Gradient Expansions for Distribution Functions and Derivation of Moment Equations

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1 Introduction

The aim of this paper is a new presentation and a generalization of the so-called quasigasdynamic (QGD) moment equations that were obtained nearly fifteen years ago (e.g. [1]) and were used as an alternative to Navier-Stokes (NS) equations. It will be shown that the distribution functions associated with QGD equations are as realistic as those associated with NS equations. The formalism used to derive QGD equations will be generalized to include translational or rotational nonequilibrium.

The classical way to obtain NS equations consists in retaining the first order terms in a series expansion of the distribution function. The form of this approximation (function f^{NS}) is obtained as a result of the Chapman-Enskog procedure. The formal change $f \to f^{NS}$ in the convective term of Boltzmann equation (BE) results in the approximation

$$\frac{\partial f}{\partial t} + (\vec{\xi}\nabla) f^{NS} = \mathcal{I},$$

and finally in the NS equation system after multiplication by collisional invariants and averaging over velocity space.

In place of f^{NS} the authors propose to use other variants of series expansions. The first variant of such an expansion allows to derive QGD equations that describe viscous continuum flows. Increasing the Knudsen number results first in a violation of translational and rotational equilibrium. The other variants presented below are generalizations of the QGD gradient expansion (QGDT and QGDR expansions) that allow to derive moment equations that describe flows with translational and rotational nonequilibrium, respectively.

2 QGD gradient expansion

The first variant (QGD gradient expansion) is, e.g., [1]

$$f^{QGD} = f_0 - \tau(\vec{\xi}\nabla)f_0,$$

where f_0 is the local Maxwellian distribution function, τ is the Maxwellian relaxation time $\tau = \mu/p$, μ is the usual viscosity and p is the pressure. τ is close to the mean collisional time. A physical interpretation of this expansion can be found, e.g. in [2]. The formal change $f \to f^{QGD}$ in the convective term of BE results in

$$\frac{\partial f}{\partial t} + (\vec{\xi}\nabla)f_0 - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla)f_0 = \mathcal{I}.$$

Averaging this approximation after multiplication by collisional invariants (and introducing Prandtl number Pr and specific heat ratio γ for generalization purpose) results in a system of moment equations that describes viscous and heat conductive flows, namely quasigasdynamic (QGD) equations:

$$\begin{aligned}
\frac{\partial}{\partial t}\rho + \nabla_i \rho\, u^i &= \nabla_i \tau\, (\nabla_j \rho\, u^i u^j + \nabla^i p), \\
\frac{\partial}{\partial t}\rho\, u^k + \nabla_i \rho\, u^i u^k + \nabla^k p &= \nabla_i\, \tau\, (\nabla_j \rho\, u^i u^j u^k + \\
&\quad \nabla^i\, p\, u^k + \nabla^k\, p\, u^i) + \nabla^k\, \tau\, \nabla_i\, p\, u^i, \\
\frac{\partial}{\partial t}E + \nabla_i u^i (E + p) &= \nabla_i\, \tau\, (\nabla_j (E + 2p) u^i u^j + \frac{1}{2}\nabla^i u_k u^k p) + \\
&\quad \frac{\gamma}{\gamma - 1}\nabla_i\, \tau\, \frac{p}{\rho}\nabla^i\, p + Pr^{-1}\frac{\gamma}{\gamma - 1}\nabla_i\, \tau\, p\, \nabla^i \frac{p}{\rho},
\end{aligned}$$

where $E = (\rho\vec{u}^2)/2 + p/(\gamma - 1), p = \rho RT$. Here and below usual notations are used. For stationary flows, QGD equations turn into NS ones, with an additional contribution of order $O(\tau^2)$ and with the simple approximation of the second viscosity coefficient ψ in the form [2] $\psi = \mu(5/3 - \gamma)$. The QGD system was used successfully to describe viscous gas flows, including rarefied ones and presented some advantages compared with NS one (e.g. [4]). In [3] QGD equations have been obtained from a continuum mechanics approach, where their relation with the classical gasdynamic models is established. QGD equations can be derived also as a differential approach to kinetical-consistent difference schemes based on space-constant approximation of distribution function [5].

QGD and NS distribution functions. When differentiating function f_0 (in cartesian coordinates) with respect to x_i, f^{QGD} writes

$$f^{QGD} = f_0(1 + \tau\mathcal{P}_3^{QGD}(\xi_i)).$$

where $\mathcal{P}_3^{QGD}$ is a polynomial of degree 3 in ξ_i. Similarly, accounting for $\mu = p/\tau$, the NS distribution function writes

$$f^{NS} = f_0(1 + \tau \mathcal{P}_3^{NS}(\xi_i)),$$

Thus both NS and QGD distribution functions can be written as a series expansion in τ. In the particular case $\gamma = 5/3$, $Pr = 1$, the coefficients for the terms containing ξ_i^3 are identical. Most other coefficients are identical except for the numerical factors. Thus the functions f^{NS} and f^{QGD} have the same asymptotic behavior along the axes for large values of ξ_i [2].

3 QGDT and QGDR gradient expansions

QGDT equations. Another gradient expansion (QGDT) allows to generalize QGD equations to flows of monoatomic gas with translational nonequilibrium, i.e., with anisotropy of the distribution function. Details are given in [2]. We use the approximation

$$f \to f^{QGDT} \text{ where } f^{QGDT} = f_e - \tau(\vec{\xi}\nabla) f_e$$

and $f_e = f_{0x} \times f_{0y} \times f_{0z}$ is an ellipsoidal distribution function, built as a product of Maxwellian distribution functions with different translational temperatures T_i in the different directions of a cartesian system. Now the approximation of BE is

$$\frac{\partial f}{\partial t} + (\vec{\xi}\nabla) f_e - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla) f_e = \mathcal{I}.$$

This equation is multiplied successively by 1, $\vec{\xi}$, $\xi_i^2/2$ and averaged over the velocity space to yield the QGDT equations. Components of pressure and total energy, connected with the three space coordinates are calculated as $p_i = \rho R T_i$, $E_i = (\rho u_i^2 + p_i)/2$. The QGDT equation system is obtained as

$$\frac{\partial \rho}{\partial t} + \nabla_i \rho u_i = \nabla_i \tau \nabla_j (\rho u_i u_j + P_{ij}),$$

$$\frac{\partial \rho u_k}{\partial t} + \nabla_i (\rho u_i u_k + P_{ik}) = \nabla_i \tau \nabla_j (\rho u_i u_j u_k + u_i P_{jk} + u_j P_{ik} + u_k P_{ij}),$$

$$\frac{\partial}{\partial t} E_\alpha + \nabla_i (E_\alpha u_i + p_\alpha u_\alpha \delta_{i\alpha}) =$$

$$\nabla_i \tau \nabla_j (E_\alpha u_i u_j + u_\alpha p_\alpha (u_j \delta_{i\alpha} + u_i \delta_{j\alpha}) + \frac{u_\alpha^2}{2} P_{ij}) +$$

$$Pr^{-1} \nabla_i \tau (\frac{P_{ij}}{2} + \delta_{i\alpha}\delta_{j\alpha} p_\alpha) \nabla_j R T_\alpha + \nabla_i \tau \frac{p_\alpha}{\rho} \nabla_j (\frac{P_{ij}}{2} + \delta_{i\alpha}\delta_{j\alpha} p_\alpha) + S_\alpha.$$

Here E_α and p_α are scalar quantities. Subscripts i, j, k, α refer to any of the space directions x, y, z and ∇_i denotes the i-component of gradients. Summation occurs for repeated i and j subscripts and

$$P_{ij} = \begin{pmatrix} p_x & 0 & 0 \\ 0 & p_y & 0 \\ 0 & 0 & p_z \end{pmatrix}.$$

As for QGD equations, the Prandtl number does not appear in the described treatment and is introduced artificially. Because the ξ_i^2 are not collisional invariants, exchange terms S_α appear in the equations that govern the evolution of energy in the different directions. They are calculated based on a relaxation model for the collision integral and they are found to be $S_i = (p - p_i)/(2\tau_{rel})$, where p is the average pressure $p = (p_x + p_y + p_z)/3$. In the present work, τ_{rel} is taken as the mean collisional time τ_c [6].

Application to shock wave structure. The QGDT system has been applied to the classical problem of shock wave structure. A DSMC calculation has been carried out on the same problem to serve as a reference, using the code DISIRAF developed at the Laboratoire d'Aérothermique. Details are given in [2]. The only difference between the present work and that presented in [2] is the expression of τ_{rel} which is now taken equal to τ_c rather than $\tau = \mu/p$. This change improved significantly the agreement between DSMC and QGDT results. The test-case presented here is that of a shock wave at Mach number $Ma = 10$ in a monoatomic hard-sphere gas ($\omega = 0.5$). Results obtained at smaller Mach numbers exhibit even better agreement with DSMC ones.

The profiles of density and velocity are given in Fig.1, as obtained by solving NS, QGD and QGDT equations. They are compared with those obtained by DSMC calculations. Abscissae are reduced by the upstream mean free path and ordinates are presented in the usual form based on upstream (1) and downstream (2) Rankine-Hugoniot values. The origin of abscissae is the point where the reduced density is equal to 1/2, the computational grid step $h = 0.25\lambda_1$.

QGD profiles present comparable or better agreement than NS ones, when compared with DSMC results. The introduction of translational nonequilibrium (QGDT) improves considerably the agreement of ρ and u profiles. Profiles of transverse and longitudinal temperatures (T_y and T_x, respectively) are presented in Fig.2 as obtained from QGDT equations and DSMC method. The qualitative features of the profiles are found, including the overshoot of T_x. However, quantitative agreement is not achieved.

The inverse reduced shock wave thickness λ_1/δ is plotted against Mach number in Fig.3. While QGD results differ little from NS ones, introducing translational nonequilibrium (QGDT equations) shifts the results much closer to DSMC ones.

For NS equations, the conductive heat transfer within a gas is equal to

$$Q^{NS} = -\kappa \frac{\partial T}{\partial x},$$

where κ is the thermal conductivity. For QGD equations, it was established [3] that

$$Q^{QGD} = -\kappa \frac{\partial T}{\partial x} - \tau \rho T u^2 \frac{\partial s}{\partial x},$$

where s is the entropy. In DSMC calculations, it is obtained by sampling as

$$Q^{DSMC} = \overline{\rho (c_x (c_x^2 + c_y^2 + c_z^2)/2)}.$$

The distribution of heat flux is presented in Fig.4, non-dimensionalized by $\rho_1 a_1^3$. The agreement of QGD and QGDT results with DSMC ones is considerably better than the agreement between NS and DSMC results.

Distribution function. When differentiating function f_e with respect to x_i, f^{QGDT} writes as

$$f^{QGDT} = f_e(1 + \tau \mathcal{P}_3^{QGDT}(\xi_i)).$$

The coefficients ahead of ξ_x^3, ξ_x^2, ξ_x^1 and ξ_x^0 are

$$a_{xxx}^{(3)} = -\frac{1}{2RT_x^2}\frac{\partial T_x}{\partial x}, \qquad a_{xx}^{(2)} = -\frac{1}{RT_x}\frac{\partial u}{\partial x} + \frac{u}{RT_x^2}\frac{\partial T_x}{\partial x},$$
$$a_x^{(1)} = \frac{u}{RT_x}\frac{\partial u}{\partial x} + \frac{1}{2T_x}\frac{\partial T_x}{\partial x}(1 - \frac{u^2}{RT_x}) + \frac{1}{2T_y}\frac{\partial T_y}{\partial x} + \frac{1}{2T_z}\frac{\partial T_z}{\partial x} - \frac{1}{\rho}\frac{\partial \rho}{\partial x_i},$$
$$a^{(0)} = 0.$$

The distribution functions associated with NS, QGD and QGDT models were compared with the distribution function obtained by sampling during the DSMC calculation. The results at abscissae $x/\lambda_1 = -1$ and 0 are shown in Figs.5 and 6, respectively. The distribution functions are plotted against ξ_x after integration over ξ_y and ξ_z velocities.

The distribution functions are very sensitive to the models used. NS distribution functions exhibit unrealistic negative values, while QGDT distribution functions appear to be closer to DSMC results. This comparison confirms that QGD and QGDT equations are associated with a reasonable approximation of the actual distribution function.

QGDR gradient expansion. To model rarefied flows with nonequilibrium between translational and rotational temperatures, a QGDR approximation for the distribution function was used

$$f^{QGDR} = f_{0r} - \tau(\vec{\xi}\nabla) f_{0r},$$

where $f_{0r} = f_0 \times f_r$, and f_r is the Hinshelwood distribution function for rotational energy in di- or polyatomic molecules [6]. The formal change $f \to f^{QGDR}$ results in an approximation for BE

$$\frac{\partial f}{\partial t} + (\vec{\xi}\nabla) f_{0r} - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla) f_{0r} = \mathcal{I}$$

that results finally in QGDR moment equations for a gas with 2 or 3 rotational degrees of freedom. This system is described and used in a companion paper [7]. In the equilibrium case, the QGDR system turns into the QGD system with the corresponding γ value.

The formalism used to derived QGD equations is currently being generalized to obtain a system of equations for gas mixtures.

Limits of the continuum approach. To illustrate the limits of the approaches presented above, a 2-D jet expansion from a slit of height d in direction y was calculated. The flow conditions were the same as for the DSMC calculation presented in [8]: exit Mach and Knudsen numbers equal to 2 and 0.1, respectively. The gas consists again in monoatomic hard-sphere molecules. The evolution of density, velocity and average temperature obtained by QGDT equations are consistent with DSMC ones close to the slit, i.e. where molecular collisions are sufficient to maintain a situation close to equilibrium (Fig.7). Unfortunately the evolution of direction-dependent temperatures obtained by DSMC was not available for these flow conditions. However, the results obtained from QGDT equations (Fig.8) are in qualitative agreement with those obtained for other flow conditions.

4 Conclusion

Approximations of the distribution function in the form of gradient expansions allow to derive moment equations that are consistent with Navier-Stokes equations in the limit $Kn \to 0$.

These equations can be generalized to describe flows with translational (QGDT) or rotational (QGDR) nonequilibrium.

The comparison of distribution functions confirms that these expansions are associated with reasonable approximations of the actual distribution function.

When applied to the problem of shock wave structure, QGDT profiles of flow parameters are in better agreement with DSMC ones than those obtained by NS or QGD equations.

Thus the family of equation systems described in the present paper can be regarded as an valuable alternative to the classical NS equation system.

References

[1] Elizarova T.G., Chetverushkin B.N., *Kinetic Algorithms for Calculating Gasdynamic Flows,* J.Comput. Mathem. and Mathem. Phys., 1985, No.5, v.25, pp.164–169.

[2] Graur I.A., Elizarova T.G., Lengrand J.C., *Quasigasdynamic Equations with Multiple Translational Temperatures*, Laboratoire d'Aérothermique du CNRS, Meudon (Fr), R 97-1,1997.

[3] Sheretov Yu.V., *Quasi Hydrodynamic Equations as a Model for Viscous Compressible Heat Conductive Flows*, in book: *Implementation of Functional Analysis in the Theory of Approaches*, Tver University, 1997, pp.127–155 (in Russian).

[4] Elizarova T.G, Graur I.A, Lengrand J.C, Chpoun A., *Rarefied Gas Flow Simulation Based on Quasigasdynamic Equations*, AIAA J., 1995, V.33, No.12, pp.2316–2324.

[5] Abalakin I.V., Chetverushkin B.N., *Kinetical Consistent Difference Schemes as a Model for Description of Gasdynamic Flows*, J. Mathematical Modelling, 1996, v.8, No.8, pp.17–36 (in Russian).

[6] Bird G.A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford, 1994.

[7] Chirokov I.A., Elizarova T.G., Lengrand J.C., *Numerical Study of Shock Wave Structure Based on Quasigasdynamic Equations with Rotational Nonequilibrium*, this symposium.

[8] Lengrand J.C., *Méthode de Monte Carlo appliquée à un jet raréfié bidimensionnel*, Laboratoire d'Aérothermique du CNRS, Meudon (Fr), R 95-1,1995.

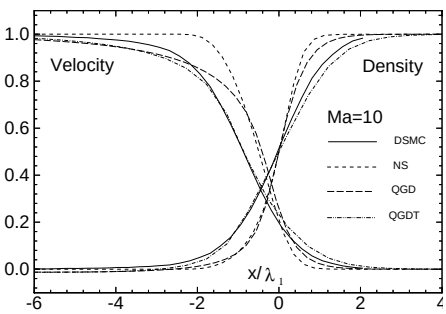

Figure 1: ρ and u profiles

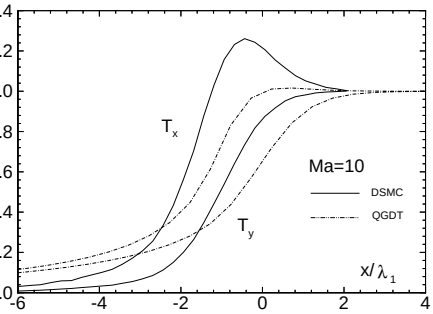

Figure 2: Profiles of temperatures

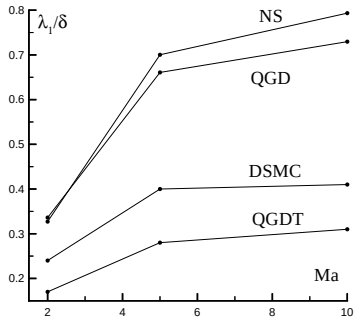

Figure 3: Inverse shock wave thickness of a shock wave

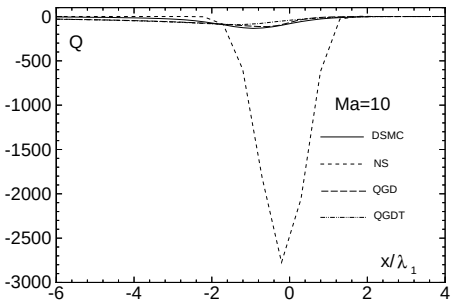

Figure 4: Profiles of conductive heat transfer in a shock wave

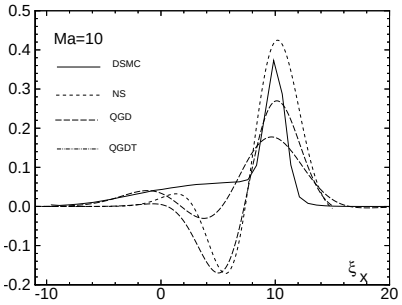

Figure 5: Distribution function in a shock wave at $x = -\lambda_1$

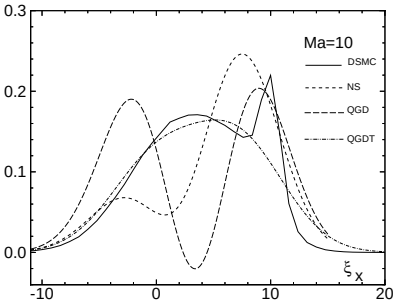

Figure 6: Distribution function in a shock wave at $x = 0$

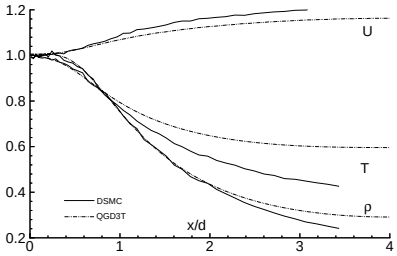

Figure 7: Evolution of flow parameter in a 2D jet expansion

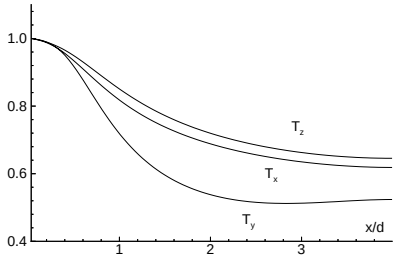

Figure 8: Evolution of direction-dependent temperatures in a 2D jet expansion