walls are studied [1]. However, dependency of specific heat capacities on temperature becomes relevant when chemical species with several thermodynamic degrees of freedom are considered; for instance, the case of carbon-dioxide represents a fitting example of a nonpolar molecule whose heat capacities strongly vary within temperature, and it is widely studied for applications like atmospheric re-entry. In this context, Direct Numerical Simulations (DNS) represent a powerful and reliable tool when it comes to build a physical understanding of configurations with severe thermo-fluid dynamic conditions, especially within an *ad hoc* numerical treatment of the discretized equations that aims to consistently represent important properties and symmetries of the continuous system also in the discrete framework [2]. In this work, computations of high-speed wall bounded flows are carried out with thermally perfect (TP) gas laws in the open-source, GPU-accelerated code STREAmS 2.1 [3]. We consider both channel flows and turbulent boundary layer, with the latter case being compared with the literature results in [1].

Organization of the Text

The three-dimensional Navier-Stokes equations are solved for a viscous, heat-conducing, Newtonian fluid

$$\partial_t \rho + \partial_{x_j}(\rho u_j) = 0 \tag{1}$$

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$$\partial_t(\rho u_i) + \partial_{x_j}\left(\rho u_j u_i + p\delta_{ij}\right) - \partial_{x_j}\tau_{ij} - f_1\delta_{i1} = 0 \quad (2)$$

$$\partial_t(\rho E) + \partial_{x_j}\left(\rho u_j H\right) - \partial_{x_j}\left[\left(u_j\tau_{ij} - q_j\right)\right] + \Phi - f_1 u_1 = 0 \quad (3)$$

with ρ the density of the fluid, u_i the Cartesian components of the velocity field, p the thermodynamic pressure, $E = e + u_i u_i/2$, the total energy and $H = E + p/\rho$ the total enthalpy. The standard constitutive relation are assumed for the dissipative part of the stress tensor $\tau_{ij} = \mu\left(\partial_{x_j}u_i + \partial_{x_i}u_j - 2/3\ \partial_{x_k}u_k\delta_{ij}\right)$, and the heat flux $q_j = -k\partial_{x_j}T$. Dynamic viscosity μ depends on temperature according to the Sutherland's law, whose general expression is $\mu/\mu_e = (T/T_e)^{1/2}(1 + C/T_e)/(1 + C/T)$, and it is linked to the thermal conductivity $\mu c_p\ /Pr$, with C the Sutherland's constant and the subscript "e " to indicate the asymptotic conditions. Finally, $T_e = 298.15$ K and Prandtl number is $Pr = 0.72$. The production terms Φ, f_i will only be taken into account to simulate compressible channel flows with a constant bulk temperature and mass flow rate. The system is closed upon specification of the equation of state $p = \rho RT$ and the relation that links internal energy to intensive thermodynamic variables, which, for thermally perfect gases, takes the form $de = c_v(T)dT$. Given the Mayer's relation $c_p - c_v = R$, the functional law for $c_v(T)$ is assumed from the 7-coefficient polynomial fittings of the NASA Glenn Coefficients [4].

Numerical treatment of the system of equations Eqs. (1) - (3) is carried out in a semi-discretized framework, where the spatial discretization enforces the Kinetic-Energy Preserving (KEP) property for all the compared simulations, such that the total energy equation is represented by the sum of the contributions of the (induced) kinetic energy and internal energy [2,5]. Additionally, a novel Entropy-Conserving (EC) formulation is considered [6], where the internal energy equation is discretized to ensure exact entropy-conservation by convection, that is no spurious contributions occur from the convective terms for interior points.

Given this background, Tab.1 reports the physical parameters and the computational setup for the presented simulations. The viscous scaling is given by the standard definitions $\delta_v = \nu_w/u_\tau$, $u_\tau = (\tau_w/\rho)^{1/2}$, with the subscript "$w$ " denoting conditions at the wall. Thus, we have$\Delta x^+ = \Delta x/\delta_v$ and $\Delta z^+ = \Delta z/\delta_v$, which are discretized with evenly-spaced points, and $\Delta y^+ = \Delta y/\delta_v$ clustered near the walls. To generate a turbulent inflow for the boundary layer case, the recycling-rescaling procedure in STREAmS is employed, setting the recycling plane at $x_{rec} = 80\delta_{in}$. Profiles and statistics are computed at $Re_\tau = \delta/\delta_v \approx 450$ with δ being the boundary layer thickness, to carry out the comparison with the results in [1]. On the other hand, the supersonic channel flow case is performed at a constant mass flow rate and enabling the cooling term Φ in total energy equation to keep the bulk temperature constant. As far as it concerns notations, we use the symbol $\overline{\phi}$ to denote the both in time and in spanwise direction - assuming homogeneity along z -direction itself- while the Favre averaging will be denoted as $\tilde{\phi} = \overline{\rho\phi}/\overline{\rho}$ for which we denote $\phi = \tilde{\phi} + \phi''$ instead of the standard Reynolds' decomposition.

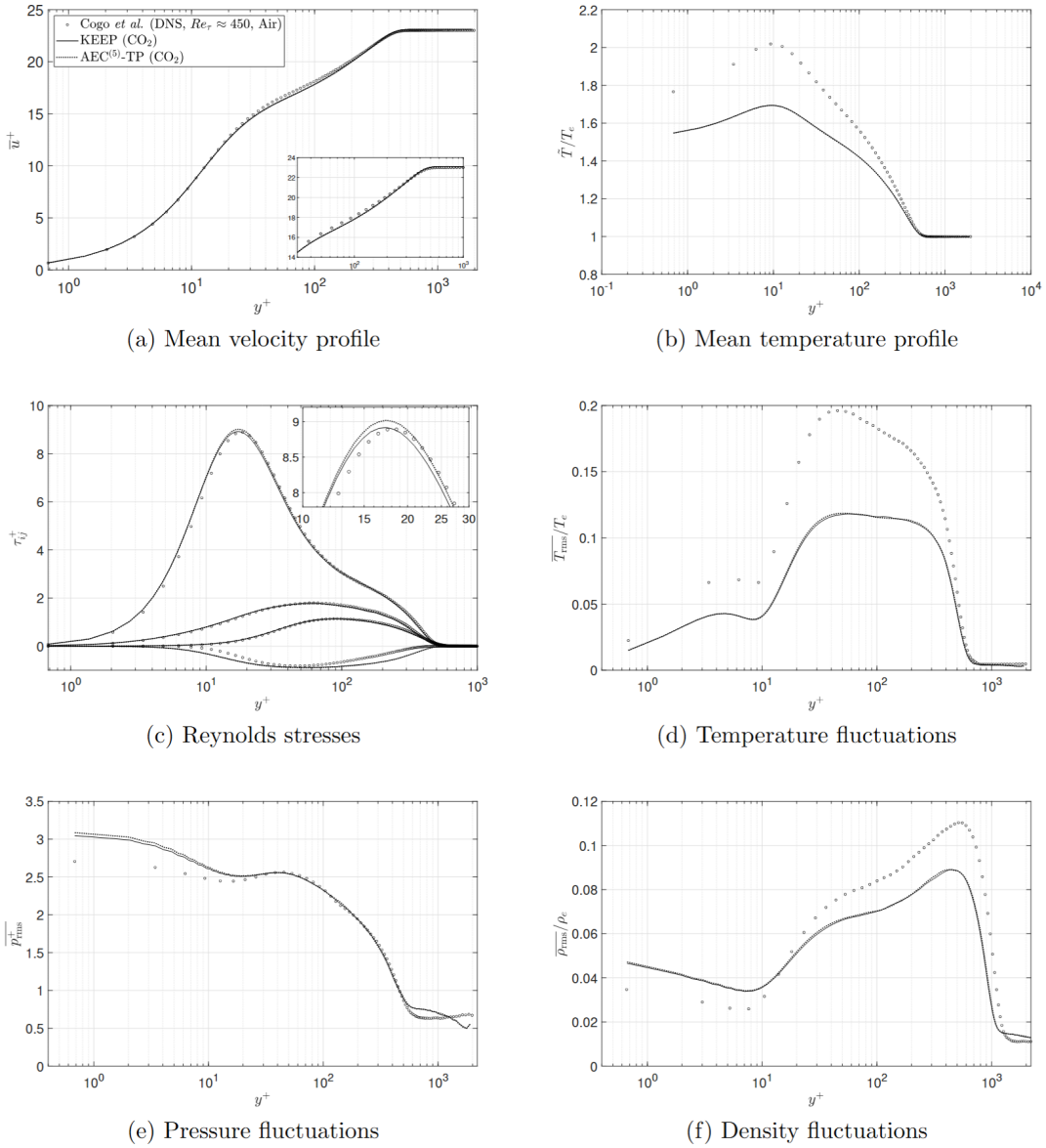
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Table 1: *Indication of the main flow and computational parameters for supersonic boundary layer at $M_e = 4.0$ (BLM4) and supersonic channel flow at $M_b = 2.0$ (CFM2). The definitions for the Mach numbers employed are $M_e = U_e/\sqrt{\gamma_e R\, T_e}$ and $M_b = U_b/\sqrt{\gamma_b R T_b}$. Recovery temperature, T_r, is likewise derived from the isentropic relations $T_r/T_e = 1 + rM_e^2(\gamma_e - 1)/2$ for the boundary layer case and, dually, $T_r/T_b = 1 + rM_b^2(\gamma_b - 1)/2$ for the channel flow case, with $r = P\, r^{1/3}$ the recovery factor. Finally, h is the half-height of the channel.*

	Gas	M	Re_τ	T_w/T_r	L_x	L_y	L_z	Δx^+	Δy_w^+	Δz^+
BLM4–CP	Air	4.0	443.6	0.44	$100\delta_{in}$	$15\delta_{in}$	$9\delta_{in}$	4.4	0.7	3.9
BLM4–TP	CO_2	4.0	443.5	0.44	$100\delta_{in}$	$12\delta_{in}$	$8\delta_{in}$	7.3	0.7	4.1
CFM2–CP	CH_4	2.0	215	0.36	$4\pi h$	$2h$	$2\pi h$	7.6	0.4	3.8
CFM2–TP	CH_4	2.0	215	0.36	$4\pi h$	$2h$	$2\pi h$	7.6	0.4	3.8

Results and discussion

Fig.1 shows both velocity and temperature profiles, where the TP case is carried out with both the built-in "KEEP" discretization in STREAmS, EC for ideal gases only, and the EC formulation specifically designed for TP gases. Inner-scaled velocity profiles present an upward shift with respect to the incompressible log-law, which is due to the combined effects of compressibility and heat transfer at the wall. On the other hand, Fig.1(b) shows that air and CO_2, given the same asymptotic conditions, produce remarkably different temperature distributions. Specifically, higher values of c_p lead to smaller temperature variations. The region associated to larger $\partial_y T$ is indeed the one that better highlights the effects of the variable $c_p(T)$. Looking at Fig.1(b)-(d), the logarithmic layer and the buffer layer are the ones that exhibit the strongest deviation from the ideal gas behaviour, especially in temperature fluctuations, whose peaks appear to largely differ. Density fluctuations behave similarly, while pressure fluctuations have also been reported, showing higher values for the TP case around 15 % at the wall. As far as it concerns the role of the numerical discretization, the KEEP scheme and the Asymptotically Entropy-Conserving (AEC) [7] only differ in the treatment of the energy equation, and research is ongoing to understanding the impact on the final results, already observed for higher-order statistics. To check the generality of the previous results, we observe that similar trends are found for the channel flow case, although both physical and computational parameters are different. This time we carry out a comparison with the same chemical specie, once modelled as a CP gas and once as a TP gas. For the CP test, γ is evaluated at bulk temperature and kept constant. Results are shown in Fig.2, with the same definitions for scaling described in Fig.1. Given the more extreme cold wall conditions considered for the channel flow, the higher variation of $c_p(T)$ for methane and the lower Reynolds number, differences between the two gas models are emphasized in this case, still holding the same trend shown for the boundary layer simulations. A final, noteworthy observation addresses the effect of the heat capacities on the skin friction coefficients, defined as $c_f = 2\overline{\tau_w}/(\rho_e U_e^2)$ - for boundary layer, $\rho_b U_b^2$ used for channels instead - and the heat transfer coefficient $B_q = \overline{q_w}/\overline{\rho_w} c_p u_\tau T_w$.



(a) Mean velocity profile

(b) Mean temperature profile

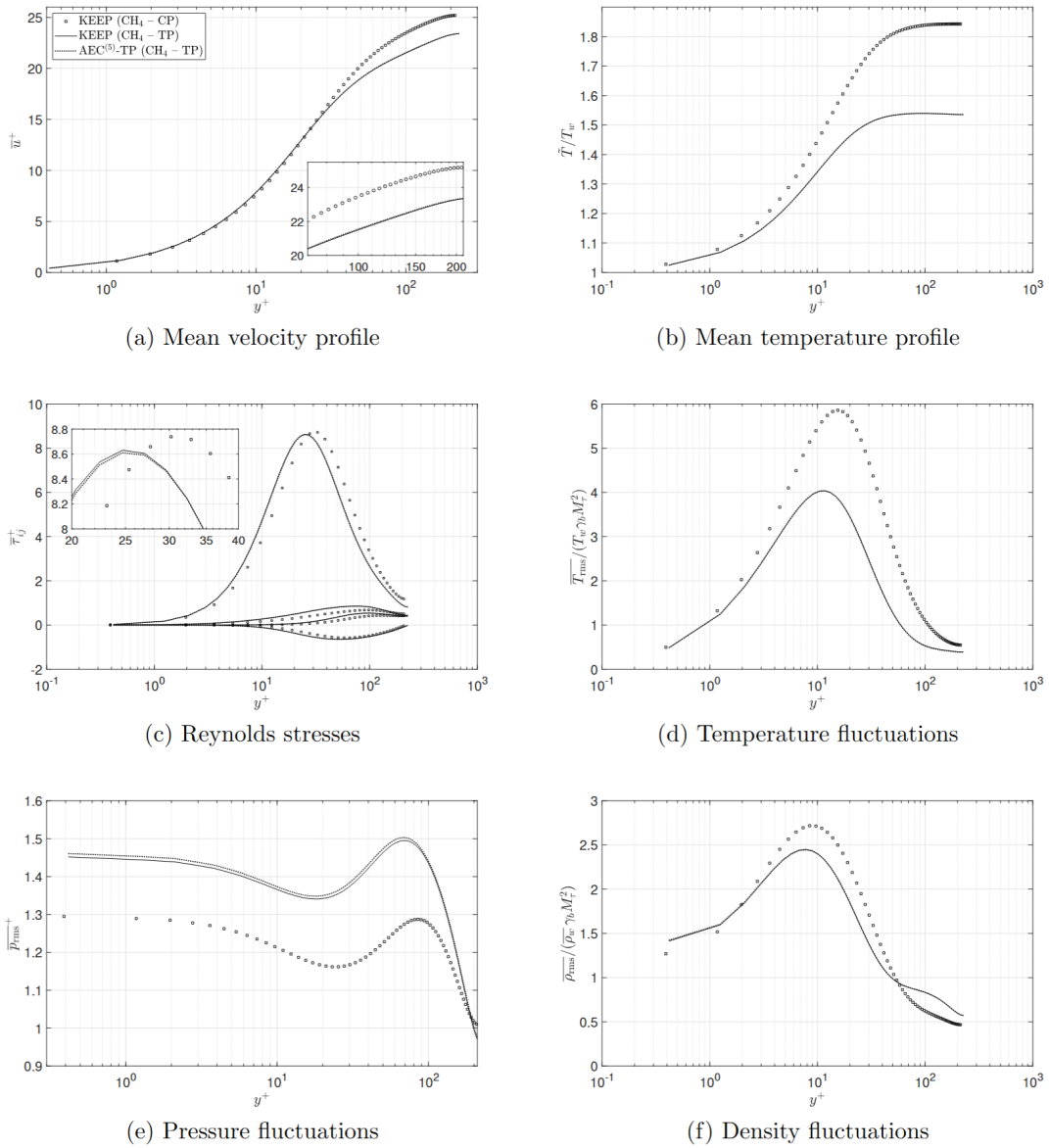
(c) Reynolds stresses

(d) Temperature fluctuations

(e) Pressure fluctuations

(f) Density fluctuations

Figure 1. *Thermo-fluid dynamic profiles for the supersonic boundary layer. Reynolds stresses are reported in viscous units as* $\tau_{ij}^+ = \overline{\rho}\,\widetilde{u_i'' u_j''}\,/\rho_w u_\tau^2$ *while thermodynamic fluctuations are expressed as root mean squares.*



(a) Mean velocity profile (b) Mean temperature profile

(c) Reynolds stresses (d) Temperature fluctuations

(e) Pressure fluctuations (f) Density fluctuations

Figure 2. T*hermo-fluid dynamic profiles for the supersonic channel flow. Scalings are performed with* $\gamma_b = \gamma(T_b)$ *to standardize comparisons between the two different thermodynamic models. Friction Mach number is defined, as usual, as* $M_\tau = u_\tau/(\gamma_b R T_w)$.

While we have not identified a general behaviour for the first one yet, exhibiting a variation with respect to the CP case within a range of ± 10 % in the second one tends to be closer to zero for higher values of $c_p$at the wall, consistent with the linear relation between the heat flux and the temperature variation, $\delta q = c_p dT$. Further research is however required to characterize both the physical and the numerical aspects of new thermodynamic frameworks.

Summary

We have presented simulations of wall-bounded supersonic flows using thermally perfect gas models and an *ad hoc* numerical formulation implemented in highly scalable GPU-based codes. Such results have been compared with the classical calorically perfect gas cases. Significant physical differences were observed, indicating that the calorically perfect gas assumption proves too restrictive in such configurations. Further research is ongoing to achieve improved modeling and numerical characterizations.

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