Local non-equilibrium phase density reconstruction with Grad and Chapman-Enskog methods

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Abstract. The study of the non-equilibrium velocity gas distribution function reconstruction was carried out due to extended gas dynamics methods. The bimodal Mott-Smith solution for a plane shock wave was used as a reference distribution function. The shock-wave solutions were considered in the range of Mach numbers from \(Ma = 2.0\) to \(Ma = 8.0\). The reconstruction of the original function was carried out using the Navier-Stokes-Fourier, 13-moment, regularized 13-moment and 26-moment approximating functions.

1. Introduction
The physical gas flow non-equilibrium is associated with the presence of a difference between the molecular distribution function (phase density) and Maxwell equilibrium distribution function. Significant differences appear in the case of a small number of collisions between molecules. It happens when the mean free path becomes comparable with the characteristic linear scale of the problem. This flow regime is called transitional (from continuum regime to free-molecular one). The classical Navier-Stokes equations allow adequate gas description only in case of moderate rarefaction. The classical approach ceases to be applicable with an increase in the degree of gas rarefaction \([1]\). The kinetic approach is a natural alternative to the continuum approach. These include Direct Simulation Monte-Carlo method (DSMC) \([2, 3]\) or deterministic solution of Boltzmann equation \([4, 5]\) or kinetic model equations \([1, 6, 7]\). The complexity of the kinetic approach applying for a moderately rarefied gas is in the high requirements of these models and methods to computational resources. Another possible way to take into account non-equilibrium is the extended gas dynamics equations. These include the Burnett equations and their modifications obtained from the Boltzmann kinetic equation due to Chapman-Enskog method \([8, 1]\), as well as the Grad moment equations \([9, 1]\). The advantage of these methods is that the continuum approach of partial differential equations is still used to describe the flow. Taking into account greater deviations from equilibrium is possible due to expansion in a small parameter (Burnett equation) or expansion in terms of Hermite polynomials (moment method). It allows expanding the applicability range of the continuum approach of description towards rarefaction (greater difference of the distribution function of molecules from equilibrium) in the comparison with the Navier-Stokes equations \([10, 11, 12, 13, 14]\).

Of course, the most detailed description of gas medium provides the knowledge of flow behavior at the microscopic level. The local velocity distribution function allows obtaining any local gas gas-dynamic parameter. Therefore, it can be said that the local distribution function
determining is an excessive goal [15]. The main goal of the extended gas dynamics methods is the correct description of moderately non-equilibrium flows at the macroscopic level with a much lower requirement for computational resources and computational time in comparison with the kinetic approaches. At the same time, the question of the degree of adequacy of the continuum methods application for the qualitative and quantitative description of the microscopic level still remains open [16]. The problem of restoring a non-equilibrium distribution function, in addition to academic interest, also has practical value in some areas. An example is the need to know the cluster distribution function during evaporation and condensation [17, 18, 19].

Here we continue the study of the possibility of restoring the non-equilibrium velocity distribution function due to the known local gas-dynamic parameters [20]. On the example of considering the analytical solution of Mott-Smith [21] for a one-dimensional shock wave, the local distribution function was reconstructed at various degrees of non-equilibrium due to Grad distribution function [9, 22] and Chapman-Enskog one [8, 1].

2. Problem formulation
The problem of the structure of a plane shock wave in a monatomic gas is used as an example of a strongly non-equilibrium flow. This flow is a classical problem of the Rarefied Gas Dynamics. There is a huge amount of studies devoted to the analytical [23, 21, 24, 25, 26, 4], numerical [27, 28, 29, 30, 31, 32, 13, 33] and experimental [34, 35, 36, 37, 38, 39, 40] study of this problem. On the one hand, the popularity of this problem is explained by its geometric simplicity (one-dimensionality in physical space). On the other hand, this flow is a clear example of the transition from one equilibrium state of the gas (before the shock wave) to another equilibrium state (behind the shock).

For this study, the analytical Mott-Smith solution for the plane shock wave structure was chosen as an example of a non-equilibrium distribution function. This solution is a bimodal solution for the velocity distribution function as the sum of two Maxwellians [21, 41].

\[
    f(c, x) = \frac{\rho_1(x)}{2\pi \theta_1} \exp \left[ -\frac{(c - v_1)^2}{2\theta_1} \right] + \frac{\rho_2(x)}{2\pi \theta_2} \exp \left[ -\frac{(c - v_2)^2}{2\theta_2} \right],
\]

where \( c \) is the particle velocity. \( \rho(x) = \rho_1(x) + \rho_2(x) \) is gas density. \( \theta = \frac{kT}{m} \) is temperature in energy units, where \( k \) is Boltzmann constant, \( m \) is molecular mass, and \( T \) is gas temperature in Kelvins. \( \rho_1(-\infty), v_1 \) and \( \theta_1 \) are the quantities before the shock wave. The corresponding parameters \( \rho_2(+\infty), v_2 \) and \( \theta_2 \) behind the shock wave are determined due to Rankine-Hugoniot...
relations for a given Mach number $Ma$ [42]. The spatial distribution of $\rho_1(x)$ and $\rho_2(x)$ were obtained in [21]. Figure 1 demonstrates the density and temperature profiles for Mach numbers $Ma = 2.0$ and $Ma = 8.0$. The space coordinate is normalized by free stream average free path. Density and temperature were normalized here as follows

$$
\hat{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1}, \quad \hat{T} = \frac{T - T_1}{T_2 - T_1}
$$

(2)

This solution is not a reference solution from the point of view of describing the flow macro-parameters’ behavior inside a shock wave [1]. On the other hand, it allows obtaining an excellent qualitative description of the distribution function changing inside a shock wave for any Mach number. With an increase in the Mach number, this solution allows a better quantitative description of the shock wave structure in terms of gas-dynamic parameters. This is due to the strengthening of the bimodal nature of the true distribution function [39]. Figure 2 presents the variation of phase density in different points ($\hat{\rho} = 0.1, 0.3, 0.5, 0.7, 0.9$) of two shock wave examples (for $Ma = 2.0$ and $Ma = 8.0$) in $x$–direction. The $x$–dependence function and the non-dimension molecular velocity $\hat{c}_x$ are obtained as follows

$$
f(c_x, x) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(c_x, c_y, c_z, x) dc_y dc_z, \quad \hat{c}_i = \frac{c_i}{2\theta_i}.
$$

(3)

Later, an analytical solution was proposed in the form of the superposition of three functions (with an extra Chapman function) [24]. This modification allows refining of gas-dynamic parameters behavior inside a shock. E.g. it allows obtaining a temperature overshoot at Mach numbers $Ma > 3.9$ [43, 44].

3. Phase density approximations

The Chapman-Enskog method allows obtaining the Euler, Navier-Stokes-Fourier, Barnett, super-Barnett equations directly from the Boltzmann kinetic equation [1, 10]. 13 and 26 moment systems of equations can be obtained due to Grad method [1, 10]. The regularized moment system of equations can be obtained using the Order of magnitude method [10]. The goal of this work is to consider the hierarchy of macroscopic approaches as applied to the reconstruction of the local non-equilibrium distribution function. Knudsen number $Kn$ can be considered as a small parameter [13]. Maxwell equilibrium phase density $f_M$ is considered as zero-order
approximation. Corresponding Euler equations are of order \(Kn^0\). The next step (\(Kn^1\)) is Navier-Stokes-Fourier (NSF) equations with the following phase density

\[
f_{NSF} = f_M \left[ 1 + \frac{\sigma_{ij}^{NSF}}{2p\theta} c_{<i}c_{j>} + \frac{2}{5} \frac{q_k^{NSF}}{p\theta} c_k \left( \frac{c^2}{2\theta} - \frac{5}{2} \right) \right],
\]

where \(p\) and \(\theta\) are local pressure and temperature. The angular brackets in the subscripts indicate the trace-free and symmetric part of the tensor. The components of stress tensor \(\sigma_{ij}^{NSF}\) and heat flux \(q_i^{NSF}\) are calculated in NSF approach via velocity and temperature gradients correspondingly

\[
\sigma_{ij}^{NSF} = -2\mu \frac{\partial v_{(i}}}{\partial x_{j)}}, \quad q_i^{NSF} = -\frac{15}{4} \frac{\mu}{\theta} \frac{\partial \theta}{\partial x_i},
\]

where \(\mu\) is local viscosity. 13-moment Grad distribution function (G13) gives the equations of the second order (\(Kn^2\)). G13 distribution function \(f_{G13}\) is equal to \(f_{NSF}\) with the replacement of \(\sigma_{ij}^{NSF} = \sigma_{ij}\) and \(q_i^{NSF} = q_i\). Here these quantities have to be calculated as the integrals of true distribution function (in our consideration it is (1)) with the corresponding weights.

R13 equations with the corresponding distribution function is the third order approach. It leads to the appearance of extra contributions \(m_{ijk}\), \(R_{ij}\), and \(\Delta\). This expansion around equilibrium can be written as follows [10]

\[
f_{R13} = f_M \left[ 1 + \frac{\sigma_{ij}}{2p\theta} c_{<i}c_{j>} + \frac{2}{5} \frac{q_k}{p\theta} c_k \left( \frac{c^2}{2\theta} - \frac{5}{2} \right) - \frac{R_{ij}}{4p\theta^2} c_{<i}c_{j>} \left( 1 - \frac{c^2}{7\theta} \right) \right.
\]

\[
\left. + \frac{m_{ijk}}{6p\theta^3} c_{<i}c_{j}c_{k>} + \frac{\Delta}{8p\theta} \left( \frac{c^2}{3\theta} - \frac{1}{15\theta^2} \right) \right],
\]

Higher order moments can be calculated via first 13 moments. There are several nonlinear variants of R13 equations which are different in higher order moment relations [22, 10, 45, 13, 46, 47]. The linear variant of R13 equations has been used in the present study [48]. In the linear case (gradient transport mechanism, GTM [49]), higher-order moments have the following form [50]:

\[
m_{ijk} = -2\tau \frac{\partial \sigma_{ij}}{\partial x_k}, \quad R_{ij} = -\frac{24}{5} \frac{\tau}{\theta} \frac{\partial q_{(i}}}{\partial x_{j)}}, \quad \Delta = -12\tau \frac{\partial q_i}{\partial x_i},
\]

where \(\tau = \mu/p\) is the relaxation time. 26-moment Grad (G26) distribution function (\(Kn^4\) order) also can be obtained applying the same way as for 13-moment Grad distribution function (with
the replacement). In this case $m_{ijk}$, $R_{ij}$, and $\Delta$ should be calculated due to the integration of (1) [10]

$$m_{ijk} = m \int c_i c_j c_k f dc,$$

$$R_{ij} = m \int c^2 c_i c_j f dc - 70\sigma_{ij},$$

$$\Delta = m \int c^4 (f - f_M) dc,$$

where $f$ and $f_M$ are Mott-Smith and Maxwell molecular distribution functions correspondingly.

4. Results and discussion

4.1. $Ma = 2.0$

At a small Mach number of the shock wave the difference between the velocity distribution function and the Maxwellian equilibrium function is not very large (see Fig. 2a). This fact can also explain the applicability of the classical NSF equations for describing the internal structure of a shock wave for weak shocks [12]. In Figure 3 the reconstructing results of two local distribution functions for points with densities $\hat{\rho} = 0.1$ and $\hat{\rho} = 0.3$ at the Mach number $Ma = 2.0$ are presented. Figure shows the original distribution of the longitudinal and transverse components of the molecular velocity and all the approximations considered in the previous section. The most difficult region of the shock wave structure to describe by macroscopic methods is the supersonic part (leading front) [51]. As it can be see from Fig. 3 a, at the first considered point of the shock wave, the local function already begins to differ noticeably from the Maxwell distribution. The distribution tail, which is responsible for slow molecules, begins to grow noticeably. In other words, the mode of the Mott-Smith solution, which is responsible for the equilibrium values to the right of the shock wave, begins to grow. When analyzing the results in this case, it is worth paying attention to the appearance of local maximums in the longitudinal distributions of NSF and R13. Their appearance greatly distorts the behavior of these approximations at the main maximum (the most probable velocity). At the same time, the G13 and G26 have no such distortion. G26, as expected, gives the best approximation to the original function for both velocity components. As we move to the left (see Fig. 3), with a decrease in the local Mach number, the relative error of all considered approximations decreases. The NSF result for the longitudinal velocity component still shows a kink that affects the most probable value. G13, R13 and G26 provide good convergence to the original distribution. In the shock wave center region (near $\hat{\rho} = 0.5$), this kink in NSF completely disappears and the distributions turn out to be closer and closer to each other.

4.2. $Ma = 4.0$ and $Ma = 8.0$

With an increase in free-stream Mach number, the difference between the velocities and temperatures of the gas before and behind the shock wave grows. This leads to an increase in the bimodal character of the distribution function inside the shock wave, which was mentioned above. In the previous subsection, the results of the considered approximations were demonstrated for a sufficiently weak shock wave. This subsection proposes a parallel comparison of the results for the Mach numbers $Ma = 4.0$ and $Ma = 8.0$ as we move from left to right in the direction of decreasing in local Mach number.

Figure 4 shows the results for $Ma = 4.0$ and $Ma = 8.0$ at the points where the density is $\hat{\rho} = 0.1$. These results are qualitatively different from the results for a weak shock wave. All approximations demonstrate strong oscillations for the longitudinal component of the molecular velocity. The NSF and G13 results are very close. Similar behavior is observed for the R13...
Figure 4. Phase densities at $\hat{\rho} = 0.1$ for $Ma = 4.0$ (a) and $Ma = 8.0$ (b).

Figure 5. Phase densities at $\hat{\rho} = 0.3$ for $Ma = 4.0$ (a) and $Ma = 8.0$ (b).

Figure 6. Phase densities at $\hat{\rho} = 0.5$ for $Ma = 4.0$ (a) and $Ma = 8.0$ (b).
and G26 pair. In case of the longitudinal distribution, \( f_{NSF} \) and \( f_{G13} \) turn out to be negative at high speeds. \( f_{R13} \) and \( f_{G26} \) on the one hand decrease the magnitude of this non-physical minimum at high speeds. On the other hand, a significant minimum appears in their results to the left of the first mode of the Mott-Smith distribution. Here we are faced with the restriction on the distribution of high velocity molecules discussed in [16]. There is no convergence in the considered hierarchy in this case.

Further movement to the right downstream leads to a smoother tail of the original distribution at high speeds. This leads to the absence of non-physical negative regions in all considered approximations (see Figures 5 and 6). \( f_{G26} \) for all presented cases allows to obtain the smallest error relative to the reference function.

5. Concluding remarks
The results of the hierarchy (from the zero to the fourth order) of approximating functions of the extended gas dynamics methods are presented in the paper. The Mott-Smith analytical solution allows a qualitative description of the evolution of the true distribution function inside the shock wave. The use of this solution allows generating a different degree of flow nonequilibrium depending on the shock wave Mach number and the position of the considered point inside the shock-wave structure. The leading edge of the shock wave turns out to be the most difficult part for applying all the considered macroscopic methods [51, 16]. It was confirmed by the presented reconstruction results. The obtained data allows collecting information on the possibilities of the NSF, G13, R13 and G26 approaches for the description of the gas behavior microscopic level.

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