The Translational Non-Equilibrium Stucture of Inert Shock Waves and Triple Points with Account for Heat Fluxes

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1 Introduction

The accurate prediction of the internal structure of shock waves is difficult due to the presence of strong non-equilibrium effects, such as anisotropic temperatures and rotational or vibrational non-equilibrium. For the case of Mach reflections, previous studies have theorized that non-equilibrium effects in regions of wave interactions can lead to lasting large-scale differences in flow structures [1–3]. Unfortunately, the relevant scales tend to exist in the so-called transition regime, between classical continuum flow and free-molecular flows. The lack of reliable and affordable models for this regime has greatly limited the study of these situations.

Moment closures are an increasingly popular method for the prediction of gas flows for non-equilibrium regimes. These meso-scale models continue to produce physically valid solutions in transitional and non-equilibrium regimes when continuum models lose accuracy, without requiring the prohibitive computational cost associated with particle-based methods. Moment methods can be seen as a way to directly model the evolution of an expanded set of statistics of the distribution of gas-particle velocities. The inclusion of higher-order statistics, usually ignored in traditional models, allows for the direct treatment of thermal non-equilibrium effects. The first-order hyperbolic nature of the resulting partial differential equations (PDEs) bring computational advantages that lead to numerical solutions that are less sensitive to the grid quality [4] and can often be computed more efficiently than classical diffusive models, such as the Navier-Stokes equations, due to less strict time-step restrictions for explicit methods.

Until very recently the promise of moment methods as a practical tool has been limited by several factors. The original closures of Grad [5] do not remain mathematically well-posed for any significant deviation from equilibrium. The maxium-entropy technique; proposed by Dreyer [6], Müller and Ruggeri [7], and Levermore [8]; produces mathematically robust models that are too computationally expensive to be used in practical calculations if a treatment for heat transfer is included. More recently, the first general models that are both mathematically robust and numerically affordable have been proposed by Fox and Laurent [9], as well as Morin and McDonald [10]. However, these models are only applicable to non-physical one-dimensional gases for which all gas particles can only have velocities in a single direction. This presentation demonstrates a new model, inspired by these previous one-dimensional models, that extends the closures to realistic three-dimensional gas flows in multi-dimensional geometries, while maintaining all desirable mathematical and computational properties. The application of this new model to the study of inert shock waves and triple points is the subject of this presentation.

Following a summary of motivation, this presentation first covers the background of kinetic theory relevant to the new method, including the classical ten-moment and a novel twenty-moment closure. The ability for these closure models to accurately and efficiently predict the strong non-equilibrium effects within a shock wave is then demonstrated for shock waves with a range of Mach numbers. Finally, the structure of isolated and interacting triple points, typical of Mach-reflections, is considered. The degree to which non-equilibrium phenomena are predicted and the effects non-equilibrium has on the global structure is explored through comparison to classical models and experimental results.

2 Background in Kinetic Theory

Moment closures of gaskinetic theory begin by modelling the gas probabilistically, with the number density of particles at position, x_i, with velocity, v_i, at time, t, being represented by a distribution function, $\mathcal{F}(x_i, v_i, t)$. Macroscopic properties of the gas can be found by taking velocity moments of this distribution. This involves multiplying $\mathcal{F}$ by the particle mass, m, and monomials of the particle velocity, $w(v_i)$, as weights, then integrating over all velocity space. Relevant low-order moments are

$$w(v_i) = 1 : \qquad \iiint_{\infty} m\mathcal{F}(x_i, v_i, t) dv_i = \langle m\mathcal{F} \rangle = \rho \,, \tag{1}$$

$$w(v_i) = v_i : \qquad \langle m v_i \mathcal{F} \rangle = \rho u_i \,, \tag{2}$$

$$w(v_i) = v_i v_j : \qquad \langle m v_i v_j \mathcal{F} \rangle = \rho u_i u_j + P_{ij} \,, \tag{3}$$

$$w(v_i) = v_i v_j v_k : \qquad \langle m v_i v_j v_k \mathcal{F} \rangle = \rho u_i u_j u_k + P_{ij} u_k + P_{ik} u_j + P_{jk} u_i + Q_{ijk} \,, \tag{4}$$

corresponding to the mass, momentum, energy, and heat-flux densities of the gas. The notation $\langle \cdots \rangle$ is used for brevity, and represents integration over the entire velocity space. The variables ρ, u_i, P_{ij}, and Q_{ijk} correspond to the mass density, bulk velocity, anisotropic pressure tensor, and generalized heat-flux tensor of the gas, respectively. The pressure tensor is related to the traditional hydrostatic pressure and viscous stresses, τ_{ij}, through the relation $P_{ij} = p\delta_{ij} - \tau_{ij}$. The pressure tensor is simply the negative of the traditional fluid-stress tensor. However, by providing separate PDEs for the evolution of each of its components, moment methods can naturally predict deviations from the continuum Navier-Stokes form of these stresses when non-equilibrium becomes relevant. An anisotropic temperature tensor, $\Theta_{ij} = P_{ij}/\rho$, can also be defined that allows a gas to display different temperatures in different directions. Such effects are well-known in transition-regime flows and manifest at locations where gas-particles velocities have a wider spread in one direction then another. This non-equilibrium phenomenon is known to be important in shock waves, where the temperature of the gas normal to the shock increases more rapidly than in other directions. Particle collisions then redistribute the thermal energy into all modes though a relaxation process.

The deviatoric velocity of an individual particle can be defined as the difference between its velocity and the local average, $c_i = v_i - u_i$. Moments of this deviatoric velocity can also be taken,

$$w(v_i) = c_i c_j : \qquad \langle m c_i c_j \mathcal{F} \rangle = P_{ij} \,, \tag{5}$$

$$w(v_i) = c_i c_j c_k : \qquad \langle m c_i c_j c_k \mathcal{F} \rangle = Q_{ijk} \,, \tag{6}$$

$$w(v_i) = c_i c_j c_k c_l : \qquad \langle m c_i c_j c_k c_l \mathcal{F} \rangle = R_{ijkl} \,. \tag{7}$$

In general, moments of arbitrarily high-order in velocity can be computed. The physical interpretation of these moments becomes less obvious for higher-order moments, however, their treatment can remain important in accurately modelling non-equilibrium flows.

The time evolution of the distribution function is governed by the Boltzmann equation, written as

$$\frac{\partial \mathcal{F}}{\partial t} + v_i \frac{\partial \mathcal{F}}{\partial x_i} = \frac{\delta \mathcal{F}}{\delta t}\,, \tag{8}$$

in the absence of any external acceleration fields. The left-hand side of this equation describes the evolution of gas-particle motion in time and space, while the right-hand side models the effects of inter-particle collisions on the distribution function. For the present work, the BGK collision operator [11] is used,

$$\frac{\delta \mathcal{F}}{\delta t} \approx -\frac{\mathcal{F} - \mathcal{M}}{\tau}\,, \tag{9}$$

Multiplying Eq. (8) by a weight vector, $\boldsymbol{w}$, containing velocity weights for all the desired properties of study, and then taking moments of this set of equations, leads to Maxwell's equation of change,

$$\frac{\partial}{\partial t} \langle m\boldsymbol{w}\mathcal{F}\rangle + \frac{\partial}{\partial x_i} \langle m\boldsymbol{w}v_i\mathcal{F}\rangle = \left\langle m\boldsymbol{w}\frac{\delta \mathcal{F}}{\delta t}\right\rangle\,, \tag{10}$$

which describes the time-evolution of the moments. This gives rise to the problem of moment closure. Compared to the solution vector, the spatial derivative term has an additional velocity weight, ensuring the flux of each moment is a moment one order higher. For the final known moment, this means that its flux is generally not a function of the elements of the solution vector, and some form of closing flux must be chosen. Equation (10) can be re-expressed as

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}_i}{\partial x_i} = \frac{\partial \boldsymbol{U}}{\partial t} + \frac{\mathrm{dF_i}}{\mathrm{dU}}\frac{\partial \boldsymbol{U}}{\partial x_i} = \boldsymbol{S}\,, \tag{11}$$

where $\boldsymbol{U}$ is the vector of the known moments, $\boldsymbol{F}$ is the vector of the fluxes, and $\boldsymbol{S}$ is the vector of collision source effects. If the fluxes are assumed to be a function of the known moments, then the matrix $\frac{\mathrm{dF_i}}{\mathrm{dU}}$ is the flux Jacobian relating the current state of the gas to its fluxes. The hyerbolicity and well-posedness of moment closures is related to the eigenstructure of this matrix. The difficulty of moment closure construction is in the definition of closing fluxes that remain physically accurate while maintaining all desirable mathematical properties.

Many possible forms of closing fluxes have been proposed, with most proposing a form for the distribution function based on the known moments, and then integrating to find the closing flux [5–8, 12]. However, these can either have narrow ranges of physical applicability, as is the case with the original Grad hierarchy [5], or propose forms of the distribution function that cannot be integrated in closed form and instead rely on computationally costly numerical integration, as with the maximum entropy hierarchy [6–8, 12]. Recent advances [9, 10] have given rise to generalizable moment closures that primarily rely on maintaining the resulting mathematical structure of the PDEs, instead of an assumed distribution function. These closures are globally hyperbolic for all realizable states of the gas (meaning they are well-posed), in balance-law form, and have a wide range of numerical methods available for their solution. However, the application of these closures is restricted to academic cases with a one-dimensional velocity space.

The closure used in the present work is a twenty-moment extension of the robust one-dimensional closures described above. This new closure comprises twenty first-order hyperbolic PDEs for the evolution of the gas mass density, momentum, the six entries of the symmetric pressure tensor, and the ten entries of the symmetric third-order generalized heat-flux tensor, Q_{ijk}. This tensor describes the conduction of thermal energy associated with each available energy mode separately, as different modes conduct at different rates when the flow is out of thermal equilibrium.

As the new closure directly tracks all moments up to third-order, approximations for the fourth moment, R_{ijkl}, are needed to close the system. These relations are proposed as three-dimensional extensions of the models developed by Morin and McDonald [10]. The ten closing x-direction fluxes take the form

$$R_{xxxx} = 2\frac{Q_{xxx}^2}{P_{xx}} + 3\frac{P_{xx}^2}{\rho}\,, \tag{12}$$

$$R_{xxxy} = 2\frac{Q_{xxx}Q_{xxy}}{P_{xx}} + 3\frac{P_{xx}P_{xy}}{\rho}\,, \tag{13}$$

$$R_{xxyy} = \frac{Q_{xxy}^2}{P_{xx}} + \frac{Q_{xyy}^2}{P_{yy}} + \frac{P_{xx}P_{yy}}{\rho} + 2\frac{P_{xy}^2}{\rho}\,, \tag{14}$$

$$R_{xyyy} = 2\frac{Q_{xyy}Q_{yyy}}{P_{yy}} + 3\frac{P_{xy}P_{yy}}{\rho}\,, \tag{15}$$

$$R_{xxyz} = \frac{Q_{xxy}Q_{xxz}}{P_{xx}} + \frac{Q_{xxx}Q_{xyz}}{P_{xx}} + \frac{P_{xx}P_{yz}}{\rho} + 2\frac{P_{xy}P_{xz}}{\rho}\,, \tag{16}$$

$$R_{xyyz} = \frac{Q_{xyy}Q_{yyz}}{P_{yy}} + \frac{Q_{yyy}Q_{xyz}}{P_{yy}} + \frac{P_{xz}P_{yy}}{\rho} + 2\frac{P_{xy}P_{yz}}{\rho}\,, \tag{17}$$

with other permutations of the y- and z-directions having similar forms. One can observe the relative simplicity of the moment equations, with fluxes all being polynomial expressions of the known moments. The resulting system can be shown to be robustly hyperbolic and to remain well-posed.

3 Preliminary Numerical Results

In order to demonstrate the enhanced physical fidelity of the new twenty-moment model, two demonstration calculations are shown. First, the flow of a gas through a strong planar shock wave is investigated to demonstrate the prediction of non-equilibrium effects. Second, a Mach-reflection case is considered to demonstrate the robustness of the new technique for real multi-dimensional problems.

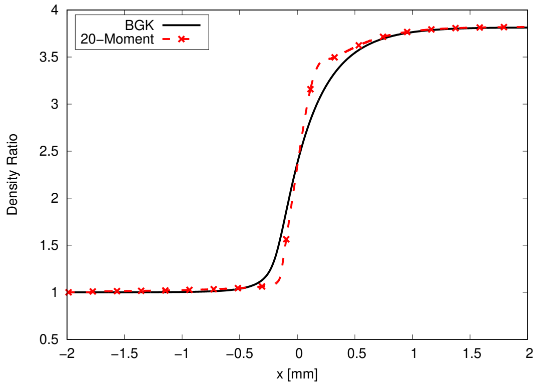
3.1 One-Dimensional Shock Structure Prediction

As a first problem of interest, the structure of a stationary, one-dimensional Mach 8 shock wave in a monatomic gas is studied. The ratios between the down-stream and up-stream states are

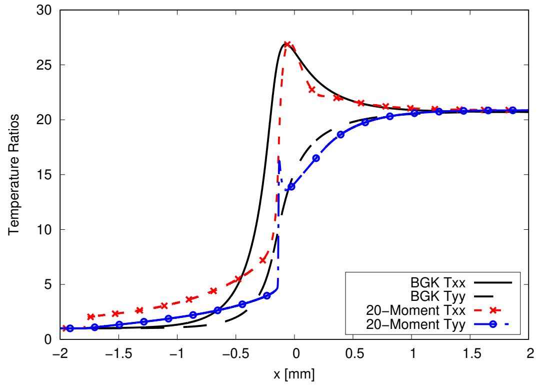
$$\frac{\rho_R}{\rho_L} = 3.368\,, \qquad \frac{u_{x_R}}{u_{x_L}} = 0.262\,, \qquad \frac{p_R}{p_L} = 79.75\,, \tag{18}$$

and an x-direction domain of $4\,\mathrm{mm} \leq x \leq 2\,\mathrm{mm}$ is used to capture the structure. A collision timescale of $\tau = 1 \times 10^{-7}\,\mathrm{s}$ is used. A more realistic collision frequency would only affect the size of the domain. The numerical solutions for the moment methods were produced using a first-order Discontinuous Galerkin (DG) scheme at a resolution of $10\,000$ cells, and were run until the solution converged to steady state. The reference solutions were produced by expensive direct numerical integration of the BGK kinetic equations, again solved using a first-order DG scheme. Due to the additional discretization of velocity space for the BGK model, the reference solutions are computed at a reduced resolution of 2048 cells, but with a resolution of 1000×500 cells in velocity space.

Figure 1 shows density and anisotropic temperature profiles through the shock wave. One can see that the moment model predicts a density profile that is in good agreement with the kinetic solution. Significant temperature anisotropies are observed, typically invisible for single-temperature models. As incoming particles that encounter the shock wave first experience a rise in kinetic energy in the direction



(a) Density profile



(b) Anisotropic temperature profiles

Figure 1: Mach 8 shock profiles as predicted by the twenty-moment closure and BGK equation

normal to the shock. This energy is then redistributed through a relaxation process. The moment method predictions are again in good agreement with the kinetic prediction. Small differences in shock-structure between the BGK and twenty-moment models are expected, but the twenty-moment prediction comes at a reduced computational cost while still capturing the non-equilibrium effects.

3.2 Multi-Dimensional Double Mach Reflection Prediction

The next case shows the robustness of the new method and solution procedure for multi-dimensional flows with strong interacting discontinuities. A double Mach reflection, previously studied by Deschambault and Glass [1] is considered. The situation involves the impingement of a shock wave with a Mach number of 7.1 on an wedge with an angle of $49°$. The ratio of the post-shock to pre-shock states is

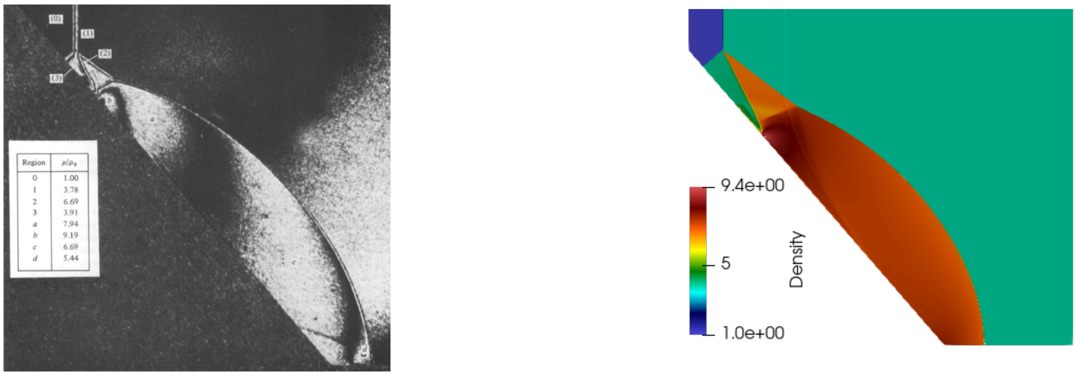
$$\frac{\rho_R}{\rho_L} = 3.775\,, \qquad \frac{u_{x_R}}{c_{x_L}} = 6.738\,, \qquad \frac{p_R}{p_L} = 62.76\,. \tag{19}$$

This flow produces a complex wave interaction including shock waves, slip steams, and triple points.

Preliminary numerical solutions were produced on a 2560×2048 grid, using a third-order-accurate discontinuous-Galerkin-Hancock scheme. Comparison between the experimental results of Deschambault and Glass and the twenty-moment numerical solution are presented in Figure 2. The density profiles show good agreement with the experimental results. The ability for this moment method to compute a complex, multi-dimensional flow problem with strong discontinuities demonstrates the robustness of both the model itself and the numerical method used to produce solutions.

4 Conclusion and Scope

This presentation briefly reviews the construction of the new twenty-moment model for non-equilibrium heat-conducting monatomic gas flows. This model offers an affordable and robust method for the prediction of general non-equilibrium gas flows. High-resolution solutions of the moment model are computed and used to investigate the non-equilibrium structure of inert shock waves and triple points. Comparisons with classical continuum models and experimental results are made. The degree to which non-equilibrium features are present and influence these flows are highlighted. Comments on extending the model to more settings, such as reactive flows, non-monatomic gases, and formulation of realistic boundary-conditions, conclude the talk.



(a) Experimental density profile [1]

(b) Numerical density profile

Figure 2: Double Mach reflection case, experimental and numerical results

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