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KINETIC MODELS WITH ROTATIONAL DEGREES OF FREEDOM FOR HYBRID METHODS

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Abstract. Flow fields where localised rarefaction phenomena are relevant, occur in various engineering applications such as supersonic/hypersonic and micro-flows. The methods that are commonly employed to simulate rarefied flows, Direct Simulation Monte Carlo (DSMC) and discrete-velocity methods for kinetic Boltzmann equations, require higher computational cost than continuum methods. This has motivated the development of hybrid techniques which restrict the use of the expensive non-continuum approaches to regions where significant non-equilibrium effects occur. In the present work, a computational framework which includes methods for the kinetic Boltzmann equations, and has been successfully employed for different monoatomic cases [1], is improved and used to predict rarefied high speed flows. A novel aspect of the method is the parallelisation of the computational load. While in the literature, a split of either the physical space or the phase space among the processors is employed, the current framework allows both levels of parallelisation at the same time. For rarefied gas flows at high velocities it is necessary to take into account the excitation of the internal degrees of freedom; these flows are characterised by large non-equilibrium regions with multiple temperatures (translational, rotational and vibrational temperature). For this reason, the framework has been recently developed with the addition of kinetic models for diatomic gases, presented in [2, 3], which are based on the assumption that the fraction of collisions involving the excitation of the rotational degrees of freedom is a given constant or is a function of the flow temperatures. As a first stage the rotational degrees of freedom has been taken into account for the cases of normal shocks, and a flat plate. Furthermore, kinetic models for diatomic gases are not yet established in the context of the hybrid approaches and the coupling between a diatomic kinetic model and a Navier-Stokes solver still presents a number of challenging tasks. Among them, the evaluation of a different way of coupling in order to increase the efficency of the hybrid approach is also objective of the present work. Indeed, to reduce the computational cost of hybrid simulations by reducing the region where the expensive method is needed, a Gas-Kinetic Scheme based on the Rykov model is proposed.

1 INTRODUCTION

With the increased interest in hypersonic vehicles, there is a need for efficient and accurate prediction of the flow field, aerodynamics and heat transfer throughout their flight regime. Hypersonic vehicles generate flow fields that can range from completely rarefied to continuum. At intermediate altitudes, the flow around hypersonic aircraft can be characterised as being mainly continuum with localised areas (generated by the rapid expansion in the wake of the vehicle as well as by strong gradients in shock waves and boundary layers) that display translational non-equilibrium effects. The flow conditions near the vehicle surface and in the wake determine the drag and the heat transferred to the vehicle and its payload, so it is important that these regions are simulated accurately using appropriate physical models. If the gradients of the macroscopic variables become so steep that their scale length is of the same order as the average distance travelled by molecules between collisions, the number of impacts is not enough to drive the fluid towards a local thermodynamic equilibrium. In this condition the flow can no longer be considered a continuum flow and the transport terms in the Navier-Stokes equations fail since the constitutive relation is not valid. The mathematical model at molecular level is the Boltzmann equation (BTE) [4], and for the regions of the flow field where highly non-equilibrium effects occur the Direct Simulation Monte Carlo method [5] is employed to statistically estimate the solution of the BTE. Alternatively a discrete velocity method can be used to solve a kinetic model approximation of the BTE [6, 7, 2]. These approaches require a cost in computational time and memory considerably higher than the flux evaluations commonly employed to simulate continuum flows. For this reason, to simulate flow fields where continuum and rarefied regime coexist, hybrid techniques have been introduced, [8]. In these methods the expensive approach is employed only where needed and is coupled with a finite-volume scheme for the Navier-Stokes equations that is used where the flow is in thermal equilibrium. Usually an hybrid technique couples two different simulation methods by means of an exchange of information between the parts of the domain where they are employed. In recent works, this has been achieved using an overlap region where flow state variables or numerical fluxes are exchanged between the two models, [9], or employing a buffer region where the two models are blended at equation level [10]. Recent works on multi-physics methods focused on rarefied high Mach flow can be found in [11, 12, 13]. All these works follow the principle defined above, while an alternative approach is presented in [14, 15]. Indeed, the Unified Gas-Kinetic Scheme (UGKS) uses a finite-volume method where the numerical fluxes are based on the solution of the Shakhov model [7] for a monoatomic gas, or the Rykov model [2] for a diatomic gas with rotational non-equilibrium. This allows the UGKS to simulate flows in both continuum and rarefied regime. The framework presented in [1] has been recently developed with the addition of the Rykov model and an Ellipsoidal-Statistical (ES) model for diatomic gases [3] which will be evaluated and compared in the first part of the paper. In order to reduce the computational cost of an hybrid simulation it is possible to pursue

a way of reducing the region where the expensive method is needed and to do so, in the second part of the work, we propose a Gas-Kinetic Scheme (GKS) based on the Chapman-Enskog (CE) expansion for the non-dimensional Rykov model, 2. The GKS enables the simulation of flows in near continuum regime at a lower cost than that of the discrete velocity kinetic solver. This approach, due to the use of the CE expansion, is limited to near-continuum regions but is simpler than the UGKS for diatomic gases presented in [15].

2 NON-DIMENSIONAL RYKOV MODEL

We will consider the flow of a diatomic gas and we will assume that the gas temperature is not too high, so that the vibrational degrees of freedom are not excited, and not too low, so that the rotational degrees of freedom may be considered fully excited. In this case the particle distribution function $f(\mathbf{x}, \mathbf{c}, t, \epsilon_r)$, which describes the state of the gas, will be a function not only of the spatial coordinate $\mathbf{x}$, the particle velocity $\mathbf{c}$ and the time t, but also of the rotational degrees of freedom ϵ_r. The Rykov model has been proved to be a reliable kinetic approximation of the Boltzmann equation for this kind of flow, [2, 16, 17, 15], and will be employed in the present work. Substituting the non-dimensional variables defined in appendix A in the Rykov model, [2], written in terms of $F = mf$ we obtain

$$
\begin{aligned}
&\tfrac{\partial F_0}{\partial t} + \mathbf{c}\tfrac{\partial F_0}{\partial \mathbf{x}} = \tfrac{F_0^{eq} - F_0}{\tau} \quad ; \quad \tfrac{\partial F_1}{\partial t} + \mathbf{c}\tfrac{\partial F_1}{\partial \mathbf{x}} = \tfrac{F_1^{eq} - F_1}{\tau} \\
&F_0^{eq} = \tfrac{1}{Z_r} F_0^r + \left(1 - \tfrac{1}{Z_r}\right) F_0^t \quad ; \quad F_1^{eq} = \tfrac{1}{Z_r} F_1^r + \left(1 - \tfrac{1}{Z_r}\right) F_1^t \\
&F_0^r = F_M(T)\left[1 + \tfrac{8}{15}\omega_0 \tfrac{q_i^t}{p}\tfrac{c'_i}{T}\left(\tfrac{c'^2}{T} - \tfrac{5}{2}\right)\right] \\
&F_0^t = F_M(T_t)\left[1 + \tfrac{8}{15}\tfrac{q_i^t}{p_t}\tfrac{c'_i}{T_t}\left(\tfrac{c'^2}{T_t} - \tfrac{5}{2}\right)\right] \\
&F_1^r = T F_M(T)\left[1 + \tfrac{8}{15}\omega_0 \tfrac{q_i^t}{p}\tfrac{c'_i}{T}\left(\tfrac{c'^2}{T} - \tfrac{5}{2}\right) + 4\omega_1(1-\delta)\tfrac{q_i^r c'_i}{pT}\right] \\
&F_1^t = T_r F_M(T_t)\left[1 + \tfrac{8}{15}\tfrac{q_i^t}{p_t}\tfrac{c'_i}{T_t}\left(\tfrac{c'^2}{T_t} - \tfrac{5}{2}\right) + 4(1-\delta)\tfrac{q_i^r c'_i}{p_t T_r}\right]
\end{aligned}
\tag{1}
$$

where

$$
F_M(T) = \tfrac{\rho}{(\pi T)^{3/2}} \exp\left(-\tfrac{c'^2}{T}\right) \tag{2}
$$

and the total collision time τ is expressed as μ_t/p_t with the viscosity determined from the translational temperature. The model is based on the assumption that the fraction of collisions involving the excitation of the rotational degrees of freedom is a given constant or a function of the flow temperatures by means of the collision number, Z_r, which is discussed in appendix B. In order to make the system (1) complete, an expression for

μ is necessary (see appendix C) and the value of the constants δ, ω_0 and ω_1, need to be determined. In [18] $\omega_0 = 0.2354$ and $\omega_1 = 0.3049$ or $\omega_0 = 0.5$ and $\omega_1 = 0.286$ are given for diatomic gases. Both pairs of values have been successfully employed in [16, 17, 18, 19] with $\delta^{-1} = 1.55$. The dimensionless macroscopic quantities can be obtained from F_0 and F_1 by means of the formulas of appendix D.

3 NON-DIMENSIONAL ELLIPSOIDAL-STATISTICAL MODEL FOR DIATOMIC GAS

In [3], for the polyatomic ES model, a parameter K_{int} is introduced to define the number of internal degrees of freedom. For a diatomic molecule without vibrational excitation, two rotational degrees of freedom are present, i.e. $K_{int} = 2$. The model introduces a modified BGK collision operator by replacing the Maxwellian equilibrium function by a generalised Gaussian function with a corresponding modification to the collision operator. Considering the non-dimensional variables defined in appendix A

$$\frac{\partial F_0}{\partial t} + \mathbf{c}\frac{\partial F_0}{\partial \mathbf{x}} = \frac{F_0^{ES} - F_0}{\tau\Big(1-\nu+\theta\nu\Big)} \quad ; \quad \frac{\partial F_1}{\partial t} + \mathbf{c}\frac{\partial F_1}{\partial \mathbf{x}} = \frac{F_1^{ES} - F_1}{\tau\Big(1-\nu+\theta\nu\Big)} \tag{3}$$

where the equilibrium function is an anisotropic Gaussian

$$\begin{aligned} F_0^{ES} &= \frac{\rho}{\sqrt{det(\pi\mathbf{\Lambda})}} \exp\Big(-\mathbf{c}' \cdot \mathbf{\Lambda}^{-1} \cdot \mathbf{c}' \Big) \\ F_1^{ES} &= T_{rel} F_0. \end{aligned} \tag{4}$$

The matrix $\mathbf{\Lambda}$ is defined as

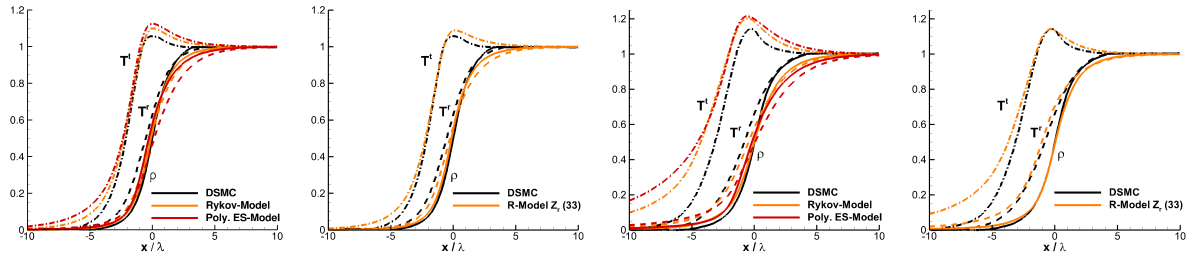
$$\mathbf{\Lambda} = \big(1-\theta\big)\Big(\big(1-\nu\big)T_{tr}\mathbf{I} + \nu\mathbf{\Theta}\Big) + \theta T_{eq}\mathbf{I} \quad ; \quad \rho\mathbf{\Theta} = \int_{-\infty}^{\infty} \mathbf{c}' \otimes \mathbf{c}' F_0 d\vec{u} \tag{5}$$

with $\rho\mathbf{\Theta}$ the opposite of the stress tensor and $0 < \theta < 1$ and $-1/2 \leq \nu < 1$ two relaxation parameters . The macroscopic variables and T_{rel} definitions can be found in appendix E.

4 EVALUATION OF THE RYKOV AND THE ELLIPSOIDAL-STATISTICAL MODELS FOR DIATOMIC GAS

For a monoatomic gas the Rykov and the polyatomic ES models reduce, respectively, to the Shakhov model and the monoatomic ES model [23]. In [24] a comparison of the latter monoatomic models is presented showing that the Shakhov model predicts more accurate numerical solutions than the ES model in most of the test cases presented except when the flow is mostly driven by heat transfer. In the present work, the two diatomic kinetic models are firstly compared with the DSMC results reported in [20], for normal shocks at Mach numbers 2.8 and 10. From figures 1a and 1c the Rykov model achieves a slightly better agreement with the DSMC results that the polyatomic ES model. Agreement

that can be further improved employing a variable collision number. Looking at figures 1b and 1d, it is clear that using equation (34) to approximate variations of Z_r with rotational and translational temperatures improves the agreement between the DSMC method and the Rykov model. Note that in the ES model the relaxation parameter θ is related to the collision number as $\theta = 1/Z_r$ and at the moment the model does not consider a variation with translational and rotational temperature. As a further step, the



(a) M= 2.8 (b) M= 2.8 (c) M= 10 (d) M= 10

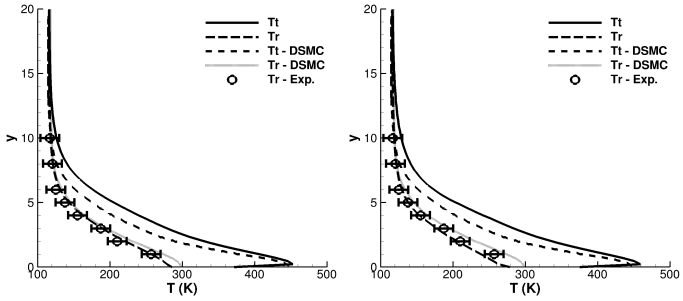
Figure 1: Non-dimensional density, rotational (T^r) and translational (T^t) temperature profiles for normal shocks in a diatomic gas. DSMC results from [20].

kinetic models have been used to predict the 2D flow field around a flat plat for which experimental data of temperature profiles in the boundary layer are available in [22]. Details of the experiment and DSMC simulation can be found in table 1. For this case, a novel implementation of the discrete velocity method for kinetic Boltzmann equations has been employed. To reduce the large computational time and memory requirement of discrete velocity methods, a two-level parallelisation is considered in the computational framework to make the solver more flexible when running on a large number of cores. This allows to split among the cores not only the physical space but also the phase space. The basic concept is straightforward; if we divide the phase space on n cores, running the simulation on m cores will lead the physical space to be divided among m/n groups of cores. For this particular case a structured grid of $250K$ points divided in 48 blocks and a velocity space discretised in 60 points per direction have been chosen.

Mach number $M = 4.89$
Knudsen number $(L = 5mm)$ $Kn = 0.024$
Reynolds number $(L = 5mm)$ $Re = 422$
$T_\infty = 116K$
$T_{plate} = 290K$

Table 1: Flat plate test case conditions [22].

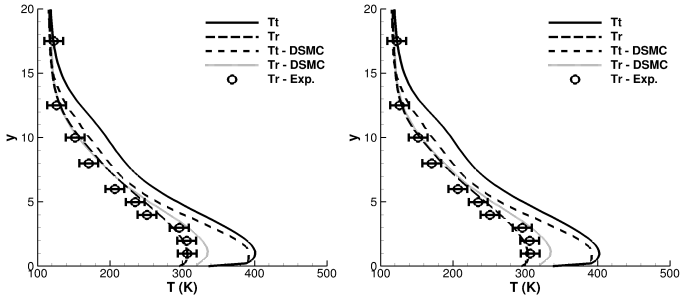
Dividing the velocity space on 16 cores, 4 per direction, the case has been run employing 512 cores on the Chadwick cluster [25] of The University of Liverpool, which means 32 groups of 16 cores among which the 48 blocks are allocated. The Rykov model with Z_r given by equation (34) leads to good agreement with both experimental and DSMC results, but it slightly over-predicts the translational temperature in the thermal layer, as it can be seen from figure 2a. Looking at figure 2b, it is clear that the polyatomic ES model slightly under-predicts the rotational temperature near the wall, leading also to a higher temperature gradient at the wall compared to the Rykov model with Z_r from equation (34). As the Rykov model, the polyatomic ES model predicts a higher translational temperature in the thermal layer. Considering figures 3a and 3b, the same behaviour is noticed at $20mm$ from the plate leading edge.



(a) Rykov model with variable Z_r eq. (33)

(b) ES model with θ=1/3.02 and ν=−0.50

Figure 2: Dimensional rotational and translational temperature profiles at $x = 5mm$ from the flat plate leading edge. DSMC and experimental results from [22].



(a) Rykov model with variable Z_r eq. (33)

(b) ES model with θ=1/3.02 and ν=−0.50

Figure 3: Dimensional rotational and translational temperature profiles at $x = 20mm$ from the flat plate leading edge. DSMC and experimental results from [22].

5 THE BGK-NS METHOD AND THE UNIFIED GAS-KINETIC SCHEME

Among the gas-kinetic schemes a successful approach is represented by the BGK-NS method, [26, 27]. The basic idea of the BGK-NS scheme is the following. Integrating in time the non-dimensional BGK equation [6] for a one-dimensional flow in a control volume dx with a continuous particle velocity c_x and discretised space x_i and time t^n one obtains

$$F|_i^{n+1} = F|_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} \left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) dt + \frac{\Delta t}{2}\left(\frac{F_M|_i^{n+1} - F|_i^{n+1}}{\tau^{n+1}} + \frac{F_M|_i^n - F|_i^n}{\tau^n}\right), \tag{6}$$

where the trapezoidal rule has been employed for the collision term integral and $[c_x F]|_{i\mp 1/2}$ are the fluxes of the distribution function across the cell interface. Then, taking the moments $\hat{\mathbf{\Psi}} = (1,\ c_x,\ \mathbf{c}^2)^T$ of equation (6), the update of the conservative variables can be found as

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}\left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) d\mathbf{c}dt \tag{7}$$

due to the compatibility conditions for the BGK model

$$\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}\frac{F_M|^n - F|^n}{\tau^n} d\mathbf{c} = (0,\ 0,\ 0,\ 0)^T. \tag{8}$$

It is known that the BGK model recovers the incorrect Prandtl number in the continuum limit and for this reason a simple correction consists in scaling the energy numerical flux, as proposed in [26]. To finally obtain the BGK-NS scheme, a time-dependent gas distribution function at the cell interfaces needs to be reconstructed in order to evaluate the numerical fluxes. The latter approach has been applied in [28, 29] to a multi-temperature BGK model where a multi-temperature intermediate equilibrium state, F_{eq}, is introduced and the same assumption that the fraction of collisions exciting the rotational degrees of freedom is a given constant or a function of the flow temperatures is considered as in the Rykov model. In this case only mass, momentum and total energy are conserved during a particle collision

$$\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}\left(\frac{F_{eq}|^n - F|^n}{\tau^n} + \frac{F_M|^n - F_{eq}|^n}{Z_r\tau^n}\right) d\mathbf{c} = (0,\ 0,\ 0,\ 0)^T + (0,\ 0,\ 0,\ s)^T \tag{9}$$

then, the update of the macroscopic variables results

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}\left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) d\mathbf{c}dt + \frac{\Delta t}{2}\left(\mathbf{S}_i^{n+1} + \mathbf{S}_i^n\right) \tag{10}$$

with the source terms S modelled through the Landau-Teller-Jeanes-type relaxation model, [29]. In [14] and [30] the BGK-NS method has been successfully employed with the

Shakhov kinetic model, [7], and improved, resulting in the Unified Gas Kinetic Scheme (UGKS), by considering a discrete integration method in the phase space with $c_x|_m$ the mth discrete velocity. Then, equation (7) in the UGKS becomes

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x} \sum_m \int_{t^n}^{t^{n+1}} \hat{\mathbf{\Psi}} \left([c_x|_m F]|_{i-1/2} - [c_x|_m F]|_{i+1/2} \right) dt \tag{11}$$

where the aforementioned Prandtl correction is not anymore needed, with F reconstructed on the basis of the equilibrium distribution function of the Shakov model. Recently, in [15], a UGKS for diatomic gas flow has been developed employing the Rykov model, (1). Also in this case, as for the modified BGK model discussed above, a source term, that needs to be determined, arises in the update of the macroscopic variables

$$\begin{aligned} \mathbf{W}_i^{n+1} = \; & \mathbf{W}_i^n + \tfrac{1}{\Delta x} \textstyle\sum_m \int_{t^n}^{t^{n+1}} \hat{\mathbf{\Psi}}_0 \left([c_x|_m F_0]|_{i-1/2} - [c_x|_m F_0]|_{i+1/2} \right) dt + \\ & + \tfrac{1}{\Delta x} \textstyle\sum_m \int_{t^n}^{t^{n+1}} \hat{\mathbf{\Psi}}_1 \left([c_x|_m F_1]|_{i-1/2} - [c_x|_m F_1]|_{i+1/2} \right) dt + \tfrac{\Delta t}{2} \left(\mathbf{S}_i^{n+1} + \mathbf{S}_i^n \right) \end{aligned} \tag{12}$$

where $\hat{\mathbf{\Psi}}_0 = (1,\ c_x,\ \mathbf{c}^2,\ 0)^T$ and $\hat{\mathbf{\Psi}}_1 = (0,\ 0,\ 1,\ 1)^T$. The method is not complete till a procedure to reconstruct a time-dependent gas distribution function at the cell interfaces is defined. In [26, 27, 30, 14, 15] the following general solution of the kinetic model equation, under the assumption of a locally constant collision time, has been employed with the BGK, Shakhov and Rykov models

$$\begin{aligned} F(x_{i+1/2}, t, c_x|_m) = \; & \tfrac{1}{\tau} \int_{t^n}^{t} F_{eq}(t', c_x|_m, x_{i+1/2} - c_x|_m (t - t')) \exp\left(-\tfrac{t-t'}{\tau}\right) dt' + \\ & + \exp\left(-\tfrac{t}{\tau}\right) F^0(t^n, \mathbf{c}|_m, x_{i+1/2} - c_x|_m (t - t^n)). \end{aligned} \tag{13}$$

The kinetic model equilibrium distribution function F_{eq} and the initial distribution function F^0 are expressed as Taylor expansions with coefficients that can be determined considering the macroscopic variables relations, as example equations (36) for the Rykov model, and the relative compatibility conditions, equations (8) or (9). A different approach has been followed for the multi-temperature BGK model in [28, 29], where the following time dependant distribution function has been used

$$F = F_{eq} - \tau^* \left(\frac{\partial F_{eq}}{\partial t} + \mathbf{c} \frac{\partial F_{eq}}{\partial \mathbf{x}} \right) + t \frac{\partial F_{eq}}{\partial t}. \tag{14}$$

The latter is based on the Chapman-Enskog expansion where the collision time is replaced by a generalised one which depends on not only the local macroscopic variables, but also

their gradients, and is obtained in order to have the kinetic equation satisfied. Indeed, substituting equation (14) in the extended BGK model [28, 29] it is possible to obtain

$$\tau^* = \frac{\tau}{1+\tau(D^2 F_{eq}/DF_{eq})} \tag{15}$$

where

$$D = \frac{\partial}{\partial t} + \mathbf{c}\frac{\partial}{\partial \mathbf{x}} \quad ; \quad D^2 = \frac{\partial D}{\partial t} + \mathbf{c}\frac{\partial D}{\partial \mathbf{x}} \tag{16}$$

In [28, 29], the derivative of the equilibrium distribution function are then expressed as Taylor expansions with the coefficients that can be obtained by means of the macroscopic variables formulas. The time derivatives of the macroscopic variables are defined in terms of the spatial derivatives thanks to the compatibility conditions. The latter approach is simpler than the former, but, being based on the Chapman-Enskog solution of the kinetic model, is, strictly speaking, valid only for small perturbances from the equilibrium.

6 GAS-KINETIC SCHEME FOR NEAR-CONTINUUM DIATOMIC FLOWS BASED ON THE RYKOV MODEL

In order to extend the domain of validity of the continuum formulation of the solver employed in the present work, we propose a Gas-Kinetic Scheme based on the Chapman-Enskog expansion for the Rykov model (section 2). This approach, due to the use of the Chapman-Enskog expansions, is limited to near-continuum regions but is simpler than the UGKS for diatomic gases presented in [15]. For this reason it fits our object of extending the continuum formulation without drastically increasing its computational cost. Integrating in time the non-dimensional reduced Rykov model system (1), as example for a one-dimensional flow problem, it is possible to obtain the following equations for the update of the distributions functions

$$F_0|_i^{n+1} = F_0|_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} \left([c_x|_m F_0]_{i-1/2} - [c_x|_m F_0]_{i+1/2}\right) dt + \frac{\Delta t}{2}\left(\frac{F_0^{eq}|^{n+1} - F_0|^{n+1}}{\tau^{n+1}} + \frac{F_0^{eq}|^n - F_0|^n}{\tau^n}\right)$$

$$F_1|_i^{n+1} = F_1|_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} \left([c_x|_m F_1]_{i-1/2} - [c_x|_m F_1]_{i+1/2}\right) dt + \frac{\Delta t}{2}\left(\frac{F_1^{eq}|^{n+1} - F_1|^{n+1}}{\tau^{n+1}} + \frac{F_1^{eq}|^n - F_1|^n}{\tau^n}\right)$$

with

$$F_0^{eq} = \frac{1}{Z_r}F_0^r + \left(1 - \frac{1}{Z_r}\right)F_0^t \quad ; \quad F_1^{eq} = \frac{1}{Z_r}F_1^r + \left(1 - \frac{1}{Z_r}\right)F_1^t. \tag{17}$$

Taking the moments $\hat{\mathbf{\Psi}}_0 = (1,\ c_x,\ \mathbf{c}^2,\ 0)^T$ of F_0 and $\hat{\mathbf{\Psi}}_1 = (0,\ 0,\ 1,\ 1)^T$ of F_1 the updated non-dimensional macroscopic variables are given by equation (12) where the source term, as discussed in appendix F, is

$$\frac{\Delta t}{2}\left(\mathbf{S}_i^{n+1} + \mathbf{S}_i^n\right) = \frac{\Delta t}{2}\left(0,\ 0,\ 0,\ \frac{\rho(T|_i^{n+1} - T_r|_i^{n+1})}{Z_r \tau_i^{n+1}} + \frac{\rho(T|_i^n - T_r|_i^n)}{Z_r \tau_i^n}\right)^T. \tag{18}$$

Here we propose to reconstruct the time dependant distribution functions at the inter-cells, i.e. $F_0|_{i\pm1/2}$ and $F_1|_{i\pm1/2}$, based on the Chapman-Enskog expansions around F_0^{eq} and F_1^{eq} given by equations (17)

$$F_0 = F_0^{eq} - \tau\left(\frac{\partial F_0^{eq}}{\partial t} + c_x\frac{\partial F_0^{eq}}{\partial x}\right) + t\frac{\partial F_0^{eq}}{\partial t} \quad ; \quad F_1 = F_1^{eq} - \tau\left(\frac{\partial F_1^{eq}}{\partial t} + c_x\frac{\partial F_1^{eq}}{\partial x}\right) + t\frac{\partial F_1^{eq}}{\partial t} \tag{19}$$

without employing a generalised collision time. Moreover, instead of employing Taylor expansions, we intend to proceed analytically and obtain the derivatives of the equilibrium distribution functions in terms of the macroscopic variables and their derivatives. These can then be evaluated at the interface knowing the values at the cells centres. Thus, deriving equations (17) we obtain

$$\frac{\partial F_0^{eq}}{\partial\alpha} = \frac{1}{Z_r}\frac{\partial F_0^r}{\partial\alpha} + \left(1-\frac{1}{Z_r}\right)\frac{\partial F_0^t}{\partial\alpha} \quad ; \quad \frac{\partial F_1^{eq}}{\partial\alpha} = \frac{1}{Z_r}\frac{\partial F_1^r}{\partial\alpha} + \left(1-\frac{1}{Z_r}\right)\frac{\partial F_1^t}{\partial\alpha} \tag{20}$$

where $\alpha = x, t$. The derivatives of F_0^r, F_0^t, F_1^r and F_1^t can be written as follows

$$\begin{aligned}
\frac{\partial F_0^r}{\partial\alpha} &= F_0^r\left(\frac{1}{F_M(T)}\frac{\partial F_M(T)}{\partial\alpha} + \frac{\omega_0}{\phi_0(T)}\frac{\partial\phi_0(T)}{\partial\alpha}\right)\\
\frac{\partial F_0^t}{\partial\alpha} &= F_0^t\left(\frac{1}{F_M(T_t)}\frac{\partial F_M(T_t)}{\partial\alpha} + \frac{1}{\phi_0(T_t)}\frac{\partial\phi_0(T_t)}{\partial\alpha}\right)\\
\frac{\partial F_1^r}{\partial\alpha} &= F_1^r\left[\frac{1}{T}\frac{\partial T}{\partial\alpha} + \frac{1}{F_M(T)}\frac{\partial F_M(T)}{\partial\alpha} + \frac{1}{1+\omega_0\phi_0(T)+\omega_1\phi_1(T)}\left(\omega_0\frac{\partial\phi_0(T)}{\partial\alpha} + \omega_1\frac{\partial\phi_1(T)}{\partial\alpha}\right)\right]\\
\frac{\partial F_1^t}{\partial\alpha} &= F_1^t\left[\frac{1}{T_r}\frac{\partial T_r}{\partial\alpha} + \frac{1}{F_M(T_t)}\frac{\partial F_M(T_t)}{\partial\alpha} + \frac{1}{1+\phi_0(T_t)+\phi_1(T_r)}\left(\frac{\partial\phi_0(T_t)}{\partial\alpha} + \frac{\partial\phi_1(T_t,T_r)}{\partial\alpha}\right)\right]
\end{aligned} \tag{21}$$

with the introduction of the following notation

$$\phi_0(T) = \frac{8}{15}\frac{q_x^t c'_x}{\rho T^2}\left(\frac{c'^2}{T} - \frac{5}{2}\right) \quad ; \quad \phi_1(T_1,T_2) = 4(1-\delta)\frac{q_x^r c'_x}{\rho T_1 T_2} \tag{22}$$

where the ideal gas law has been used. The derivative of the Maxwellian, F_M, and the Rykov model corrections, ϕ_0 and ϕ_1, can be found in appendix G. In order to remove the time derivatives we remember that the time and space derivative of the macroscopic variables can be linked by means of the compatibility condition for the currently employed Chapman-Enskog expansion

$$\int_{-\infty}^{+\infty}\left[\hat{\mathbf{\Psi}}_0\left(\frac{\partial F_0^{eq}}{\partial t} + c_x\frac{\partial F_0^{eq}}{\partial x}\right) + \hat{\mathbf{\Psi}}_1\left(\frac{\partial F_1^{eq}}{\partial t} + c_x\frac{\partial F_1^{eq}}{\partial x}\right)\right]d\mathbf{c} = \mathbf{S} \tag{23}$$

Thus, we obtain

$$\frac{\partial\mathbf{W}}{\partial t} = \mathbf{S} - \int_{-\infty}^{+\infty}\left(\hat{\mathbf{\Psi}}_0 c_x\frac{\partial F_0^{eq}}{\partial x} + \hat{\mathbf{\Psi}}_1 c_x\frac{\partial F_1^{eq}}{\partial x}\right)d\mathbf{c} \tag{24}$$

which, as explained in appendix H, leads to

$$\frac{\partial \mathbf{W}}{\partial t} = \mathbf{S} - \frac{\partial \mathbf{Q}}{\partial x} \tag{25}$$

where

$$\mathbf{Q} = \begin{bmatrix} \rho u_x \\ \frac{1}{2}\rho\left(T_t + \frac{T-T_t}{Z_r}\right) + \rho u_x^2 \\ \frac{3}{2}\rho\left(T_t + \frac{T-T_t}{Z_r}\right)u_x + \rho u_x^3 + \frac{2}{3}\frac{Z_r+\omega_0-1}{Z_r}q_x^t + \rho\left(T_r + \frac{T-T_r}{Z_r}\right)u_x + 2(1-\delta)\frac{Z_r+\omega_1-1}{Z_r}q_x^r \\ \rho\left(T_r + \frac{T-T_r}{Z_r}\right)u_x + 2(1-\delta)\frac{Z_r+\omega_1-1}{Z_r}q_x^r \end{bmatrix} \tag{26}$$

Regarding the heat fluxes time derivatives, needed for the derivatives of the Rykov corrections (22); multiplying the first and the second equations of the Rykov model (1) by ${c'}_x {c'}^2/2$ and ${c'}_x$, respectively, and integrating, the following expressions can be obtained as discussed in appendix H

$$\frac{\partial q_x^t}{\partial t} = \left(\frac{\omega_0-1}{3Z_r} - \frac{2}{3}\right)\frac{q_x^t}{\tau} \quad ; \quad \frac{\partial q_x^r}{\partial t} = \left((1-\delta)\frac{\omega_1-1}{Z_r} - \delta\right)\frac{q_x^r}{\tau} \tag{27}$$

7 CONCLUSIONS AND FUTURE WORKS

In the first part of the paper the Rykov and the Ellipsoidal-Statistical kinetic models for diatomic gases have been evaluated with respect to experimental and DSMC results, showing that both models are reliable to simulate high Mach flows with rotational degrees of freedom. However, the Rykov model leads to slightly better predictions when compared to the ES model, mainly due to the temperature dependant collision number. In the second part of the work the Rykov model has been employed to formulate a Gas Kinetic Scheme for near continuum flow simulations. The scheme will be employed in future works in hybrid methods in order to reduce the computational domain where the expensive discrete velocity methods for kinetic Boltzmann equations are needed.

A THE NON-DIMENSIONAL VARIABLES

To obtain a non-dimensional form of this kinetic model, we define the following dimensionless quantities

$$\begin{array}{lll} \rho = \hat{\rho}/\rho_\infty & ; \quad T = \hat{T}/T_\infty & ; \quad u = \hat{c}/\sqrt{2RT_\infty} \\ t = \hat{t}/(\mu_\infty p_\infty^{-1}) & ; \quad \mathbf{x} = \hat{\mathbf{x}}/\left(\sqrt{2RT_\infty}\mu_\infty p_\infty^{-1}\right) & ; \quad p = \hat{p}/(\rho_\infty R T_\infty) \\ \mu = \hat{\mu}/\mu_\infty & ; \quad q = \hat{q}/\left(\rho_\infty (2RT_\infty)^{3/2}\right) & ; \quad \tau = \hat{\nu}/(\mu_\infty p_\infty^{-1}) \end{array} \tag{28}$$

where the dimensional variables are denoted with a hat and $c_\infty = \sqrt{2RT_\infty}$ represents the most probable molecular velocity magnitude at equilibrium at the reference temperature T_∞. Then, the non-dimensional distribution functions are

$$F_0 = \hat{F}_0 / \left(\rho_\infty (2RT_\infty)^{-3/2}\right) \quad ; \quad F_1 = \hat{F}_1 / \left(mRT_\infty \rho_\infty (2RT_\infty)^{-3/2}\right). \tag{29}$$

B THE PARTICLE COLLISION NUMBER Z_r

In a system of colliding particles, energy is transferred between the various internal modes. These collisions tend to drive the internal energy distributions towards their respective equilibrium state and the number of them necessary to push a particular mode to the equilibrium is the collision number, Z, associated to that mode, [31]. It is well known that generally

$$Z_{translation} < Z_{rotation} < Z_{vibration} \tag{30}$$

therefore, the number of collisions required for the vibrational mode to reach the equilibrium is greater than the one required for the rotational energy which in turn is higher than the one associated with the translational mode. This implies that the time required for the different modes to relax towards the equilibrium state is different. Indeed, if we define the collision times $\tau_{t,r,v}$ as usual in the literature

$$\tau_{t,r,v} = Z_{t,r,v}\tau \tag{31}$$

where τ is the mean time between collisions, from relation (30) it is immediate to find that

$$\tau_{translation} < \tau_{rotation} < \tau_{vibration}. \tag{32}$$

We will focus now on the rotational degrees of freedom. Considering the rotational collision number as a constant over the entire flow field, any temperature dependence is neglected and this is in direct contrast with the theoretical results of [32] and [33]. For this reason, several works provide an expression of Z_R as a function of the temperature in the flow field. Probably the first attempt to appear in the literature is the theoretical work in [32], where, employing an empirical non impulsive model and by assuming a zero initial energy in the rotational mode, the following approximate expression in the continuum limit is obtained

$$Z_r = \frac{(Z_r)_\infty}{1+(\pi^{3/2}/2)(T^*/T)^{1/2}+(\pi^2/4+\pi)(T^*/T)} \tag{33}$$

where $T* = 91.5K$ is the characteristic temperature of the intermolecular potential and $(Z_R)_\infty = 23.5$ is the limiting value. While Parker's expression, (33), is derived involving a large number of simplifying assumption the overall dependence on the temperature is in agreement with the more rigorous treatment of [33]. However, this expression, being derived in the continuum regime, does not involve any dependence on the different translational and rotational temperatures. Thus, in the recent literature, formulas derived

from data fitting, either from numerical or experimental results, have been employed. Among them an expressions for $Z_R(T_t, T_r)$ derived from molecular dynamics simulations can be found in [21]. The latter is written as

$$Z_r = \left[a_1 \left(\frac{T_t}{1K}\right)^{1/4} + a_2 \left(\frac{T_t}{1K}\right)^{-1/4} - a_3 \left(\frac{T_t}{1K} - 1000\right)\right] \left[1 - b\left(1 - \frac{T_r}{T_t}\right)\right] \tag{34}$$

where $a_1 = 1.33868$, $a_2 = -6.19992$, $a_3 = -0.00107942$ and $0 < b \leq 1$.

C THE VISCOSITY LAW

For the viscosity variations the power law has been adopted

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}}\right)^{\omega} \tag{35}$$

with an exponential factor of 0.72 or 0.81. For Nitrogen, a power law with an exponential $\omega = 0.81$ represents better viscosity variations at low temperatures, while $\omega = 0.72$ is more suitable at high temperatures.

D THE NON-DIMENSIONAL MACROSCOPIC VARIABLES FOR THE RYKOV MODEL

The non-dimensional macroscopic quantities can be obtained from the distribution functions F_0 and F_1 of system (1) employing the following formulas

$$\begin{gathered}
\rho = \int_{-\infty}^{+\infty} F_0 d\mathbf{c} \quad ; \quad \rho u_i = \int_{-\infty}^{+\infty} c_i F_0 d\mathbf{c} \quad ; \quad \tfrac{3}{2}\rho T_t + \rho(u_x^2 + u_y^2 + u_z^2) = \int_{-\infty}^{+\infty} c^2 F_0 d\mathbf{c} \\
\rho T_r = \int_{-\infty}^{+\infty} F_1 d\mathbf{c} \quad ; \quad \tfrac{5}{2}T = \tfrac{3}{2}T_t + T_r \quad ; \quad p_t = \rho T_t \quad ; \quad p = \rho T \\
q_i^t = \int_{-\infty}^{+\infty} c'_i \tfrac{c'^2}{2} F_0 d\mathbf{c} \quad ; \quad q_i^r = \int_{-\infty}^{+\infty} \tfrac{c'_i}{2} F_1 d\mathbf{c}.
\end{gathered} \tag{36}$$

E THE NON-DIMENSIONAL MACROSCOPIC VARIABLES FOR THE ES MODEL

We then find for the equivalent continuum density, velocity and energy,

$$\begin{gathered}
\rho = \int_{-\infty}^{\infty} F_0 d\mathbf{c} \quad ; \quad \rho u_i = \int_{-\infty}^{\infty} c_i F_0 d\mathbf{c} \quad ; \quad \tfrac{3}{2}\rho T_t + \rho(u_x^2 + u_y^2 + u_z^2) = \int_{-\infty}^{+\infty} c^2 F_0 d\mathbf{c} \\
\tfrac{5}{2}T = \tfrac{3}{2}T_t + T_r \quad ; \quad \rho T_r = \int_{-\infty}^{\infty} F_1 d\mathbf{c}.
\end{gathered} \tag{37}$$

The pressure is assumed to depend on the equilibrium temperature T, and furthermore a relaxation temperature is introduced to represent the thermodynamic non-equilibrium between the translational and internal degrees of freedom,

$$p = \rho T \quad ; \quad T_{rel} = \theta T + (1-\theta) T_{rot}. \tag{38}$$

F THE MOMENTS OF THE RYKOV MODEL COLLISION TERM

With $\hat{\mathbf{\Psi}}_0 = (1,\ c_x,\ \mathbf{c}^2,\ 0)^T$ and $\hat{\mathbf{\Psi}}_1 = (0,\ 0,\ 1,\ 1)^T$ the moments of the Rykov model collision term result

$$\int_{-\infty}^{+\infty} \left[\hat{\mathbf{\Psi}}_0 \left(\tfrac{F_0^t - F_0}{\tau} + \tfrac{F_0^r - F_0^t}{\tau} \right) + \hat{\mathbf{\Psi}}_1 \left(\tfrac{F_1^t - F_1}{\tau} + \tfrac{F_1^r - F_1^t}{\tau} \right) \right] d\mathbf{c} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{\rho(T-T_r)}{Z_r \tau} \end{pmatrix}. \tag{39}$$

Indeed

$$\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 \tfrac{F_0^t - F_0}{\tau} = (0,\ 0,\ 0,\ 0)^T \quad ; \quad \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 \tfrac{F_0^r - F_0^t}{\tau} = \left(0,\ 0,\ \tfrac{3}{2}\tfrac{\rho(T-T_t)}{Z_r \tau},\ 0\right)^T \tag{40}$$

and

$$\int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 \tfrac{F_1^t - F_1}{\tau} = (0,\ 0,\ 0,\ 0)^T \quad ; \quad \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 \tfrac{F_1^r - F_1^t}{\tau} = \left(0,\ 0,\ \tfrac{\rho(T-T_r)}{Z_r \tau},\ \tfrac{\rho(T-T_r)}{Z_r \tau}\right)^T \tag{41}$$

from which, remembering the link between T, T_t and T_r defined in equations (36), it is straightforward to find equations (39)

G MAXWELLIAN AND RYKOV CORRECTIONS DERIVATIVES

For the derivative of the Maxwellian we have

$$\frac{\partial F_M(T)}{\partial \alpha} = F_M(T) \left[\frac{1}{\rho}\frac{\partial \rho}{\partial \alpha} + \left(\frac{c'^2}{T} - \frac{3}{2} \right) \frac{\partial T}{\partial \alpha} + 2\frac{c'_x}{T}\frac{\partial u_x}{\partial \alpha} \right] \tag{42}$$

while the derivatives of ϕ_0 and ϕ_1 in equation (21) result

$$\begin{aligned} \frac{\partial \phi_0(T)}{\partial \alpha} &= \phi_0(T) \left(\frac{1}{q_x^t}\frac{\partial q_x^t}{\partial \alpha} - \frac{1}{c'_x}\frac{\partial u_x}{\partial \alpha} - \frac{1}{\rho}\frac{\partial \rho}{\partial \alpha} - 2\frac{1}{T}\frac{\partial T}{\partial \alpha} \right) - \frac{\phi_0(T)}{\frac{c'^2}{T} - \frac{5}{2}} \left(2\frac{c'_x}{T}\frac{\partial u_x}{\partial \alpha} + \frac{c'^2}{T^2}\frac{\partial T}{\partial \alpha} \right) \\ \frac{\partial \phi_1(T_1,T_2)}{\partial \alpha} &= \phi_1(T) \left(\frac{1}{q_x^r}\frac{\partial q_x^r}{\partial \alpha} - \frac{1}{c'_x}\frac{\partial u_x}{\partial \alpha} - \frac{1}{\rho}\frac{\partial \rho}{\partial \alpha} - \frac{1}{T_1}\frac{\partial T_1}{\partial \alpha} - \frac{1}{T_2}\frac{\partial T_2}{\partial \alpha} \right) \end{aligned} \tag{43}$$

where the ideal gas law has been used.

H THE MACROSCOPIC VARIABLES TIME-DERIVATIVE FOR THE GAS-KINETIC SCHEME

From equation (21) follows that

$$\frac{\partial \mathbf{W}}{\partial t} = \mathbf{S} - \frac{\partial}{\partial x} \int_{-\infty}^{+\infty} \left(\hat{\mathbf{\Psi}}_0 c_x F_0^{eq} + \hat{\mathbf{\Psi}}_1 c_x F_1^{eq} \right) d\mathbf{c}. \tag{44}$$

Considering equations (20)

$$\begin{aligned} \int_{-\infty}^{+\infty} \left(\hat{\mathbf{\Psi}}_0 c_x F_0^{eq} + \hat{\mathbf{\Psi}}_1 c_x F_1^{eq} \right) d\mathbf{c} = \; & \tfrac{1}{Z_r} \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 c_x F_0^r d\mathbf{c} + \left(1 - \tfrac{1}{Z_r}\right) \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 c_x F_0^t d\mathbf{c} + \\ & + \tfrac{1}{Z_r} \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 c_x F_1^r d\mathbf{c} + \left(1 - \tfrac{1}{Z_r}\right) \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 c_x F_1^t d\mathbf{c} \end{aligned} \tag{45}$$

with

$$\begin{aligned} & \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 c_x F_0^r d\mathbf{c} = \left(\rho u_x,\ \tfrac{1}{2}\rho T + \rho u_x^2,\ \tfrac{3}{2}\rho T u_x + \rho u_x^3 + \tfrac{2}{3}\omega_0 q_x^t,\ 0 \right)^T \\ & \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_0 c_x F_0^t d\mathbf{c} = \left(\rho u_x,\ \tfrac{1}{2}\rho T_t + \rho u_x^2,\ \tfrac{3}{2}\rho T_t u_x + \rho u_x^3 + \tfrac{2}{3} q_x^t,\ 0 \right)^T \\ & \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 c_x F_1^r d\mathbf{c} = \left(0,\ 0,\ \rho T u_x + 2\omega_1(1-\delta) q_x^r,\ \rho T u_x + 2\omega_1(1-\delta) q_x^r \right)^T \\ & \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}}_1 c_x F_1^r d\mathbf{c} = \left(0,\ 0,\ \rho T_r u_x + 2(1-\delta) q_x^r,\ \rho T_r u_x + 2(1-\delta) q_x^r \right)^T \end{aligned} \tag{46}$$

equations (25) can be closed. Finally, obtaining equations (27) is straightforward considering definitions (17), the macroscopic relations (36) and the following integrals

$$\begin{aligned} & \int_{-\infty}^{+\infty} c'_x \tfrac{c'^2}{2} F_0^r d\mathbf{c} = \tfrac{\omega_0}{3} q_x^t \quad ; \quad \int_{-\infty}^{+\infty} c'_x \tfrac{c'^2}{2} F_0^t d\mathbf{c} = \tfrac{1}{3} q_x^t \\ & \int_{-\infty}^{+\infty} c'_x F_1^r d\mathbf{c} = \omega_1(1-\delta) q_x^r \quad ; \quad \int_{-\infty}^{+\infty} c'_x F_1^t d\mathbf{c} = (1-\delta) q_x^r \end{aligned} \tag{47}$$

REFERENCES

[1] Steijl, R. and Barakos, G. Computational Fluid dynamics of Partially Rarefied Flows with Coupled Kinetic Boltzmann/Navier-Stokes Methods. *ECCOMAS 2012*, 10-14 September 2012, Vienna, Austria.

[2] Rykov, V. A Model Kinetic Equation for a Gas with Rotational Degrees of Freedom. *Fluid Dynamics* (1975) **10**:959–966.

[3] Andries, P., LeTallec, P., Perlat, J.-P., and Perthame, B. The Gaussian-BGK Model of Boltzmann Equation with Small Prandtl Number. *European Journal of Mechanics - B/Fluids* (2000) **19**:813–830.

[4] Vincenti, W. and Kruger, C. *Introduction to Pysical Gas Dynamics* (1965). John Wiley and Sons, Inc.

[5] Bird, G. *The DSM Method* (2013). https://www.createspace.com/3689652.

[6] Bhatnagar, P., Gross, E., and Krook, M. A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems. *Physical Review* (1954) **94**:511–525.

[7] Shakhov, E. (1968) Generalization of the Krook Kinetic Relaxation Equation. *Mekhanika Zhidkosti i Gaza* (1968) **3**:142–145.

[8] Bourgat, J.-F., Le Tallec, P., and Tidriri, M. Coupling Boltzmann and Navier-Stokes Equations by Friction. *Journal of Computational Physics* (1996) **127**:227–245.

[9] Schwartzentruber, T. *A Modular Particle-Continuum Numerical Algorithm for Hypersonic Non-equilibrium Flows* (2007). PhD dissertation, The Univeristy of Michigan.

[10] Degond, P., Jin, S., and Mieussens, L. A Smooth Transition Model Between Kinetic and Hydrodnamic Equaions. *Journal of Computational Phsics* (2005) **209**:665–694.

[11] Deschenes, T. and Boyd, I. (2011) Extension of a Modular Particle-Continuum Method to Vibrationally Exited, Hypersonic Flows. *AIAA Journal*, **49**.

[12] Degond, P., Dimarco, G., and Mieussens, L. A multiscale kinetic-fluid solver with dynamic localization of kinetic effects. *Journal of Computational Physics* (2010) **229**:4907–4933.

[13] Degond, P. and Dimarco, G. Fluid simulations with localised Boltzmann upscaling by direct simulation Monte-Carlo. *Journal of Computational Physics* (2012) **231**:2414–2437.

[14] Xu, K. and Huang, J.-C. An Improved Unified Gas-Kinetic Scheme and the Study of Shock Structures. *IMA Journal of Applied Mathematics* (2011) **76**:698–711.

[15] Liu, S., Pubing, Y., Xu, K., and Zhong, C. Unified Gas-Kinetic Scheme for Diatomic Molecular Simulations in all Flow Regimes. *Journal of Computational Physics* (2014) **259**:96–113.

[16] Rykov, V., Titarev, V., and Shakhov, E. Numerical Study of the Transverse Supersonic Flow of a Diatomic Rarefied Gas past a Plate. *Computational Mathematics and Mathematical Physics* (2007) **47**:136–150.

[17] Rykov, V., Titarev, V., and Shakhov, E. Shock Wave Structure in a Diatomic Gas Based on a Kinetic Model. *Fluid Dynamics* (2008) **43**:316–326.

[18] Larina, I. and Rykov, V. Kinetic Model of the Boltzmann Eqaution for a Diatomic Gas with Rotational Degrees of Freedom. *Computational Mathematics and Mathematical Physics* (2010) **50**:2118–2130.

[19] Larina, I. and Rykov, V. Computation of a Rarefied Diatomic Gas Flows through a Plane Microchannel. *Computational Mathematics and Mathematical Physics* (2010) **52**:637–648.

[20] Alsmeyer, H. Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorptiobn of an Electron Beam. *Journal of Fluid Mechanics* (1976) **74**:497–513.

[21] Valentini, P., Zhang, C., and Schwartzentruber, T. Molecular Dynamics Simulation of Rotational Relaxation in Nitrogen: Implications for Rotational Collision Number Models. *Physics of Fluids* (2012) 106101:1–23.

[22] Tsuboi, N. and Matsumoto, Y. Experimental and Numerical Study of Hypersonic Rarefied Gas Flow over Flat Plates. *AIAA Journal* (2005) **43**:1243–1255.

[23] Holway, L. J. Kinetic Theory of Shock Structure Using an Ellipsoidal Distribution Function. *Rarefied Gas Dynamics, Proceedings of the Fourth International Symposium held at the Institute for Aerospace Studies, 1964 Toronto, Canada* (1965) **1**, 193–215.

[24] Chen, S., Xu, K., and Cai, Q. A Comparison and Unification of Ellipsoidal Statistical and Shakhov BGK Models. *arXiv:1304.0865v2 [physics.flu-dyn]* (2013).

[25] For more information about The University of Liverpool High Performance Computing visit *http://www.liv.ac.uk/csd/projects/hpc/*

[26] Xu, K. A Gas-Kinetic BGK Scheme for the NavierStokes Equations and its Connection with Artificial Dissipation and Godunov Method. *Journal of Computational Physics* (2001) **171**:289–335.

[27] Xu, K. A Multidimansional Gas-Kinetic BGK Scheme for Hypersonic Viscous Flow. *Journal of Computational Physics* (2005) **203**:405–421.

[28] Xu, K. and Josyula, E. Continuum Formulation for Non-equilibrium Shock Structure Calculation. *Communications in Computational Physics* (2006) **1**:425–450.

[29] Xu, K., He, X., and Cai, C. Multiple Temperature Kinetic Model and Gas-Kinetic Method for Hypersonic Non-equilibrium Flow Computations. *Journal of Computational Physics* (2008) **227**:6779–6794.

[30] Xu, K. and Huang, J.-C. A Unified Gas-Kinetic Scheme for Continuum and Rarefied Flows. *Journal of Computational Physics* (2010) **229**:7747–7764.

[31] Boyd, I. Rotational-Translational Energy Transfer in Rarefied Non-equilibrium Flows. *Physics of Fluids A* (1990) **2**:447–452.

[32] Parker, J. Rotational and Vibrational Relaxation in Diatomic Gases. *Physics of Fluids* (1959) **2**:449–462.

[33] Lordi, J. and Mates, R. Rotational Relaxation in Nonpolar Diatomic Gases. *Physics of Fluids* (1970) **9**:291–308.