3. Classical Method of Moments for Monatomic Gas

Coverage of this section:

- Overview of Moment Closure Methods
- Chapman-Enskog Method
- Grad's Method of Moments (Moment Closures)
- Recovery of Navier-Stokes Equations
- Order of Magnitude Approach
- Application of Classical Moment Methods
- Summary of Classical Moment Methods

3.1 Overview of Moment Closure Methods

3.1.1 Approximate Solution Method

- As discussed in the introduction to the course, moment closure methods essentially provide a means of constructing approximate solutions to the governing kinetic equation
- Generally involve approximating the NDF by some assumed form involving a number of free parameters, the latter which can be related to selected macroscopic quantities or moments associated with the NDF solution
- Rather than solving the kinetic equation directly, solutions are instead sought to the transport equations for the moments

3.1 Overview of Moment Closure Methods

3.1.2 Desirable Properties and Characteristics

- Moment closures provide complexity reduction with reduced models that bridge macroscopic and microscopic scales
- Moment equations present a number of other advantages:
  - mathematical
  - physical modelling
  - computational

Moment Closure Methods

Mathematical Advantages:

- reduction in dimensionality of the problem: much less complicated and expensive than direct-discretization and particle simulation techniques (e.g., DSMC and Lagrangian methods)
- if one is careful, mathematically elegant: well-defined entropy, fully-realizable moments, strictly hyperbolic transport equations (symmetric hyperbolic system, Godunov, 1961, classical Friedrichs-Lax hyperbolic system, Friedrichs & Lax, 1971)

Physical Modelling Advantages:

- finite propagation speeds for transport of solution information
- provides description of both near-equilibrium and extended description of more general non-equilibrium flows

Moment Closure Methods

Computational Advantages:

- first-order, quasi-linear hyperbolic systems with relaxation (source terms — potentially stiff)
- do not require discretization of second (or higher) derivatives (unlike conventional fluid treatments)
- well-suited for solution by schemes devised for hyperbolic conservation laws (e.g., Godunov-type finite-volume or discontinuous-Galerkin schemes)
- development of schemes which handle conservation equations of mixed type (i.e., with elliptic and hyperbolic nature) has proven difficult on irregular meshes
- can gain an extra order of spatial accuracy for the same reconstruction stencil when compared to PDEs involving second derivatives
- less sensitive to grid irregularities — more amenable to adaptive-mesh-refinement or embedded-boundary techniques

3.1 Overview of Moment Closure Methods

3.1.3 Maxwell's Equation of Change (Maxwell, 1867)

As a reminder, for a given macroscopic moment of interest, M, given by

$$M(\vec{x}, t) = \langle\, V(v_i)\mathcal{F}\,\rangle \;,$$

Maxwell's equation of change is given by

$$\frac{\partial}{\partial t}(M) + \frac{\partial}{\partial x_i}\left[\langle\, v_i V(v_i)\mathcal{F}\,\rangle\right] - \left\langle\, a_i \frac{\partial V}{\partial v_i}\mathcal{F}\,\right\rangle = \left\langle\, V(v_i)\frac{\delta \mathcal{F}}{\delta t}\,\right\rangle \;,$$

where the moment flux, F_i, is given by

$$F_i = \langle\, v_i V(v_i)\mathcal{F}\,\rangle \;.$$

The preceding is the so-called conservation form of Maxwell's equation of change.

3.1.3 Maxwell's Equation of Change

The non-conservation form of Maxwell's equation of change can be formulated for a macroscopic moment of interest, $M_\circ$, expressed in terms of the random particle velocity, c_i, and given by

$$M_\circ(\vec{x},t) = \langle\, V(c_i)\mathcal{F} \,\rangle \,,$$

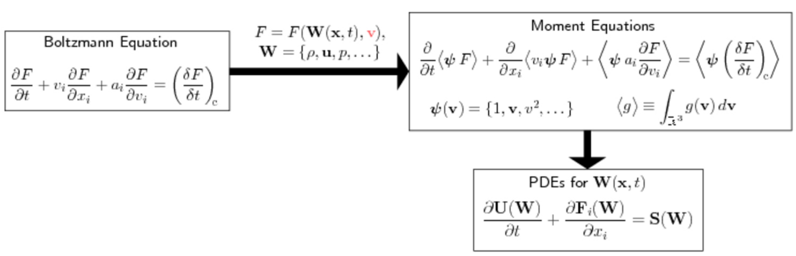
Maxwell's equation of change is given by

$$\begin{aligned}\frac{\partial}{\partial t}(M_\circ) + \frac{\partial}{\partial x_i}(u_i M_\circ) + \frac{\partial}{\partial x_i}\left[\langle\, c_i V(c_i)\mathcal{F} \,\rangle\right] \\ + \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right)\left[\left\langle \frac{\partial V}{\partial c_i}\mathcal{F} \right\rangle\right] + \frac{\partial u_i}{\partial x_j}\left[\left\langle c_j \frac{\partial V}{\partial c_i}\mathcal{F} \right\rangle\right] \\ - \left\langle a_i \frac{\partial V}{\partial c_i}\mathcal{F} \right\rangle = \left\langle V(c_i)\frac{\delta \mathcal{F}}{\delta t} \right\rangle \,,\end{aligned}$$

where the next higher-order moment flux is now given by

$$\langle\, c_i V(c_i)\mathcal{F} \,\rangle \,.$$

3.1 Overview of Moment Closure Methods



3.1.4 The Closure Problem

- Given a selected finite set of N velocity moments, $\mathbf{V}^{(N)} = [1, \vec{v}, \vec{v}\vec{v}, v^2, \dots]^{\mathrm{T}}$:

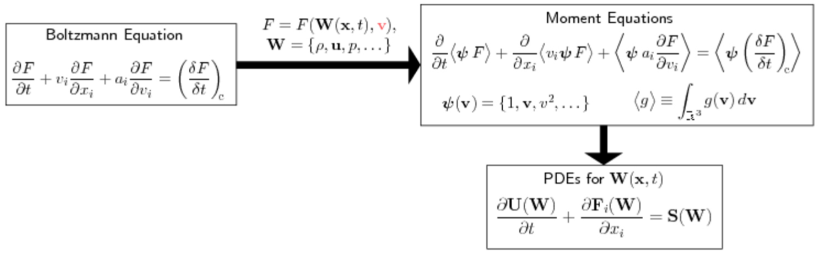
$$\mathbf{M}^{(N)} = m \iiint\limits_{\infty} \mathbf{V}^{(N)} \mathcal{F}(\vec{x},\vec{v},t)\,\mathrm{d}^3 v \;= \left\langle \mathbf{V}^{(N)}\mathcal{F} \right\rangle$$

- Resulting moment equations (first-order, quasi-linear, PDEs with relaxation):

$$\frac{\partial}{\partial t}\left(\mathbf{M}^{(N)}\right) + \vec{\nabla}\cdot\left\langle\, \vec{v}\,\mathbf{V}^{(N)}\mathcal{F} \,\right\rangle - \left\langle\, \vec{a}\cdot\left(\vec{\nabla}_v \mathbf{V}^{(N)}(\vec{v})\right)\mathcal{F} \,\right\rangle = \left\langle \mathbf{V}^{(N)}\frac{\delta \mathcal{F}}{\delta t} \right\rangle$$

- Unfortunately, an infinite set of moments is required to describe an arbitrary NDF associated with a non-equilibrium solution.

3.1.4 The Closure Problem



- Closure problem: next highest-order velocity moment must be specified
$$\vec{\mathbf{F}}^{(N)} = \left\langle \vec{v}\, \mathbf{V}^{(N)} \mathcal{F} \right\rangle = ?$$
- As we will see, closure is generally achived by assuming a form for $\mathcal{F}$
$$\mathcal{F} \approx \mathcal{F}^{(N)}(\vec{x}, \vec{v}, t; \mathbf{M}^{(N)})$$
- Closure is then provided by
$$\vec{\mathbf{F}}^{(N)} = \left\langle \vec{v}\, \mathbf{V}^{(N)} \mathcal{F} \right\rangle \approx \left\langle \vec{v}\, \mathbf{V}^{(N)} \mathcal{F}^{(N)}(\vec{v}; \mathbf{M}^{(N)}) \right\rangle$$

3.1 Overview of Moment Closure Methods

3.1.5 Difficulties and Challenges

- Formal convergence of the moment closure approach to the solution of the Boltzmann equation is difficult to show (general argument: the more moments the merrier!)
- Which moments should be included in the selected set and is there an optimal set?
- Closures can also suffer from some form of breakdown and/or loss of hyperbolicity
- Validity of the closures for full range of physically realizable moments can also be a challenge
- Finally, theres is a need for robust and efficient numerical solution schemes for the resulting moment equations

3.2 Chapman-Enskog Method

In this section of the course we will review so-called classical moment closure methods as represented by the method of Grad (1949). However prior to doing so, we will first review the Chapman-Enskog method. As discussed previously, this approximate solution technique for the Boltzmann equation predates the moment methods and is based on a formal perturbative expansion for the NDF, $\mathcal{F}$, and results in a hierarchy of increasingly more accurate approximate solutions to the kinetic equation.

3.2 Chapman-Enskog Method

3.2.1 BGK Kinetic Equation

Assuming that there are no external forces (i.e., $a_i = 0$) and adopting a relaxation time approximation for the collision operator of the type first proposed by Bhatnagar *et al.* (1954), the Chapman-Enskog method will be applied here to so-called BGK kinetic equation describing the time-evolution of the NDF, $\mathcal{F}$, given by

$$\frac{\partial \mathcal{F}}{\partial t} + v_i \frac{\partial \mathcal{F}}{\partial x_i} = \frac{\delta \mathcal{F}}{\delta t} = -\frac{\mathcal{F} - \mathcal{M}}{\tau}, \tag{1}$$

where $\mathcal{M}$ is the Maxwell-Boltzmann distribution function and τ is the characteristic relaxation time for collision processes. The Maxwell-Boltzmann distribution function is given by

$$\mathcal{M} = \frac{\rho}{m\,(2\pi p/\rho)^{3/2}} \exp\left(-\frac{1}{2}\frac{\rho c^2}{p}\right) = \frac{\rho}{m\,(2\pi\theta)^{3/2}} \exp\left(-\frac{1}{2}\frac{c^2}{\theta}\right), \tag{2}$$

where $\theta = p/\rho$.

3.2 Chapman-Enskog Method

3.2.2 Chapman-Enskog Perturbative Expansion Technique

In the Chapman-Enskog perturbative expansion technique approximate solutions to a scaled version of the kinetic equation

$$\frac{\partial \mathcal{F}}{\partial t} + v_i \frac{\partial \mathcal{F}}{\partial x_i} = -\frac{\mathcal{F} - \mathcal{M}}{\epsilon \tau}\,, \tag{3}$$

are sought which have the following form:

$$\mathcal{F} = \mathcal{M}\left(f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \epsilon^3 f^{(3)} + \ldots\right)\,, \tag{4}$$

where ϵ is a scaling parameter introduced for the purposes of the perturbative solution analysis with the understanding that $\epsilon \ll 1$. In general, $\epsilon \propto \mathrm{Kn}$. This implies that the relaxation time, τ, is small and that we are interested in perturbative solutions from local thermodynamic equilibrium. The corresponding solution to the unscaled kinetic equation (i.e., Eq. (1) given above) is then given by

$$\mathcal{F} = \mathcal{M}\left(f^{(0)} + f^{(1)} + f^{(2)} + f^{(3)} + \ldots\right)\,, \tag{5}$$

3.2.2 Chapman-Enskog Perturbative Expansion Technique

with the assumptions that

$$f^{(0)} = O(1)\,, \quad f^{(1)} = O(\epsilon)\,, \quad f^{(2)} = O(\epsilon^2)\,, \quad f^{(3)} = O(\epsilon^3)\,, \quad \text{etc.} \tag{6}$$

Substituting the scaled expansion into the scaled kinetic equation yields

$$\begin{aligned}
\mathcal{M}\frac{\left(f^{(0)} - 1\right)}{\tau} \quad &+ \quad \epsilon\left[\frac{\partial}{\partial t}\left(f^{(0)}\mathcal{M}\right) + v_i \frac{\partial}{\partial x_i}\left(f^{(0)}\mathcal{M}\right) + \frac{f^{(1)}\mathcal{M}}{\tau}\right] \\
&+ \quad \epsilon^2\left[\frac{\partial}{\partial t}\left(f^{(1)}\mathcal{M}\right) + v_i \frac{\partial}{\partial x_i}\left(f^{(1)}\mathcal{M}\right) + \frac{f^{(2)}\mathcal{M}}{\tau}\right] \\
&+ \quad \epsilon^3\left[\frac{\partial}{\partial t}\left(f^{(2)}\mathcal{M}\right) + v_i \frac{\partial}{\partial x_i}\left(f^{(2)}\mathcal{M}\right) + \frac{f^{(3)}\mathcal{M}}{\tau}\right] \\
&+ \quad \cdots \\
&= \quad 0\,.
\end{aligned} \tag{7}$$

For non-trivial solutions, require each term of this expansion for the kinetic equation in powers of ϵ to vanish.

3.2 Chapman-Enskog Method

3.2.2 Chapman-Enskog Perturbative Expansion Technique

At this point, it is very important to point out the distinctions between the Chapman-Enskog and Grad-type (moment closure) expansion techniques! The Chapman-Enskog approach is formally a perturbative expansion in a small parameter, with each term adding only the next higher-order correction to the solution. As will be shown, the Grad approach is a truncated power series expansion where each term can contain solution content of all orders.

3.2.3 Zeroth-Order Solution: The Euler Equations

To zeroth order in the small parameter, ϵ, the solution of the kinetic equation must satisfy

$$\mathcal{M}\frac{\left(f^{(0)}-1\right)}{\tau}=0\,. \tag{8}$$

This condition yields

$$f^{(0)}=1\,, \tag{9}$$

and

$$\mathcal{F}\approx\mathcal{M}\,, \tag{10}$$

3.2.4 Zeroth-Order Solution: The Euler Equations

where

$$\mathcal{M}=\mathcal{M}(\rho,u_i,p)=\mathcal{M}(\rho,u_i,\theta)\,. \tag{11}$$

Thus, to zeroth-order in ϵ, the particle NDF can be approximated by a local Maxwell-Boltzmann distribution, $\mathcal{M}$, which depends on the local values of ρ, u_i, and p (or θ). This is the so-called local thermal equilibrium (LTE) approximation. In this case, the unscaled kinetic equation can be written as

$$\frac{\partial\mathcal{M}}{\partial t}+v_i\frac{\partial\mathcal{M}}{\partial x_i}=0\,, \tag{12}$$

or

$$\frac{\partial\mathcal{M}}{\partial t}+(u_i+c_i)\frac{\partial\mathcal{M}}{\partial x_i}-\left[\frac{\partial u_i}{\partial t}+(u_j+c_j)\frac{\partial u_i}{\partial x_j}\right]\frac{\partial\mathcal{M}}{\partial c_i}=0\,. \tag{13}$$

The latter is the non-conservative form of the kinetic equation expressed in terms of the random particle velocity, c_i. Note that the value of the BGK collision operator is zero at this level of approximation. Moment equations describing the transport of ρ, u_i, and p (or θ) can be obtained taking the velocity moments m, mc_i, and $mc^2/2$ of the approximate kinetic equation.

3.2.4 Zeroth-Order Solution: The Euler Equations

These transport equations can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0\,, \tag{14}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} = 0\,, \tag{15}$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} = 0\,. \tag{16}$$

These well-known moment equations are referred to as the Euler equations governing inviscid gaseous flows and complete the specification of the zeroth-order solution.

3.2 Chapman-Enskog Method

3.2.5 First-Order Solution: The Navier-Stokes Equations

The first-order correction, $f^{(1)}$, to the zeroth-order result given above must satisfy

$$\frac{\partial \mathcal{M}}{\partial t} + v_i \frac{\partial \mathcal{M}}{\partial x_i} + \frac{f^{(1)}\mathcal{M}}{\tau} = 0\,. \tag{17}$$

This condition yields

$$f^{(1)} = -\frac{\tau}{\mathcal{M}}\left[\frac{\partial \mathcal{M}}{\partial t} + v_i \frac{\partial \mathcal{M}}{\partial x_i}\right]\,, \tag{18}$$

where the NDF is now approximated by

$$\mathcal{F} \approx \mathcal{M}\left(1 + f^{(1)}\right)\,. \tag{19}$$

Substituting this first-order approximation for the distribution function into the unscaled kinetic equation yields the following approximate kinetic equations:

$$\frac{\partial}{\partial t}\left[(1+f^{(1)})\mathcal{M}\right] + v_i \frac{\partial}{\partial x_i}\left[(1+f^{(1)})\mathcal{M}\right] = -\frac{f^{(1)}\mathcal{M}}{\tau}\,, \tag{20}$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

or

$$\frac{\partial}{\partial t}\left[(1+f^{(1)})\mathcal{M}\right] + (u_i + c_i)\frac{\partial}{\partial x_i}\left[(1+f^{(1)})\mathcal{M}\right] - \left[\frac{\partial u_i}{\partial t} + (u_j + c_j)\frac{\partial u_i}{\partial x_j}\right]\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right] = -\frac{f^{(1)}\mathcal{M}}{\tau}. \quad (21)$$

For consistency with the zeroth-order solution, it is required that

$$m\left\langle f^{(1)}\mathcal{M}\right\rangle = 0\,, \quad (22)$$

$$m\left\langle v_i f^{(1)}\mathcal{M}\right\rangle = 0\,, \quad m\left\langle c_i f^{(1)}\mathcal{M}\right\rangle = 0\,, \quad (23)$$

$$\frac{m}{2}\left\langle v^2 f^{(1)}\mathcal{M}\right\rangle = 0\,, \quad \frac{m}{2}\left\langle c^2 f^{(1)}\mathcal{M}\right\rangle = 0\,. \quad (24)$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

These consistency conditions follow from the definition of the Maxwellian, $\mathcal{M}$, for which

$$m\langle \mathcal{M}\rangle = \rho\,, \quad (25)$$

$$m\langle v_i\mathcal{M}\rangle = \rho u_i\,, \quad m\langle c_i\mathcal{M}\rangle = 0\,, \quad (26)$$

$$\frac{m}{2}\left\langle v^2\mathcal{M}\right\rangle = \frac{3}{2}p + \frac{1}{2}\rho u^2\,, \quad \frac{m}{2}\left\langle c^2\mathcal{M}\right\rangle = \frac{3}{2}p\,, \quad (27)$$

$$m\langle v_i v_j\mathcal{M}\rangle = \rho u_i u_j + \delta_{ij}p\,, \quad m\langle c_i c_j\mathcal{M}\rangle = \delta_{ij}p\,, \quad (28)$$

and the definitions of the velocity moments of any distribution function, for which we require that

$$m\left\langle (1+f^{(1)})\mathcal{M}\right\rangle = \rho\,, \quad (29)$$

$$m\left\langle v_i(1+f^{(1)})\mathcal{M}\right\rangle = \rho u_i\,, \quad m\left\langle c_i(1+f^{(1)})\mathcal{M}\right\rangle = 0\,, \quad (30)$$

$$\frac{m}{2}\left\langle v^2(1+f^{(1)})\mathcal{M}\right\rangle = \frac{3}{2}p + \frac{1}{2}\rho u^2\,, \quad \frac{m}{2}\left\langle c^2(1+f^{(1)})\mathcal{M}\right\rangle = \frac{3}{2}p\,, \quad (31)$$

in the case that $\mathcal{F} = \mathcal{M}(1+f^{(1)})$.

As with the zeroth-order approximation, if we now take velocity moments m, mc_i, and $mc^2/2$ of the non-conservative form of the approximate kinetic equation, the moment equations for the first-order solution can be obtained.

3.2.5 First-Order Solution: The Navier-Stokes Equations

For the continuity equation one can write

$$\left\langle m\frac{\partial}{\partial t}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle + \left\langle m\,(u_i+c_i)\,\frac{\partial}{\partial x_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle - \left\langle m\left[\frac{\partial u_i}{\partial t}+(u_j+c_j)\,\frac{\partial u_i}{\partial x_j}\right]\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle = -\left\langle m\frac{f^{(1)}\mathcal{M}}{\tau}\right\rangle,$$

which can then be evaluated in stages as follows:

$$\frac{\partial}{\partial t}\left\langle m(1+f^{(1)})\mathcal{M}\right\rangle + u_i\frac{\partial}{\partial x_i}\left\langle m(1+f^{(1)})\mathcal{M}\right\rangle + \frac{\partial}{\partial x_i}\left\langle mc_i(1+f^{(1)})\mathcal{M}\right\rangle - \left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left\langle m\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle - \frac{\partial u_i}{\partial x_j}\left\langle mc_j\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle = -\frac{1}{\tau}\left\langle mf^{(1)}\mathcal{M}\right\rangle,$$

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3.2.5 First-Order Solution: The Navier-Stokes Equations

$$\frac{\partial\rho}{\partial t}+u_i\frac{\partial\rho}{\partial x_i}-\frac{\partial u_i}{\partial x_j}\left\langle m\frac{\partial}{\partial c_i}\left[c_j(1+f^{(1)})\mathcal{M}\right]\right\rangle+\frac{\partial u_i}{\partial x_j}\left\langle m\frac{\partial c_j}{\partial c_i}(1+f^{(1)})\mathcal{M}\right\rangle=0,$$

$$\frac{\partial\rho}{\partial t}+u_i\frac{\partial\rho}{\partial x_i}+\rho\,\delta_{ij}\frac{\partial u_i}{\partial x_j}=0,$$

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0. \qquad (32)$$

For the momentum equation one can write

$$\left\langle mc_\alpha\frac{\partial}{\partial t}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle + \left\langle mc_\alpha\,(u_i+c_i)\,\frac{\partial}{\partial x_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle - \left\langle mc_\alpha\left[\frac{\partial u_i}{\partial t}+(u_j+c_j)\,\frac{\partial u_i}{\partial x_j}\right]\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle = -\left\langle mc_\alpha\frac{f^{(1)}\mathcal{M}}{\tau}\right\rangle,$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

which can then be evaluated in stages as follows:

$$
\begin{aligned}
\frac{\partial}{\partial t}\left\langle\, mc_\alpha(1+f^{(1)})\mathcal{M}\,\right\rangle + u_i\frac{\partial}{\partial x_i}\left\langle\, mc_\alpha(1+f^{(1)})\mathcal{M}\,\right\rangle & \\
+\frac{\partial}{\partial x_i}\left\langle\, mc_\alpha c_i(1+f^{(1)})\mathcal{M}\,\right\rangle & \\
-\left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left\langle\, mc_\alpha\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\,\right\rangle & \\
-\frac{\partial u_i}{\partial x_j}\left\langle\, mc_\alpha c_j\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\,\right\rangle & \\
=-\frac{1}{\tau}\left\langle\, mc_\alpha f^{(1)}\mathcal{M}\,\right\rangle\,, &
\end{aligned}
$$

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3.2.5 First-Order Solution: The Navier-Stokes Equations

$$
\begin{aligned}
\frac{\partial}{\partial x_i}\langle\, mc_\alpha c_i\mathcal{M}\,\rangle + \frac{\partial}{\partial x_i}\left\langle\, mc_\alpha c_i f^{(1)}\mathcal{M}\,\right\rangle & \\
-\left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left(\left\langle\, m\frac{\partial}{\partial c_i}\left[c_\alpha(1+f^{(1)})\mathcal{M}\right]\,\right\rangle\right. & \\
\left.-\left\langle\, m\frac{\partial c_\alpha}{\partial c_i}(1+f^{(1)})\mathcal{M}\,\right\rangle\right) & \\
-\frac{\partial u_i}{\partial x_j}\left(\left\langle\, m\frac{\partial}{\partial c_i}\left[c_\alpha c_j(1+f^{(1)})\mathcal{M}\right]\,\right\rangle\right. & \\
\left.-\left\langle\, m\frac{\partial}{\partial c_i}\left[c_\alpha c_j\right](1+f^{(1)})\mathcal{M}\,\right\rangle\right) & \\
=0\,, &
\end{aligned}
$$

$$
\delta_{i\alpha}\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_i}\left\langle\, mc_\alpha c_i f^{(1)}\mathcal{M}\,\right\rangle+\delta_{i\alpha}\left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\rho=0\,,
$$

$$
\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}+\frac{1}{\rho}\frac{\partial p}{\partial x_i}+\frac{1}{\rho}\frac{\partial}{\partial x_j}\left(m< c_i c_j f^{(1)}\mathcal{M}>\right)=0\,. \tag{33}
$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

And finally, for the energy equation one can write

$$\left\langle \frac{m}{2}c^2\frac{\partial}{\partial t}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle + \left\langle \frac{m}{2}c^2(u_i+c_i)\frac{\partial}{\partial x_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle - \left\langle \frac{m}{2}c^2\left[\frac{\partial u_i}{\partial t}+(u_j+c_j)\frac{\partial u_i}{\partial x_j}\right]\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle = -\left\langle \frac{m}{2}c^2\frac{f^{(1)}\mathcal{M}}{\tau}\right\rangle,$$

which can then be evaluated in stages as follows:

$$\frac{\partial}{\partial t}\left\langle \frac{m}{2}c^2(1+f^{(1)})\mathcal{M}\right\rangle + u_i\frac{\partial}{\partial x_i}\left\langle \frac{m}{2}c^2(1+f^{(1)})\mathcal{M}\right\rangle + \frac{\partial}{\partial x_i}\left\langle \frac{m}{2}c_ic^2(1+f^{(1)})\mathcal{M}\right\rangle - \left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left\langle \frac{m}{2}c^2\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle - \frac{\partial u_i}{\partial x_j}\left\langle \frac{m}{2}c_jc^2\frac{\partial}{\partial c_i}\left[(1+f^{(1)})\mathcal{M}\right]\right\rangle = -\frac{1}{\tau}\left\langle \frac{m}{2}c^2f^{(1)}\mathcal{M}\right\rangle,$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

$$\frac{3}{2}\frac{\partial p}{\partial t} + \frac{3}{2}u_i\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}\left\langle \frac{m}{2}c_ic^2\mathcal{M}\right\rangle + \frac{\partial}{\partial x_i}\left\langle \frac{m}{2}c_ic^2f^{(1)}\mathcal{M}\right\rangle - \left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left(\left\langle \frac{m}{2}\frac{\partial}{\partial c_i}\left[c^2(1+f^{(1)})\mathcal{M}\right]\right\rangle - \left\langle \frac{m}{2}\frac{\partial}{\partial c_i}\left[c^2\right](1+f^{(1)})\mathcal{M}\right\rangle\right) - \frac{\partial u_i}{\partial x_j}\left(\left\langle \frac{m}{2}\frac{\partial}{\partial c_i}\left[c_jc^2(1+f^{(1)})\mathcal{M}\right]\right\rangle - \left\langle \frac{m}{2}\frac{\partial}{\partial c_i}\left[c_jc^2\right](1+f^{(1)})\mathcal{M}\right\rangle\right) = 0\,,$$

$$\frac{\partial p}{\partial t} + u_i\frac{\partial p}{\partial x_i} + \frac{2}{3}\frac{\partial}{\partial x_i}\left\langle \frac{m}{2}c_ic^2f^{(1)}\mathcal{M}\right\rangle + \frac{2}{3}\left(\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}\right)\left\langle mc_i(1+f^{(1)})\mathcal{M}\right\rangle + \frac{2}{3}\delta_{ij}\frac{\partial u_i}{\partial x_j}\left\langle \frac{m}{2}c^2(1+f^{(1)})\mathcal{M}\right\rangle + \frac{2}{3}\frac{\partial u_i}{\partial x_j}\left\langle mc_ic_j(1+f^{(1)})\mathcal{M}\right\rangle = 0\,,$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{2}{3}\frac{\partial}{\partial x_i}\left\langle \frac{m}{2} c_i c^2 f^{(1)} \mathcal{M} \right\rangle + p\frac{\partial u_i}{\partial x_i} + \frac{2}{3}\delta_{ij} p \frac{\partial u_i}{\partial x_j} + \frac{2}{3}\left\langle m c_i c_j f^{(1)} \mathcal{M} \right\rangle \frac{\partial u_i}{\partial x_j} = 0 ,$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} + \frac{2}{3}\frac{\partial}{\partial x_i}\left\langle \frac{m}{2} c_i c^2 f^{(1)} \mathcal{M} \right\rangle + \frac{2}{3}\left\langle m c_i c_j f^{(1)} \mathcal{M} \right\rangle \frac{\partial u_i}{\partial x_j} = 0 . \quad (34)$$

Defining the fluid stresses, τ_{ij}, and heat flux, q_i, to be

$$m\left\langle c_i c_j f^{(1)} \mathcal{M} \right\rangle = -\tau_{ij} , \quad (35)$$

$$\frac{m}{2}\left\langle c_i c^2 f^{(1)} \mathcal{M} \right\rangle = q_i , \quad (36)$$

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3.2.5 First-Order Solution: The Navier-Stokes Equations

the continuity, momentum, and energy equations for the first-order solution can be summarized as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 , \quad (37)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0 , \quad (38)$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} + \frac{2}{3}\frac{\partial q_i}{\partial x_i} - \frac{2}{3}\tau_{ij}\frac{\partial u_i}{\partial x_j} = 0 . \quad (39)$$

These are the well-known Navier-Stokes equations, which describe the time evolution of the velocity moments ρ, u_i, and p.

In order to complete the description of the first-order solution, all that remains is to determine $f^{(1)}$ and calculate expressions for the fluid stresses and heat flux.

3.2.5 First-Order Solution: The Navier-Stokes Equations

From Eq. (18) and using the fact that $\mathcal{M} = \mathcal{M}(\rho, u_i, \theta)$, can write

$$
\begin{aligned}
f^{(1)} &= -\frac{\tau}{\mathcal{M}}\left[\frac{\partial \mathcal{M}}{\partial \rho}\left(\frac{\partial \rho}{\partial t} + v_i \frac{\partial \rho}{\partial x_i}\right) + \frac{\partial \mathcal{M}}{\partial u_\alpha}\left(\frac{\partial u_\alpha}{\partial t} + v_i \frac{\partial u_\alpha}{\partial x_i}\right)\right. \\
&\qquad \left. + \frac{\partial \mathcal{M}}{\partial \theta}\left(\frac{\partial \theta}{\partial t} + v_i \frac{\partial \theta}{\partial x_i}\right)\right], \\
&= -\frac{\tau}{\mathcal{M}}\left[\frac{\partial \mathcal{M}}{\partial \rho}\left(\frac{\partial \rho}{\partial t} + [u_i + c_i] \frac{\partial \rho}{\partial x_i}\right) + \frac{\partial \mathcal{M}}{\partial u_\alpha}\left(\frac{\partial u_\alpha}{\partial t} + [u_i + c_i] \frac{\partial u_\alpha}{\partial x_i}\right)\right. \\
&\qquad \left. + \frac{\partial \mathcal{M}}{\partial \theta}\left(\frac{\partial \theta}{\partial t} + [u_i + c_i] \frac{\partial \theta}{\partial x_i}\right)\right], \\
&= -\frac{\tau}{\mathcal{M}}\left[\frac{\partial \mathcal{M}}{\partial \rho}\left(\frac{\partial \rho}{\partial t} + [u_i + c_i] \frac{\partial \rho}{\partial x_i}\right) + \frac{\partial \mathcal{M}}{\partial u_\alpha}\left(\frac{\partial u_\alpha}{\partial t} + [u_i + c_i] \frac{\partial u_\alpha}{\partial x_i}\right)\right. \\
&\qquad \left. + \frac{1}{\rho}\frac{\partial \mathcal{M}}{\partial \theta}\left(\frac{\partial p}{\partial t} + [u_i + c_i] \frac{\partial p}{\partial x_i}\right) - \frac{p}{\rho^2}\frac{\partial \mathcal{M}}{\partial \theta}\left(\frac{\partial \rho}{\partial t} + [u_i + c_i] \frac{\partial \rho}{\partial x_i}\right)\right], \\
&= -\frac{\tau}{\mathcal{M}}\left[\left(\frac{\partial \mathcal{M}}{\partial \rho} - \frac{p}{\rho^2}\frac{\partial \mathcal{M}}{\partial \theta}\right)\left(\frac{\partial \rho}{\partial t} + [u_i + c_i] \frac{\partial \rho}{\partial x_i}\right)\right. \\
&\qquad \left. + \frac{\partial \mathcal{M}}{\partial u_\alpha}\left(\frac{\partial u_\alpha}{\partial t} + [u_i + c_i] \frac{\partial u_\alpha}{\partial x_i}\right) + \frac{1}{\rho}\frac{\partial \mathcal{M}}{\partial \theta}\left(\frac{\partial p}{\partial t} + [u_i + c_i] \frac{\partial p}{\partial x_i}\right)\right], \quad (40)
\end{aligned}
$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

The next step is to use the zeroth-order moment equations (i.e., the Euler equations) to evaluate the convective derivatives of ρ, u_i, and p. This is an important approximation in the Chapman-Enskog technique. One can then rewrite the expression for $f^{(1)}$ given above as

$$
\begin{aligned}
f^{(1)} &= -\frac{\tau}{\mathcal{M}}\left[\left(\frac{\partial \mathcal{M}}{\partial \rho} - \frac{p}{\rho^2}\frac{\partial \mathcal{M}}{\partial \theta}\right)\left(-\rho \frac{\partial u_i}{\partial x_i} + c_i \frac{\partial \rho}{\partial x_i}\right)\right. \\
&\qquad \left. + \frac{\partial \mathcal{M}}{\partial u_\alpha}\left(-\frac{1}{\rho}\frac{\partial p}{\partial x_\alpha} + c_i \frac{\partial u_\alpha}{\partial x_i}\right) + \frac{1}{\rho}\frac{\partial \mathcal{M}}{\partial \theta}\left(-\frac{5}{3} p \frac{\partial u_i}{\partial x_i} + c_i \frac{\partial p}{\partial x_i}\right)\right]. \quad (41)
\end{aligned}
$$

Now, the derivatives of the Maxwell-Boltzmann NDF must be evaluated. From Eq. (2), it follows that

$$
\ln \mathcal{M} = \ln \rho - \frac{3}{2}\ln \theta - \frac{1}{2}\frac{c^2}{\theta} - \ln\left[m\,(2\pi)^{3/2}\right], \quad (42)
$$

and hence

$$
\frac{1}{\mathcal{M}}\frac{\partial \mathcal{M}}{\partial \rho} = \frac{1}{\rho}, \quad (43)
$$

$$
\frac{1}{\mathcal{M}}\frac{\partial \mathcal{M}}{\partial u_i} = -\frac{c_i}{\theta}\frac{\partial c_i}{\partial u_i} = \frac{c_i}{\theta} = \frac{\rho c_i}{p}, \quad (44)
$$

$$
\frac{1}{\mathcal{M}}\frac{\partial \mathcal{M}}{\partial \theta} = -\frac{3}{2\theta} + \frac{c^2}{2\theta^2} = -\frac{3\rho}{2p} + \frac{\rho^2 c^2}{2p^2}. \quad (45)
$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

Substituting these expressions for the derivatives of $\mathcal{M}$ into the equation for $f^{(1)}$ can write

$$\begin{aligned} f^{(1)} &= -\tau\left[\frac{1}{\rho}\left(\frac{5}{2}-\frac{\rho c^2}{2p}\right)\left(-\rho\frac{\partial u_i}{\partial x_i}+c_i\frac{\partial \rho}{\partial x_i}\right)+\frac{\rho c_\alpha}{p}\left(-\frac{1}{\rho}\frac{\partial p}{\partial x_\alpha}+c_i\frac{\partial u_\alpha}{\partial x_i}\right)\right. \\ &\quad \left.+\frac{1}{\rho}\left(-\frac{3\rho}{2p}+\frac{\rho^2 c^2}{2p^2}\right)\left(-\frac{5}{3}p\frac{\partial u_i}{\partial x_i}+c_i\frac{\partial p}{\partial x_i}\right)\right] \\ &= -\tau\left[\left(\frac{\rho^2}{2p^2}c_i c^2-\frac{5\rho}{2p}c_i\right)\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)+\frac{\rho}{p}c_i c_j\frac{\partial u_j}{\partial x_i}-\frac{\rho}{3p}c^2\frac{\partial u_i}{\partial x_i}\right]. \qquad (46) \end{aligned}$$

Noting that

$$\frac{\rho}{p}c_i c_j\frac{\partial u_j}{\partial x_i}=\frac{\rho}{2p}c_i c_j\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right),$$

the final expression for $f^{(1)}$ can be obtained and written as

$$f^{(1)}=-\tau\left[\left(\frac{\rho^2}{2p^2}c_\alpha c^2-\frac{5\rho}{2p}c_\alpha\right)\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right)+\frac{\rho}{2p}c_\alpha c_\beta\left(\frac{\partial u_\beta}{\partial x_\alpha}+\frac{\partial u_\alpha}{\partial x_\beta}\right)-\frac{\rho}{3p}c^2\frac{\partial u_\alpha}{\partial x_\alpha}\right]. \qquad (47)$$

Note the change of indices.

3.2.5 First-Order Solution: The Navier-Stokes Equations

Finally, using the definitions of the fluid stresses and heat flux given by Eqs. (35) and (36), can write

$$\begin{aligned} \tau_{ij} &= -m\left\langle\, c_i c_j f^{(1)}\mathcal{M}\,\right\rangle \\ &= m\tau\left\langle\, c_i c_j\left[\frac{\rho}{2p}c_\alpha c_\beta\left(\frac{\partial u_\beta}{\partial x_\alpha}+\frac{\partial u_\alpha}{\partial x_\beta}\right)-\frac{\rho}{3p}c^2\frac{\partial u_\alpha}{\partial x_\alpha}\right]\mathcal{M}\,\right\rangle \\ &= \frac{\rho\tau}{2p}\,m\,\langle\, c_i c_j c_\alpha c_\beta\mathcal{M}\,\rangle\left(\frac{\partial u_\beta}{\partial x_\alpha}+\frac{\partial u_\alpha}{\partial x_\beta}\right)-\frac{\rho\tau}{3p}\,m\left\langle\, c_i c_j c^2\mathcal{M}\,\right\rangle\frac{\partial u_\alpha}{\partial x_\alpha} \\ &= \frac{\rho\tau}{2p}\frac{p^2}{\rho}\left[\delta_{ij}\delta_{\alpha\beta}+\delta_{i\alpha}\delta_{j\beta}+\delta_{i\beta}\delta_{\alpha j}\right]\left(\frac{\partial u_\beta}{\partial x_\alpha}+\frac{\partial u_\alpha}{\partial x_\beta}\right) \\ &\quad -\frac{\rho\tau}{3p}\frac{p^2}{\rho}\left[\delta_{ij}\delta_{\beta\beta}+2\delta_{i\beta}\delta_{j\beta}\right]\frac{\partial u_\alpha}{\partial x_\alpha} \\ &= \tau p\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\tau p\,\delta_{ij}\frac{\partial u_\alpha}{\partial x_\alpha} \\ &= \mu\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_\alpha}{\partial x_\alpha}\right], \qquad (48) \end{aligned}$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

$$
\begin{aligned}
q_i &= \frac{m}{2}\left\langle c_i c^2 f^{(1)}\mathcal{M}\right\rangle \\
&= -\frac{m}{2}\tau\left\langle c_i c^2\left(\frac{\rho^2}{2p^2}c_\alpha c^2 - \frac{5\rho}{2p}c_\alpha\right)\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right)\mathcal{M}\right\rangle \\
&= -\frac{\rho^2\tau}{4p^2}m\left\langle c_i c_\alpha c^4\mathcal{M}\right\rangle\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right) + \frac{5\rho\tau}{4p}m\left\langle c_i c_\alpha c^2\mathcal{M}\right\rangle\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right) \\
&= -\frac{\rho^2\tau}{4p^2}\frac{p^3}{\rho^2}\left[35\delta_{i\alpha}\right]\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right) + \frac{5\rho\tau}{4p}\frac{p^2}{\rho}\left[\delta_{i\alpha}\delta_{\beta\beta} + 2\delta_{i\beta}\delta_{\alpha\beta}\right]\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right) \\
&= -\frac{35\tau p}{4}\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right) + \frac{5\tau p}{4}\left[3\delta_{i\alpha} + 2\delta_{i\alpha}\right]\frac{\partial}{\partial x_\alpha}\left(\frac{p}{\rho}\right) \\
&= -\frac{5\tau p}{2}\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right) \\
&= -\kappa\frac{\partial T}{\partial x_i}\,,
\end{aligned}
\tag{49}
$$

where $\mu = \tau p$ is the dynamic viscosity and $\kappa = 5k\tau p/(2m)$ is the thermal conductivity.

3.2.5 First-Order Solution: The Navier-Stokes Equations

The preceding expressions for the fluid stresses and heat flux vector are identical to those given previously for the Navier-Stokes equations and showing that the first-order Chapman-Enskog solution recovers the conventional fluid-dynamic limit as well as providing expressions for the transport coefficients.

An important limitation of the BGK or relaxation time collision operator is revealed by determining the Prandtl number based on the transport coefficients, μ and κ, given above. By definition the Prandtl number is

$$\mathrm{Pr} = \frac{\mu C_p}{\kappa}\,. \tag{50}$$

For a monatomic ideal gas, the specific heat at constant pressure is $C_p = \gamma R/(\gamma-1) = 5R/2 = 5k/(2m)$. Using this value for C_p and the expressions for μ and κ given above can write

$$\mathrm{Pr} = \frac{(5)2mk\tau p}{(5)2mk\tau p} = 1\,. \tag{51}$$

3.2.5 First-Order Solution: The Navier-Stokes Equations

From this it can be seen that the use of a single relaxation time in the BGK collision operator is equivalent to assuming that the Prandtl number, which is essentially the ratio of relaxation time for the diffusion of momentum to the relaxation time for the diffusion of internal energy, is unity. As only one relaxation time is introduced in the model this should be expected. In actuality, most gases have a Prandtl number somewhat less than one. A value near 0.70 is typical. The use of a hard sphere inverse potential for the collision operator yields a Prandtl number of two thirds (2/3).

3.2 Chapman-Enskog Method

3.2.6 Higher-Order Solutions

The Chapman-Enskog technique can be continued to include more and more terms in the perturbative expansion. To second- and third-order in the small parameter, ϵ, the approximate solutions of the Boltzmann equation satisfy the Burnett and super-Burnett equations, respectively, with a BGK collision operator. However, one should be cautioned that the resulting expressions for the constitutive relations become more complex and non-linear. For example,

$$\tau_{ij} = \tau_{ij}^{(0)} + \tau_{ij}^{(1)} + \tau_{ij}^{(2)} \,,$$

$$\tau_{ij}^{(0)} = 0 \,, \quad \tau_{ij}^{(1)} = \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_\alpha}{\partial x_\alpha} \right] \,,$$

$$\tau_{ij}^{(2)} = -\beta_\rho \frac{\partial^2 \rho}{\partial x_i \partial x_j} + \beta_T \frac{\partial^2 T}{\partial x_i \partial x_j} + \beta_{2,\rho} \left(\frac{\partial \rho}{\partial x_i} \right) \frac{\partial \rho}{\partial x_i} + \cdots + \,.$$

Furthermore, the inherent stability of the resulting equations has been shown to be problematic.

3.3 Grad's Method of Moments (Moment Closures)

The method of moments as originally proposed by Grad (1949) is the best known alternative to the Chapman-Enskog method described previously. Although the original approach was formulated as either a 20-moment or 13-moment closure, Grad's method can actually be thought of as a hierarchy of moment closures which includes:

- 26-Moment Closure
- 20-Moment Closure
- 13-Moment Closure
- 10-Moment Closure (equivalent to Gaussian Closure)
- 8-Moment Closure
- 5-Moment Closure (equilibrium solution, Euler Equations)

among others.

3.3 Grad's Method of Moments (Moment Closures)

3.3.1 20-Moment Closure

We will begin the discussion of the Grad methods by considering the 20-moment closure.

3.3.1 20-Moment Closure

Selected Moments

In the Grad 20-moment closure, the following set of total velocity weights is considered:

$$\mathbf{V}^{(20)}(v_i) = m\,[1, v_i, v_i v_j, v_i v_j v_k]^{\mathrm{T}} \,,$$

or the following set of random velocity weights:

$$\mathbf{V}^{(20)}(c_i) = m\,[1, c_i, c_i c_j, c_i c_j c_k]^{\mathrm{T}} \,.$$

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3.3.1 20-Moment Closure

Selected Moments

These choices correspond to the following selected macroscopic quantities:

$$
\begin{aligned}
&m \langle\, \mathcal{F} \,\rangle = \rho \,, \\
&m \langle\, v_i \mathcal{F} \,\rangle = \rho u_i \,, \\
&m \langle\, v_i v_j \mathcal{F} \,\rangle = \rho u_i u_j + P_{ij} \,, \\
&m \langle\, v_i v_j v_k \mathcal{F} \,\rangle = \rho u_i u_j u_k + P_{ij} u_k + P_{ik} u_j + P_{jk} u_i + Q_{ijk} \,,
\end{aligned}
$$

3.3.1 20-Moment Closure

Selected Moments

or

$$m \langle \mathcal{F} \rangle = \rho\,,$$
$$m \langle c_i \mathcal{F} \rangle = 0\,,$$
$$m \langle c_i c_j \mathcal{F} \rangle = P_{ij} = p\delta_{ij} - \tau_{ij}\,,$$
$$m \langle c_i c_j c_k \mathcal{F} \rangle = Q_{ijk}\,,$$

with

$$\mathbf{M}^{(20)} = [\rho, \rho u_i, \rho u_i u_j + P_{ij}, \rho u_i u_j u_k + P_{ij} u_k + P_{ik} u_j + P_{jk} u_i + Q_{ijk}]^{\mathrm{T}}\,,$$

and

$$\mathbf{W}^{(20)} = [\rho, u_i, P_{ij}, Q_{ijk}]^{\mathrm{T}}\,.$$

The former correspond to conserved variables and the latter will be referred to as primitive variables.

3.3.1 20-Moment Closure

Assumed Form for the NDF

Grad originally constructed the 20-moment closure by assuming an approximate form for the NDF, $\mathcal{F}$, in terms of polynomial series expansion in velocity space in terms of Hermite polynomials, a family of orthogonal polynomials. The use of Hermite polynomials was helpful in determine where to truncate the polynomial series expansion but is not required in order to derive the closure. Here a regular polynomial approximation or truncated power series will be used in deriving the closure.

3.3.1 20-Moment Closure

Assumed Form for the NDF

In the Grad 20-moment closure, it is assumed that

$$\mathcal{F} \approx \mathcal{F}^{(20)}(x_i, c_i, t; \rho, u_i, P_{ij}, Q_{ijk})$$
$$= \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3}) \left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_{\alpha\beta\gamma}\, c_\alpha c_\beta c_\gamma\right] ,$$

where the coefficients of the truncated power series, A_α (3 values), $B_{\alpha\beta}$ (6 values), and $D_{\alpha\beta\gamma}$ (10 values), are specified by relating them to the 20 selected or known moments for the closure. These are the so-called moment constraints on the assumed form for the NDF. Note that the preceding polynomial contains all terms up to degree three in c_i and all higher degree terms (i.e., degree 4 and above) are dropped or neglected.

3.3.1 20-Moment Closure

Moment Constraints on $\mathcal{F}^{(20)}$

The moment constraints on $\mathcal{F}^{(20)}$ are as follows:

$$m \left\langle \mathcal{F}^{(20)} \right\rangle = \rho \,,$$
$$m \left\langle c_i \mathcal{F}^{(20)} \right\rangle = 0 \,,$$
$$m \left\langle c_i c_j \mathcal{F}^{(20)} \right\rangle = P_{ij} = p\delta_{ij} - \tau_{ij} \,,$$
$$m \left\langle c_i c_j c_k \mathcal{F}^{(20)} \right\rangle = Q_{ijk} \,.$$

Moment Constraints on $\mathcal{F}^{(20)}$

If we consider the first constraint, we have

$$\begin{aligned}
\rho &= m \left\langle \mathcal{F}^{(20)} \right\rangle \\
&= m \langle \mathcal{M} [1 + A_\alpha c_\alpha + B_{\alpha\beta} c_\alpha c_\beta + D_{\alpha\beta\gamma} c_\alpha c_\beta c_\gamma] \rangle \\
&= m \langle \mathcal{M} \rangle + A_\alpha m \langle c_\alpha \mathcal{M} \rangle + B_{\alpha\beta} m \langle c_\alpha c_\beta \mathcal{M} \rangle \\
&\quad + D_{\alpha\beta\gamma} m \langle c_\alpha c_\beta c_\gamma \mathcal{M} \rangle \\
&= m \langle \mathcal{M} \rangle + B_{\alpha\beta} m \langle c_\alpha c_\beta \mathcal{M} \rangle \\
&= \rho + B_{\alpha\beta} p \delta_{\alpha\beta} \\
&= \rho + B_{\alpha\alpha} p \\
0 &= B_{\alpha\alpha} p \,,
\end{aligned}$$

or

$$B_{\alpha\alpha} = 0 \,. \tag{52}$$

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Moment Constraints on $\mathcal{F}^{(20)}$

If we consider the second constraint, we have

$$\begin{aligned}
0 &= m \left\langle c_i \mathcal{F}^{(20)} \right\rangle \\
&= m \langle c_i \mathcal{M} [1 + A_\alpha c_\alpha + B_{\alpha\beta} c_\alpha c_\beta + D_{\alpha\beta\gamma} c_\alpha c_\beta c_\gamma] \rangle \\
&= m \langle c_i \mathcal{M} \rangle + A_\alpha m \langle c_i c_\alpha \mathcal{M} \rangle + B_{\alpha\beta} m \langle c_i c_\alpha c_\beta \mathcal{M} \rangle \\
&\quad + D_{\alpha\beta\gamma} m \langle c_i c_\alpha c_\beta c_\gamma \mathcal{M} \rangle \\
&= A_\alpha m \langle c_i c_\alpha \mathcal{M} \rangle + D_{\alpha\beta\gamma} m \langle c_i c_\alpha c_\beta c_\gamma \mathcal{M} \rangle \\
&= A_\alpha p \delta_{i\alpha} + D_{\alpha\beta\gamma} \frac{p^2}{\rho} [\delta_{i\alpha}\delta_{\beta\gamma} + \delta_{i\beta}\delta_{\alpha\gamma} + \delta_{i\gamma}\delta_{\alpha\beta}] \\
&= A_i p + D_{i\beta\beta} \frac{p^2}{\rho} + D_{\alpha i\alpha} \frac{p^2}{\rho} + D_{\alpha\alpha i} \frac{p^2}{\rho} \\
0 &= A_i + \frac{3p}{\rho} D_{i\alpha\alpha} \,,
\end{aligned}$$

or

$$A_i + \frac{3p}{\rho} D_{i\alpha\alpha} = 0 \,. \tag{53}$$

Moment Constraints on $\mathcal{F}^{(20)}$

If we consider the third constraint, we have

$$\begin{aligned}
p\delta_{ij} - \tau_{ij} &= m \left\langle\, c_i c_j \mathcal{F}^{(20)} \,\right\rangle \\
&= m \langle\, c_i c_j \mathcal{M} \left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_{\alpha\beta\gamma}\, c_\alpha c_\beta c_\gamma\right] \rangle \\
&= m \langle\, c_i c_j \mathcal{M} \,\rangle + A_\alpha m \langle\, c_i c_j c_\alpha \mathcal{M} \,\rangle + B_{\alpha\beta} m \langle\, c_i c_j c_\alpha c_\beta \mathcal{M} \,\rangle \\
&\quad + D_{\alpha\beta\gamma} m \langle\, c_i c_j c_\alpha c_\beta c_\gamma \mathcal{M} \,\rangle \\
&= m \langle\, c_i c_j \mathcal{M} \,\rangle + B_{\alpha\beta} m \langle\, c_i c_j c_\alpha c_\beta \mathcal{M} \,\rangle \\
&= p\delta_{ij} + B_{\alpha\beta} \frac{p^2}{\rho} \left[\delta_{ij}\delta_{\alpha\beta} + \delta_{i\alpha}\delta_{j\beta} + \delta_{i\beta}\delta_{j\alpha}\right] \\
-\tau_{ij} &= B_{\alpha\alpha} \frac{p^2}{\rho} \delta_{ij} + B_{ij} \frac{p^2}{\rho} + B_{ji} \frac{p^2}{\rho} \\
\tau_{ij} &= -2 \frac{p^2}{\rho} B_{ij} \,,
\end{aligned}$$

or

$$\tau_{ij} = -2 \frac{p^2}{\rho} B_{ij} \,. \tag{54}$$

Moment Constraints on $\mathcal{F}^{(20)}$

If we consider the fourth and final constraint, we have

$$\begin{aligned}
Q_{ijK} &= m \left\langle\, c_i c_j c_k \mathcal{F}^{(20)} \,\right\rangle \\
&= m \langle\, c_i c_j c_k \mathcal{M} \left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_{\alpha\beta\gamma}\, c_\alpha c_\beta c_\gamma\right] \rangle \\
&= m \langle\, c_i c_j c_k \mathcal{M} \,\rangle + A_\alpha m \langle\, c_i c_j c_k c_\alpha \mathcal{M} \,\rangle + B_{\alpha\beta} m \langle\, c_i c_j c_k c_\alpha c_\beta \mathcal{M} \,\rangle \\
&\quad + D_{\alpha\beta\gamma} m \langle\, c_i c_j c_k c_\alpha c_\beta c_\gamma \mathcal{M} \,\rangle \\
&= A_\alpha m \langle\, c_i c_j c_k c_\alpha \mathcal{M} \,\rangle + D_{\alpha\beta\gamma} m \langle\, c_i c_j c_k c_\alpha c_\beta c_\gamma \mathcal{M} \,\rangle \\
&= A_\alpha \frac{p^2}{\rho} \left[\delta_{ij}\delta_{k\alpha} + \delta_{ik}\delta_{j\alpha} + \delta_{i\alpha}\delta_{jk}\right] + D_{\alpha\beta\gamma} \frac{p^3}{\rho^2} \left\{\delta_{ij}\delta_{k\alpha}\delta_{\beta\gamma}\right\}^{(15)}_{[ijk\alpha\beta\gamma]} \\
&= A_k \frac{p^2}{\rho} \delta_{ij} + A_j \frac{p^2}{\rho} \delta_{ik} + A_i \frac{p^2}{\rho} \delta_{jk} + D_{\alpha\beta\gamma} \frac{p^3}{\rho^2} \left\{\delta_{ij}\delta_{k\alpha}\delta_{\beta\gamma}\right\}^{(15)}_{[ijk\alpha\beta\gamma]} \\
&= 6 \frac{p^3}{\rho^2} D_{ijk} \,,
\end{aligned}$$

or

$$Q_{ijK} = 6 \frac{p^3}{\rho^2} D_{ijk} \,. \tag{55}$$

3.3.1 20-Moment Closure

Final Form for 20-Moment NDF

Using the preceding expressions for the coefficients, A_α, $B_{\alpha\beta}$, and $D_{\alpha\beta\gamma}$ the following expression can be obtained for $\mathcal{F}^{(20)}$:

$$\begin{aligned}\mathcal{F}^{(20)}&(x_i, c_i, t; \rho, u_i, P_{ij}, Q_{ijk})\\ &= \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3}) \left[1 + \frac{\rho}{2p^2}\left(p_{ij} - p\delta_{ij}\right)\, c_\alpha c_\beta \right.\\ &\qquad \left. + \frac{\rho^2}{6p^3}\left(Q_{\alpha\beta\gamma} c_\beta c_\gamma - \frac{3p}{\rho} Q_{\alpha\beta\beta}\right) c_\alpha\right] ,\end{aligned}$$

or

$$\begin{aligned}\mathcal{F}^{(20)}&(x_i, c_i, t; \rho, u_i, \tau_{ij}, Q_{ijk})\\ &= \mathcal{M}(\rho, u_i, p) \left[1 - \frac{\rho}{2p^2}\tau_{ij}\, c_\alpha c_\beta \right.\\ &\qquad \left. + \frac{\rho^2}{6p^3}\left(Q_{\alpha\beta\gamma} c_\beta c_\gamma - \frac{3p}{\rho} Q_{\alpha\beta\beta}\right) c_\alpha\right] .\end{aligned}$$

3.3.1 20-Moment Closure

Moment Equations

The non-conservation form of the moment equations for the 20-moment closure may then be derived by using the non-conservation form of Maxwell's equation of change which, using the relaxation-time or BGK collision operator and assuming $a_i = 0$, is given by

$$\begin{aligned}&\frac{\partial}{\partial t}(M_\circ) + \frac{\partial}{\partial x_i}(u_i M_\circ) + \frac{\partial}{\partial x_i}\left[\left\langle\, c_i V(c_i)\mathcal{F}^{(20)}\,\right\rangle\right]\\ &\quad + \left(\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j}\right)\left[\left\langle\, \frac{\partial V}{\partial c_i}\mathcal{F}^{(20)}\,\right\rangle\right] + \frac{\partial u_i}{\partial x_j}\left[\left\langle\, c_j\frac{\partial V}{\partial c_i}\mathcal{F}^{(20)}\,\right\rangle\right]\\ &\quad = -\frac{1}{\tau}\left[M_\circ - \langle\, V(c_i)\mathcal{M}\,\rangle\right] ,\end{aligned}$$

with

$$M_\circ(\vec{x}, t) = \left\langle\, V(c_i)\mathcal{F}^{(20)}\,\right\rangle , \quad \text{and} \quad V \in \mathbf{V}^{(20)}(c_i) = m\left[1, c_i, c_i c_j, c_i c_j c_k\right]^{\mathrm{T}} ,$$

3.3.1 20-Moment Closure

Moment Equations

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0\,,$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial P_{ij}}{\partial x_j} = \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0\,,$$

$$\frac{\partial P_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(u_k P_{ij}) + P_{jk}\frac{\partial u_i}{\partial x_k} + P_{ik}\frac{\partial u_j}{\partial x_k} + \frac{\partial Q_{ijk}}{\partial x_k} = -\frac{1}{\tau}(P_{ij} - p\delta_{ij}) = \frac{1}{\tau}\tau_{ij}\,,$$

$$\frac{\partial Q_{ijk}}{\partial t} + \frac{\partial}{\partial x_l}(u_l Q_{ijk}) + Q_{jkl}\frac{\partial u_i}{\partial x_l} + Q_{ikl}\frac{\partial u_j}{\partial x_l} + Q_{ijl}\frac{\partial u_k}{\partial x_l}$$
$$- \frac{P_{jk}}{\rho}\frac{\partial P_{il}}{\partial x_l} - \frac{P_{ik}}{\rho}\frac{\partial P_{jl}}{\partial x_l} - \frac{P_{ij}}{\rho}\frac{\partial P_{kl}}{\partial x_l} + \frac{\partial R_{ijkl}}{\partial x_l} = -\frac{1}{\tau}Q_{ijk}\,,$$

where the fourth-order moment, R_{ijkl}, given by

$$R_{ijkl} = m\left\langle\, c_i c_j c_k c_l \mathcal{F}^{(20)} \,\right\rangle\,,$$

remains to be evaluated for closure.

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3.3.1 20-Moment Closure

Closing Relation for R_{ijkl}

$$\begin{aligned}
R_{ijkl} &= m\left\langle\, c_i c_j c_k c_l \mathcal{F}^{(20)} \,\right\rangle \\
&= m\left\langle\, c_i c_j c_k c_l \mathcal{M}\left[1 - \frac{\rho}{2p^2}\tau_{ij}\, c_\alpha c_\beta + \frac{\rho^2}{6p^3}\left(Q_{\alpha\beta\gamma}c_\beta c_\gamma - \frac{3p}{\rho}Q_{\alpha\beta\beta}\right)c_\alpha\right]\right\rangle \\
&= m\langle\, c_i c_j c_k c_l \mathcal{M}\,\rangle - \frac{\rho}{2p^2}\tau_{ij}\; m\langle\, c_i c_j c_k c_l c_\alpha c_\beta \mathcal{M}\,\rangle \\
&\quad + \frac{\rho^2}{6p^3}Q_{\alpha\beta\gamma}\; m\langle\, c_i c_j c_k c_l c_\alpha c_\beta c_\gamma \mathcal{M}\,\rangle - \frac{3p}{\rho}Q_{\alpha\beta\beta}\; m\langle\, c_i c_j c_k c_l c_\alpha \mathcal{M}\,\rangle \\
&= m\langle\, c_i c_j c_k c_l \mathcal{M}\,\rangle - \frac{\rho}{2p^2}\tau_{ij}\; m\langle\, c_i c_j c_k c_l c_\alpha c_\beta \mathcal{M}\,\rangle \\
&= \frac{1}{\rho}\left[P_{ij}P_{kl} + P_{ik}P_{jl} + P_{il}P_{jk} - \tau_{ij}\tau_{kl} + \tau_{ik}\tau_{jl} + \tau_{il}\tau_{jk}\right]\,,
\end{aligned}$$

or

$$R_{ijkl} = \frac{1}{\rho}\left[P_{ij}P_{kl} + P_{ik}P_{jl} + P_{il}P_{jk} - \tau_{ij}\tau_{kl} + \tau_{ik}\tau_{jl} + \tau_{il}\tau_{jk}\right]\,. \qquad (56)$$

3.3 Grad's Method of Moments (Moment Closures)

3.3.2 13-Moment Closure

We will next consider the Grad 13-moment closure.

3.3.2 13-Moment Closure

Selected Moments

In the Grad 13-moment closure, the following set of total velocity weights is considered:

$$\mathbf{V}^{(13)}(v_i) = m\left[1, v_i, v_i v_j, \frac{1}{2} v_i v^2\right]^{\mathrm{T}},$$

or the following set of random velocity weights:

$$\mathbf{V}^{(13)}(c_i) = m\left[1, c_i, c_i c_j, \frac{1}{2} c_i c^2\right]^{\mathrm{T}}.$$

3.3.2 13-Moment Closure

Selected Moments

These choices correspond to the following macroscopic quantities:

$$m\langle \mathcal{F} \rangle = \rho\,,$$
$$m\langle v_i\mathcal{F} \rangle = \rho u_i\,,$$
$$m\langle v_iv_j\mathcal{F} \rangle = \rho u_iu_j + P_{ij}\,,$$
$$\frac{m}{2}\langle v_iv^2\mathcal{F} \rangle = \rho u_i\left(\frac{1}{2}u^2 + \frac{3}{2}\frac{p}{\rho}\right) - \tau_{ij}u_j + q_i\,,$$

3.3.2 13-Moment Closure

Selected Moments

or

$$m\langle \mathcal{F} \rangle = \rho\,,$$
$$m\langle c_i\mathcal{F} \rangle = 0\,,$$
$$m\langle c_ic_j\mathcal{F} \rangle = P_{ij} = p\delta_{ij} - \tau_{ij}\,,$$
$$\frac{m}{2}\langle c_ic^2\mathcal{F} \rangle = q_i\,,$$

with

$$\mathbf{M}^{(13)} = \left[\rho, \rho u_i, \rho u_iu_j + P_{ij}, \rho u_i\left(\frac{1}{2}u^2 + \frac{3}{2}\frac{p}{\rho}\right) - \tau_{ij}u_j + q_i\right]^{\mathrm{T}}\,,$$

and

$$\mathbf{W}^{(13)} = [\rho, u_i, P_{ij}, q_i]^{\mathrm{T}} = [\rho, u_i, p\delta_{ij} - \tau_{ij}, q_i]^{\mathrm{T}}\,.$$

3.3.2 13-Moment Closure

Assumed Form for the NDF

In the Grad 13-moment closure, it is assumed that

$$\begin{aligned}\mathcal{F} &\approx \mathcal{F}^{(13)}(x_i, c_i, t; \rho, u_i, P_{ij}, q_i) \\ &= \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3}) \left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_\alpha\, c_\alpha c^2\right] ,\end{aligned}$$

where the coefficients of the truncated power series, A_α (3 values), $B_{\alpha\beta}$ (6 values), and D_α (3 values), are specified by relating them to the 13 moment constraints. Note that the preceding polynomial contains all terms up to degree two plus selected third-degree terms in c_i.

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3.3.2 13-Moment Closure

Moment Constraints on $\mathcal{F}^{(13)}$

The moment constraints on $\mathcal{F}^{(13)}$ are as follows:

$$\begin{aligned} m \left\langle \mathcal{F}^{(13)} \right\rangle &= \rho \,, \\ m \left\langle c_i \mathcal{F}^{(13)} \right\rangle &= 0 \,, \\ m \left\langle c_i c_j \mathcal{F}^{(13)} \right\rangle &= P_{ij} = p\delta_{ij} - \tau_{ij} \,, \\ \frac{m}{2} \left\langle c_i c^2 \mathcal{F}^{(13)} \right\rangle &= q_i \,. \end{aligned}$$

Moment Constraints on $\mathcal{F}^{(13)}$

If we consider the first constraint, we have

$$\begin{aligned}
\rho &= m\left\langle\, \mathcal{F}^{(13)} \,\right\rangle \\
&= m\left\langle\, \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_\alpha\, c_\alpha c^2\right] \,\right\rangle \\
&= m\langle\, \mathcal{M} \,\rangle + A_\alpha m\langle\, c_\alpha \mathcal{M} \,\rangle + B_{\alpha\beta} m\langle\, c_\alpha c_\beta \mathcal{M} \,\rangle \\
&\quad + D_\alpha m\left\langle\, c_\alpha c^2 \mathcal{M} \,\right\rangle \\
&= m\langle\, \mathcal{M} \,\rangle + B_{\alpha\beta} m\langle\, c_\alpha c_\beta \mathcal{M} \,\rangle \\
&= \rho + B_{\alpha\beta} p \delta_{\alpha\beta} \\
&= \rho + B_{\alpha\alpha} p \\
0 &= B_{\alpha\alpha} p\,,
\end{aligned}$$

or

$$B_{\alpha\alpha} = 0\,. \tag{57}$$

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Moment Constraints on $\mathcal{F}^{(13)}$

If we consider the second constraint, we have

$$\begin{aligned}
0 &= m\left\langle\, c_i \mathcal{F}^{(13)} \,\right\rangle \\
&= m\left\langle\, c_i \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta + D_\alpha\, c_\alpha c^2\right] \,\right\rangle \\
&= m\langle\, c_i \mathcal{M} \,\rangle + A_\alpha m\langle\, c_i c_\alpha \mathcal{M} \,\rangle + B_{\alpha\beta} m\langle\, c_i c_\alpha c_\beta \mathcal{M} \,\rangle \\
&\quad + D_\alpha m\left\langle\, c_i c_\alpha c^2 \mathcal{M} \,\right\rangle \\
&= A_\alpha m\langle\, c_i c_\alpha \mathcal{M} \,\rangle + D_\alpha m\left\langle\, c_i c_\alpha c^2 \mathcal{M} \,\right\rangle \\
&= A_\alpha p \delta_{i\alpha} + D_\alpha 5\frac{p^2}{\rho}\delta_{i\alpha} \\
&= A_i p + 5 D_i \frac{p^2}{\rho} \\
0 &= A_i + \frac{5p}{\rho} D_i\,,
\end{aligned}$$

or

$$A_i + \frac{5p}{\rho} D_i = 0\,. \tag{58}$$

Moment Constraints on $\mathcal{F}^{(13)}$

If we consider the third constraint, we have

$$\begin{aligned}
p\delta_{ij} - \tau_{ij} &= m \left\langle \, c_i c_j \mathcal{F}^{(13)} \, \right\rangle \\
&= m \left\langle \, c_i c_j \mathcal{M} \left[1 + A_\alpha \, c_\alpha + B_{\alpha\beta} \, c_\alpha c_\beta + D_\alpha \, c_\alpha c^2 \right] \, \right\rangle \\
&= m \langle \, c_i c_j \mathcal{M} \, \rangle + A_\alpha m \langle \, c_i c_j c_\alpha \mathcal{M} \, \rangle + B_{\alpha\beta} m \langle \, c_i c_j c_\alpha c_\beta \mathcal{M} \, \rangle \\
&\quad + D_\alpha m \left\langle \, c_i c_j c_\alpha c^2 \mathcal{M} \, \right\rangle \\
&= m \langle \, c_i c_j \mathcal{M} \, \rangle + B_{\alpha\beta} m \langle \, c_i c_j c_\alpha c_\beta \mathcal{M} \, \rangle \\
&= p\delta_{ij} + B_{\alpha\beta} \frac{p^2}{\rho} \left[\delta_{ij}\delta_{\alpha\beta} + \delta_{i\alpha}\delta_{j\beta} + \delta_{i\beta}\delta_{j\alpha} \right] \\
-\tau_{ij} &= B_{\alpha\alpha} \frac{p^2}{\rho} \delta_{ij} + B_{ij} \frac{p^2}{\rho} + B_{ji} \frac{p^2}{\rho} \\
\tau_{ij} &= -2 \frac{p^2}{\rho} B_{ij} \, ,
\end{aligned}$$

or

$$\tau_{ij} = -2 \frac{p^2}{\rho} B_{ij} \, . \qquad (59)$$

Moment Constraints on $\mathcal{F}^{(13)}$

If we consider the fourth and final constraint, we have

$$\begin{aligned}
q_i &= \frac{m}{2} \left\langle \, c_i c^2 \mathcal{F}^{(13)} \, \right\rangle \\
&= \frac{m}{2} \left\langle \, c_i c^2 \mathcal{M} \left[1 + A_\alpha \, c_\alpha + B_{\alpha\beta} \, c_\alpha c_\beta + D_\alpha \, c_\alpha c^2 \right] \, \right\rangle \\
&= \frac{m}{2} \left\langle \, c_i c^2 \mathcal{M} \, \right\rangle + A_\alpha \frac{m}{2} \left\langle \, c_i c_\alpha c^2 \mathcal{M} \, \right\rangle + B_{\alpha\beta} \frac{m}{2} \left\langle \, c_i c_\alpha c_\beta c^2 \mathcal{M} \, \right\rangle \\
&\quad + D_\alpha \frac{m}{2} \left\langle \, c_i c_\alpha c^4 \mathcal{M} \, \right\rangle \\
&= A_\alpha \frac{m}{2} \left\langle \, c_i c_\alpha c^2 \mathcal{M} \, \right\rangle + D_\alpha \frac{m}{2} \left\langle \, c_i c_\alpha c^4 \mathcal{M} \, \right\rangle \\
&= A_\alpha \frac{5}{2} \frac{p^2}{\rho} \delta_{i\alpha} + D_\alpha \frac{35}{2} \frac{p^3}{\rho^2} \delta_{i\alpha} \\
&= A_i \frac{5}{2} \frac{p^2}{\rho} + D_i \frac{35}{2} \frac{p^3}{\rho^2} \\
&= 5 \frac{p^3}{\rho^2} D_i \, ,
\end{aligned}$$

or

$$q_i = 5 \frac{p^3}{\rho^2} D_i \, . \qquad (60)$$

3.3.2 13-Moment Closure

Final Form for 13-Moment NDF

Using the preceding expressions for the coefficients, A_α, $B_{\alpha\beta}$, and D_α, the following expression can be obtained for $\mathcal{F}^{(13)}$:

$$\begin{aligned}\mathcal{F}^{(13)}&(x_i, c_i, t; \rho, u_i, P_{ij}, q_i)\\ &= \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3}) \left[1 + \frac{\rho}{2p^2}\left(p_{ij} - p\delta_{ij}\right) c_\alpha c_\beta \right.\\ &\qquad\left. + \frac{\rho^2}{p^3}\left(\frac{1}{5}c^2 - \frac{p}{\rho}\right) q_\alpha c_\alpha\right] ,\end{aligned}$$

or

$$\begin{aligned}\mathcal{F}^{(13)}&(x_i, c_i, t; \rho, u_i, \tau_{ij}, q_i)\\ &= \mathcal{M}(\rho, u_i, p) \left[1 - \frac{\rho}{2p^2}\tau_{ij}\, c_\alpha c_\beta \right.\\ &\qquad\left. + \frac{\rho^2}{p^3}\left(\frac{1}{5}c^2 - \frac{p}{\rho}\right) q_\alpha c_\alpha\right] .\end{aligned}$$

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3.3.2 13-Moment Closure

Moment Equations

The non-conservation form of the moment equations for the 13-moment closure may then be derived by using the non-conservation form of Maxwell's equation of change (relaxation-time or BGK collision operator and $a_i = 0$) given by

$$\begin{aligned}&\frac{\partial}{\partial t}(M_\circ) + \frac{\partial}{\partial x_i}(u_i M_\circ) + \frac{\partial}{\partial x_i}\left[\left\langle\, c_i V(c_i)\mathcal{F}^{(13)}\,\right\rangle\right]\\ &\quad + \left(\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j}\right)\left[\left\langle\, \frac{\partial V}{\partial c_i}\mathcal{F}^{(13)}\,\right\rangle\right] + \frac{\partial u_i}{\partial x_j}\left[\left\langle\, c_j\frac{\partial V}{\partial c_i}\mathcal{F}^{(13)}\,\right\rangle\right]\\ &\quad = -\frac{1}{\tau}\left[M_\circ - \langle\, V(c_i)\mathcal{M}\,\rangle\right] ,\end{aligned}$$

with

$$M_\circ(\vec{x}, t) = \left\langle\, V(c_i)\mathcal{F}^{(13)}\,\right\rangle , \quad \text{and} \quad V \in \mathbf{V}^{(13)}(c_i) = m\left[1, c_i, c_i c_j, \frac{1}{2}c_i c^2\right]^{\mathrm{T}} ,$$

3.3.2 13-Moment Closure

Moment Equations

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0\,,$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0\,,$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} - \frac{2}{3}\tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{2}{3}\frac{\partial q_i}{\partial x_i} = 0\,,$$

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(u_k \tau_{ij}) + \tau_{jk}\frac{\partial u_i}{\partial x_k} + \tau_{ik}\frac{\partial u_j}{\partial x_k} - \delta_{ij}\tau_{kl}\frac{\partial u_k}{\partial x_l}$$
$$- p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) - \left(\frac{2}{5}\frac{\partial q_i}{\partial x_j} + \frac{2}{5}\frac{\partial q_j}{\partial x_i} - \frac{4}{15}\delta_{ij}\frac{\partial q_l}{\partial x_l}\right) = -\frac{1}{\tau}\tau_{ij}\,,$$

$$\frac{\partial q_i}{\partial t} + u_j \frac{\partial q_i}{\partial x_j} + \frac{7}{5} q_i \frac{\partial u_j}{\partial x_j} + \frac{2}{5} q_j \frac{\partial u_j}{\partial x_i} + \frac{7}{5} q_j \frac{\partial u_i}{\partial x_j} + \frac{5}{2} p \frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)$$
$$- \frac{5}{2}\tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{p}{\rho}\right) - p\frac{\partial}{\partial x_j}\left(\frac{\tau_{ij}}{\rho}\right) - \tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{\tau_{jk}}{\rho}\right) = -\frac{1}{\tau} q_i\,.$$

3.3.2 13-Moment Closure

Note that the 13-moment closure can be derived directly from the 20-moment closure by merely assuming that

$$Q_{ijk} = \frac{2}{5}\left(q_i\delta_{jk} + q_j\delta_{ik} + q_k\delta_{ij}\right)\,,$$

which is fully consistent with $Q_{ijj}/2 = q_i$.

3.3 Grad's Method of Moments (Moment Closures)

3.3.3 10-Moment Closure

We will next consider further simplifications of the Grad closures. Consider the 10-moment closure.

3.3.3 10-Moment Closure

Selected Moments

In the Grad 10-moment closure, the following set of total velocity weights is considered:

$$\mathbf{V}^{(10)}(v_i) = m\,[1, v_i, v_i v_j]^{\mathrm{T}} \ ,$$

or the following set of random velocity weights:

$$\mathbf{V}^{(10)}(c_i) = m\,[1, c_i, c_i c_j]^{\mathrm{T}} \ .$$

3.3.3 10-Moment Closure

Selected Moments

These choices correspond to the following macroscopic quantities:

$$m\langle\,\mathcal{F}\,\rangle = \rho\,,$$
$$m\langle\,v_i\mathcal{F}\,\rangle = \rho u_i\,,$$
$$m\langle\,v_iv_j\mathcal{F}\,\rangle = \rho u_iu_j + P_{ij}\,,$$

3.3.3 10-Moment Closure

Selected Moments

or

$$m\langle\,\mathcal{F}\,\rangle = \rho\,,$$
$$m\langle\,c_i\mathcal{F}\,\rangle = 0\,,$$
$$m\langle\,c_ic_j\mathcal{F}\,\rangle = P_{ij} = p\delta_{ij} - \tau_{ij}\,,$$

with

$$\mathbf{M}^{(10)} = [\rho, \rho u_i, \rho u_iu_j + P_{ij}]^{\mathrm{T}}\,,$$

and

$$\mathbf{W}^{(10)} = [\rho, u_i, P_{ij}]^{\mathrm{T}}\,.$$

3.3.3 10-Moment Closure

Assumed Form for the NDF

In the Grad 10-moment closure, it is assumed that

$$\begin{aligned}\mathcal{F} &\approx \mathcal{F}^{(10)}(x_i, c_i, t; \rho, u_i, P_{ij}) \\ &= \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3})\,[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta]\ ,\end{aligned}$$

where the coefficients of the truncated power series, A_α (3 values) and $B_{\alpha\beta}$ (6 values) are specified by relating them to the 10 moment constraints. Note that the preceding polynomial contains all terms up to degree two, but nothing beyond that.

3.3.3 10-Moment Closure

Moment Constraints on $\mathcal{F}^{(10)}$

The moment constraints on $\mathcal{F}^{(10)}$ are as follows:

$$\begin{aligned}m\left\langle\ \mathcal{F}^{(10)}\ \right\rangle &= \rho\,, \\ m\left\langle\ c_i\mathcal{F}^{(10)}\ \right\rangle &= 0\,, \\ m\left\langle\ c_ic_j\mathcal{F}^{(10)}\ \right\rangle &= P_{ij} = p\delta_{ij} - \tau_{ij}\ ,\end{aligned}$$

Moment Constraints on $\mathcal{F}^{(10)}$

If we consider the first constraint, we have

$$\begin{aligned}
\rho &= m\left\langle \mathcal{F}^{(10)} \right\rangle \\
&= m\left\langle \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta\right]\right\rangle \\
&= m\left\langle \mathcal{M} \right\rangle + A_\alpha m\left\langle c_\alpha \mathcal{M} \right\rangle + B_{\alpha\beta} m\left\langle c_\alpha c_\beta \mathcal{M} \right\rangle \\
&= m\left\langle \mathcal{M} \right\rangle + B_{\alpha\beta} m\left\langle c_\alpha c_\beta \mathcal{M} \right\rangle \\
&= \rho + B_{\alpha\beta} p \delta_{\alpha\beta} \\
&= \rho + B_{\alpha\alpha} p \\
0 &= B_{\alpha\alpha} p\,,
\end{aligned}$$

or

$$B_{\alpha\alpha} = 0\,. \tag{61}$$

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Moment Constraints on $\mathcal{F}^{(10)}$

If we consider the second constraint, we have

$$\begin{aligned}
0 &= m\left\langle c_i \mathcal{F}^{(10)} \right\rangle \\
&= m\left\langle c_i \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B_{\alpha\beta}\, c_\alpha c_\beta\right]\right\rangle \\
&= m\left\langle c_i \mathcal{M} \right\rangle + A_\alpha m\left\langle c_i c_\alpha \mathcal{M} \right\rangle + B_{\alpha\beta} m\left\langle c_i c_\alpha c_\beta \mathcal{M} \right\rangle \\
&= A_\alpha m\left\langle c_i c_\alpha \mathcal{M} \right\rangle \\
&= A_\alpha p \delta_{i\alpha} \\
&= A_i p\,,
\end{aligned}$$

or

$$A_i = 0\,. \tag{62}$$

Moment Constraints on $\mathcal{F}^{(10)}$

If we consider the third constraint, we have

$$\begin{aligned}
p\delta_{ij} - \tau_{ij} &= m \left\langle \, c_i c_j \mathcal{F}^{(10)} \, \right\rangle \\
&= m \langle \, c_i c_j \mathcal{M} \left[1 + A_\alpha \, c_\alpha + B_{\alpha\beta} \, c_\alpha c_\beta\right] \rangle \\
&= m \langle \, c_i c_j \mathcal{M} \, \rangle + A_\alpha m \langle \, c_i c_j c_\alpha \mathcal{M} \, \rangle + B_{\alpha\beta} m \langle \, c_i c_j c_\alpha c_\beta \mathcal{M} \, \rangle \\
&= m \langle \, c_i c_j \mathcal{M} \, \rangle + B_{\alpha\beta} m \langle \, c_i c_j c_\alpha c_\beta \mathcal{M} \, \rangle \\
&= p\delta_{ij} + B_{\alpha\beta} \frac{p^2}{\rho} \left[\delta_{ij}\delta_{\alpha\beta} + \delta_{i\alpha}\delta_{j\beta} + \delta_{i\beta}\delta_{j\alpha}\right] \\
-\tau_{ij} &= B_{\alpha\alpha} \frac{p^2}{\rho} \delta_{ij} + B_{ij} \frac{p^2}{\rho} + B_{ji} \frac{p^2}{\rho} \\
\tau_{ij} &= -2 \frac{p^2}{\rho} B_{ij} \, ,
\end{aligned}$$

or

$$\tau_{ij} = -2 \frac{p^2}{\rho} B_{ij} \, . \tag{63}$$

3.3.3 10-Moment Closure

Final Form for 10-Moment NDF

Using the preceding expressions for the coefficients, A_α and $B_{\alpha\beta}$, the following expression can be obtained for $\mathcal{F}^{(10)}$:

$$\begin{aligned}
&\mathcal{F}^{(10)}(x_i, c_i, t; \rho, u_i, P_{ij}) \\
&\quad = \mathcal{M}(\rho, u_i, p = \frac{P_{ii}}{3}) \left[1 + \frac{\rho}{2p^2} \left(p_{ij} - p\delta_{ij}\right) \, c_\alpha c_\beta\right] ,
\end{aligned}$$

or

$$\begin{aligned}
&\mathcal{F}^{(10)}(x_i, c_i, t; \rho, u_i, \tau_{ij}) \\
&\quad = \mathcal{M}(\rho, u_i, p) \left[1 - \frac{\rho}{2p^2} \tau_{ij} \, c_\alpha c_\beta\right] .
\end{aligned}$$

3.3.3 10-Moment Closure

Moment Equations

The non-conservation form of the moment equations for the 10-moment closure may then be derived by using the non-conservation form of Maxwell's equation of change (relaxation-time or BGK collision operator and $a_i = 0$) given by

$$\frac{\partial}{\partial t}(M_\circ) + \frac{\partial}{\partial x_i}(u_i M_\circ) + \frac{\partial}{\partial x_i}\left[\left\langle\, c_i V(c_i)\mathcal{F}^{(10)}\,\right\rangle\right] + \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right)\left[\left\langle\, \frac{\partial V}{\partial c_i}\mathcal{F}^{(10)}\,\right\rangle\right] + \frac{\partial u_i}{\partial x_j}\left[\left\langle\, c_j \frac{\partial V}{\partial c_i}\mathcal{F}^{(10)}\,\right\rangle\right] = -\frac{1}{\tau}\left[M_\circ - \langle\, V(c_i)\mathcal{M}\,\rangle\right],$$

with

$$M_\circ(\vec{x},t) = \left\langle\, V(c_i)\mathcal{F}^{(10)}\,\right\rangle, \quad \text{and} \quad V \in \mathbf{V}^{(10)}(c_i) = m\,[1, c_i, c_i c_j]^{\mathrm{T}},$$

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3.3.3 10-Moment Closure

Moment Equations

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0,$$

$$\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial P_{ij}}{\partial x_j} = \frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0,$$

$$\frac{\partial P_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(u_k P_{ij}) + P_{jk}\frac{\partial u_i}{\partial x_k} + P_{ik}\frac{\partial u_j}{\partial x_k} + \frac{\partial Q_{ijk}}{\partial x_k} = -\frac{1}{\tau}(P_{ij} - p\delta_{ij}) = \frac{1}{\tau}\tau_{ij},$$

where the third-order moment, Q_{ijk}, given by

$$Q_{ijk} = m\left\langle\, c_i c_j c_k \mathcal{F}^{(10)}\,\right\rangle.$$

remains to be evaluated for closure.

3.3.3 10-Moment Closure

Closing Relation for Q_{ijk}

$$
\begin{aligned}
Q_{ijk} &= m \left\langle\, c_i c_j c_k \mathcal{F}^{(10)} \,\right\rangle \\
&= m \left\langle\, c_i c_j c_k \mathcal{M} \left[1 - \frac{\rho}{2p^2} \tau_{ij}\, c_\alpha c_\beta \right] \right\rangle \\
&= m \langle\, c_i c_j c_k \mathcal{M} \,\rangle - \frac{\rho}{2p^2} \tau_{ij}\, m \langle\, c_i c_j c_k c_\alpha c_\beta \mathcal{M} \,\rangle \\
&= 0 \,,
\end{aligned}
$$

or

$$Q_{ijk} = 0 \,. \tag{64}$$

3.3.3 10-Moment Closure

Note that the 10-moment closure can be derived directly from the 20-moment closure by merely assuming that

$$Q_{ijk} = 0 \,,$$

i.e., by assuming the heat flux is zero.

3.3 Grad's Method of Moments (Moment Closures)

3.3.4 8-Moment Closure

Consider also a Grad 8-moment closure.

3.3.4 8-Moment Closure

Selected Moments

In the Grad 8-moment closure, the following set of total velocity weights is considered:

$$\mathbf{V}^{(8)}(v_i) = m \left[1, v_i, \frac{1}{2}v^2, \frac{1}{2}v_i v^2\right]^{\mathrm{T}} ,$$

or the following set of random velocity weights:

$$\mathbf{V}^{(8)}(c_i) = m \left[1, c_i, \frac{1}{2}c^2, \frac{1}{2}c_i c^2\right]^{\mathrm{T}} .$$

3.3.4 8-Moment Closure

Selected Moments

These choices correspond to the following macroscopic quantities:

$$
\begin{aligned}
&m \langle \mathcal{F} \rangle = \rho \,, \\
&m \langle v_i \mathcal{F} \rangle = \rho u_i \,, \\
&\frac{m}{2} \langle v^2 \mathcal{F} \rangle = \frac{1}{2}\rho u^2 + \frac{3}{2} p \,, \\
&\frac{m}{2} \langle v_i v^2 \mathcal{F} \rangle = \rho u_i \left(\frac{1}{2} u^2 + \frac{3}{2}\frac{p}{\rho} \right) - \tau_{ij} u_j + q_i \,,
\end{aligned}
$$

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3.3.4 8-Moment Closure

Selected Moments

or

$$
\begin{aligned}
&m \langle \mathcal{F} \rangle = \rho \,, \\
&m \langle c_i \mathcal{F} \rangle = 0 \,, \\
&\frac{m}{2} \langle c^2 \mathcal{F} \rangle = \frac{3}{2} p \,, \\
&\frac{m}{2} \langle c_i c^2 \mathcal{F} \rangle = q_i \,,
\end{aligned}
$$

with

$$
\mathbf{M}^{(8)} = \left[\rho, \rho u_i, \rho u_i u_j + P_{ij}, \rho u_i \left(\frac{1}{2} u^2 + \frac{3}{2}\frac{p}{\rho} \right) - \tau_{ij} u_j + q_i \right]^{\mathrm{T}} ,
$$

and

$$
\mathbf{W}^{(8)} = [\rho, u_i, p, q_i]^{\mathrm{T}} \,.
$$

3.3.4 8-Moment Closure

Assumed Form for the NDF

In the Grad 8-moment closure, it is assumed that

$$\mathcal{F} \approx \mathcal{F}^{(8)}(x_i, c_i, t; \rho, u_i, p, q_i)$$
$$= \mathcal{M}(\rho, u_i, p)\left[1 + A_\alpha\, c_\alpha + B\, c^2 + D_\alpha\, c_\alpha c^2\right] ,$$

where the coefficients of the truncated power series, A_α (3 values), B (1 value), and D_α (3 values), are specified by relating them to the 8 moment constraints. Note that the preceding polynomial contains does not contain all terms up to degree three, only selected terms in c_i.

3.3.4 8-Moment Closure

Moment Constraints on $\mathcal{F}^{(8)}$

The moment constraints on $\mathcal{F}^{(8)}$ are as follows:

$$m\left\langle\ \mathcal{F}^{(8)}\ \right\rangle = \rho\,,$$
$$m\left\langle\ c_i\mathcal{F}^{(8)}\ \right\rangle = 0\,,$$
$$\frac{m}{2}\left\langle\ c^2\mathcal{F}^{(8)}\ \right\rangle = \frac{3}{2}p\,,$$
$$\frac{m}{2}\left\langle\ c_i c^2\mathcal{F}^{(13)}\ \right\rangle = q_i\,.$$

Moment Constraints on $\mathcal{F}^{(8)}$

If we consider the first constraint, we have

$$\begin{aligned}
\rho &= m\left\langle \mathcal{F}^{(8)} \right\rangle \\
&= m\left\langle \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B\, c^2 + D_\alpha\, c_\alpha c^2\right] \right\rangle \\
&= m\left\langle \mathcal{M} \right\rangle + A_\alpha m\left\langle c_\alpha \mathcal{M} \right\rangle + Bm\left\langle c^2\mathcal{M} \right\rangle \\
&\quad + D_\alpha m\left\langle c_\alpha c^2 \mathcal{M} \right\rangle \\
&= m\left\langle \mathcal{M} \right\rangle + Bm\left\langle c^2\mathcal{M} \right\rangle \\
&= \rho + 3Bp \\
0 &= 3Bp\,,
\end{aligned}$$

or

$$B = 0\,. \tag{65}$$

Moment Constraints on $\mathcal{F}^{(8)}$

If we consider the second constraint, we have

$$\begin{aligned}
0 &= m\left\langle c_i\mathcal{F}^{(8)} \right\rangle \\
&= m\left\langle c_i\mathcal{M}\left[1 + A_\alpha\, c_\alpha + B\, c^2 + D_\alpha\, c_\alpha c^2\right] \right\rangle \\
&= m\left\langle c_i\mathcal{M} \right\rangle + A_\alpha m\left\langle c_i c_\alpha \mathcal{M} \right\rangle + Bm\left\langle c_i c^2\mathcal{M} \right\rangle \\
&\quad + D_\alpha m\left\langle c_i c_\alpha c^2 \mathcal{M} \right\rangle \\
&= A_\alpha m\left\langle c_i c_\alpha \mathcal{M} \right\rangle + D_\alpha m\left\langle c_i c_\alpha c^2 \mathcal{M} \right\rangle \\
&= A_\alpha p\delta_{i\alpha} + D_\alpha 5\frac{p^2}{\rho}\delta_{i\alpha} \\
&= A_i p + 5D_i\frac{p^2}{\rho} \\
0 &= A_i + \frac{5p}{\rho}D_i\,,
\end{aligned}$$

or

$$A_i + \frac{5p}{\rho}D_i = 0\,. \tag{66}$$

Moment Constraints on $\mathcal{F}^{(8)}$

If we consider the third constraint, we have

$$\begin{aligned}
p\delta_{ij} - \tau_{ij} &= m\left\langle\, c_i c_j \mathcal{F}^{(8)} \,\right\rangle \\
&= m\left\langle\, c_i c_j \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B\, c^2 + D_\alpha\, c_\alpha c^2\right] \,\right\rangle \\
&= m\langle\, c_i c_j \mathcal{M}\,\rangle + A_\alpha m\langle\, c_i c_j c_\alpha \mathcal{M}\,\rangle + Bm\left\langle\, c_i c_j c^2 \mathcal{M}\,\right\rangle \\
&\quad + D_\alpha m\left\langle\, c_i c_j c_\alpha c^2 \mathcal{M}\,\right\rangle \\
&= m\langle\, c_i c_j \mathcal{M}\,\rangle + Bm\left\langle\, c_i c_j c^2 \mathcal{M}\,\right\rangle \\
&= p\delta_{ij} + 5B\frac{p^2}{\rho}5\delta_{ij} \\
-\tau_{ij} &= 5B\frac{p^2}{\rho}\delta_{ij} \\
\tau_{ij} &= 0\,,
\end{aligned}$$

or

$$\tau_{ij} = 0\,. \tag{67}$$

Moment Constraints on $\mathcal{F}^{(8)}$

If we consider the fourth and final constraint, we have

$$\begin{aligned}
q_i &= \frac{m}{2}\left\langle\, c_i c^2 \mathcal{F}^{(8)} \,\right\rangle \\
&= \frac{m}{2}\left\langle\, c_i c^2 \mathcal{M}\left[1 + A_\alpha\, c_\alpha + B\, c^2 + D_\alpha\, c_\alpha c^2\right] \,\right\rangle \\
&= \frac{m}{2}\left\langle\, c_i c^2 \mathcal{M}\,\right\rangle + A_\alpha\frac{m}{2}\left\langle\, c_i c_\alpha c^2 \mathcal{M}\,\right\rangle + B\frac{m}{2}\left\langle\, c_i c^4 \mathcal{M}\,\right\rangle \\
&\quad + D_\alpha\frac{m}{2}\left\langle\, c_i c_\alpha c^4 \mathcal{M}\,\right\rangle \\
&= A_\alpha\frac{m}{2}\left\langle\, c_i c_\alpha c^2 \mathcal{M}\,\right\rangle + D_\alpha\frac{m}{2}\left\langle\, c_i c_\alpha c^4 \mathcal{M}\,\right\rangle \\
&= A_\alpha\frac{5}{2}\frac{p^2}{\rho}\delta_{i\alpha} + D_\alpha\frac{35}{2}\frac{p^3}{\rho^2}\delta_{i\alpha} \\
&= A_i\frac{5}{2}\frac{p^2}{\rho} + D_i\frac{35}{2}\frac{p^3}{\rho^2} \\
&= 5\frac{p^3}{\rho^2}D_i\,,
\end{aligned}$$

or

$$q_i = 5\frac{p^3}{\rho^2}D_i\,. \tag{68}$$

3.3.4 8-Moment Closure

Final Form for 8-Moment NDF

Using the preceding expressions for the coefficients, A_α, B, and D_α, the following expression can be obtained for $\mathcal{F}^{(8)}$:

$$\mathcal{F}^{(8)}(x_i, c_i, t; \rho, u_i, p, q_i) = \mathcal{M}(\rho, u_i, p)\left[1 + \frac{\rho^2}{p^3}\left(\frac{1}{5}c^2 - \frac{p}{\rho}\right) q_\alpha c_\alpha\right] .$$

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3.3.4 8-Moment Closure

Moment Equations

The non-conservation form of the moment equations for the 8-moment closure may then be derived by using the non-conservation form of Maxwell's equation of change (relaxation-time or BGK collision operator and $a_i = 0$) given by

$$\begin{aligned}\frac{\partial}{\partial t}(M_\circ) + \frac{\partial}{\partial x_i}(u_i M_\circ) + \frac{\partial}{\partial x_i}\left[\left\langle\, c_i V(c_i)\mathcal{F}^{(8)} \,\right\rangle\right] \\ + \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right)\left[\left\langle\, \frac{\partial V}{\partial c_i}\mathcal{F}^{(8)} \,\right\rangle\right] + \frac{\partial u_i}{\partial x_j}\left[\left\langle\, c_j \frac{\partial V}{\partial c_i}\mathcal{F}^{(8)} \,\right\rangle\right] \\ = -\frac{1}{\tau}\left[M_\circ - \langle\, V(c_i)\mathcal{M} \,\rangle\right] ,\end{aligned}$$

with

$$M_\circ(\vec{x}, t) = \left\langle\, V(c_i)\mathcal{F}^{(8)} \,\right\rangle , \quad \text{and} \quad V \in \mathbf{V}^{(8)}(c_i) = m\left[1, c_i, \frac{1}{2}c^2, \frac{1}{2}c_i c^2\right]^{\mathrm{T}} ,$$

3.3.4 8-Moment Closure

Moment Equations

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0\,,$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} = 0\,,$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} + \frac{2}{3}\frac{\partial q_i}{\partial x_i} = 0\,,$$

$$\frac{\partial q_i}{\partial t} + u_j \frac{\partial q_i}{\partial x_j} + \frac{7}{5} q_i \frac{\partial u_j}{\partial x_j} + \frac{2}{5} q_j \frac{\partial u_j}{\partial x_i} + \frac{7}{5} q_j \frac{\partial u_i}{\partial x_j} + \frac{5}{2} p \frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right) = -\frac{1}{\tau} q_i\,.$$

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3.3.4 8-Moment Closure

Note that the 8-moment closure can be derived directly from the 20-moment closure by merely assuming that

$$\tau_{ij} = 0\,,$$

and

$$Q_{ijk} = \frac{2}{5}\left(q_i \delta_{jk} + q_j \delta_{ik} + q_k \delta_{ij}\right)\,.$$

The latter is fully consistent with $Q_{ijj}/2 = q_i$.

3.3 Grad's Method of Moments (Moment Closures)

3.3.5 5-Moment Closure

Lastly, consider the 5-moment closure.

3.3.5 5-Moment Closure

Selected Moments

In the Grad 5-moment closure, the following set of total velocity weights is considered:

$$\mathbf{V}^{(5)}(v_i) = m \left[1, v_i, \frac{1}{2}v^2\right]^{\mathrm{T}} ,$$

or the following set of random velocity weights:

$$\mathbf{V}^{(5)}(c_i) = m \left[1, c_i, \frac{1}{2}c^2\right]^{\mathrm{T}} .$$

3.3.5 5-Moment Closure

Selected Moments

These choices correspond to the following macroscopic quantities:

$$m\langle\,\mathcal{F}\,\rangle = \rho\,,$$
$$m\langle\, v_i\mathcal{F}\,\rangle = \rho u_i\,,$$
$$\frac{m}{2}\langle\, v^2\mathcal{F}\,\rangle = \frac{1}{2}\rho u^2 + \frac{3}{2}p\,,$$

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3.3.5 5-Moment Closure

Selected Moments

or

$$m\langle\,\mathcal{F}\,\rangle = \rho\,,$$
$$m\langle\, c_i\mathcal{F}\,\rangle = 0\,,$$
$$\frac{m}{2}\langle\, c^2\mathcal{F}\,\rangle = \frac{3}{2}p\,,$$

with

$$\mathbf{M}^{(5)} = \left[\rho, \rho u_i, \frac{1}{2}\rho u^2 + \frac{3}{2}p\right]^{\mathrm{T}}\,,$$

and

$$\mathbf{W}^{(5)} = [\rho, u_i, p]^{\mathrm{T}}\,.$$

3.3.5 5-Moment Closure

Assumed Form for the NDF

In the Grad 5-moment closure, it is assumed that

$$\mathcal{F} \approx \mathcal{F}^{(5)}(x_i, c_i, t; \rho, u_i, p) = \mathcal{M}(\rho, u_i, p)\,,$$

3.3.5 5-Moment Closure

Moment Constraints on $\mathcal{F}^{(8)}$

The moment constraints on $\mathcal{F}^{(5)}$ are as follows:

$$m\left\langle\, \mathcal{F}^{(5)} \,\right\rangle = \rho\,,$$
$$m\left\langle\, c_i\mathcal{F}^{(5)} \,\right\rangle = 0\,,$$
$$\frac{m}{2}\left\langle\, c^2\mathcal{F}^{(5)} \,\right\rangle = \frac{3}{2}p\,,$$

3.3.5 5-Moment Closure

Moment Equations

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0\,,$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} = 0\,,$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} = 0\,.$$

Mass, momentum, and energy are collisional invariants and the 5-moment or Euler equations provides a description of flow in local thermodynamic equilibrium.

3.3.5 5-Moment Closure

Note that the 5-moment closure can be derived directly from the 20-moment closure by merely assuming that

$$\tau_{ij} = 0\,,$$

and

$$Q_{ijk} = 0\,.$$

3.4 Recovery of Navier-Stokes Equations

Consider 13-Moment Closure

Will consider the recovery of the Navier-Stokes equations (continuum-limit approximation) from the Grad moment equations. To do this will apply a Chapman-Enskog-like expansion directly to the moment equations. Will consider the 13-moment equations for this. It will be shown that the 13-moment closure formally recovers the Navier-Stokes equations. A similar procedure can be applied to the other Grad moment closures and it can be shown that the 20-moment closure also recovers the Navier-Stokes equations whereas the 10- and 8-moment closures do not. The latter are defective in that they are either missing terms associated with the heat flux or fluid stresses.

3.4 Recovery of Navier-Stokes Equations

As a reminder, the moment equations of the Grad 13-moment closure are as follows:

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \,,$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0 \,,$$

$$\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \frac{5}{3} p \frac{\partial u_i}{\partial x_i} - \frac{2}{3}\tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{2}{3}\frac{\partial q_i}{\partial x_i} = 0 \,,$$

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(u_k \tau_{ij}) + \tau_{jk}\frac{\partial u_i}{\partial x_k} + \tau_{ik}\frac{\partial u_j}{\partial x_k} - \delta_{ij}\tau_{kl}\frac{\partial u_k}{\partial x_l}$$
$$- p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) - \left(\frac{2}{5}\frac{\partial q_i}{\partial x_j} + \frac{2}{5}\frac{\partial q_j}{\partial x_i} - \frac{4}{15}\delta_{ij}\frac{\partial q_l}{\partial x_l}\right) = -\frac{1}{\tau}\tau_{ij} \,,$$

$$\frac{\partial q_i}{\partial t} + u_j \frac{\partial q_i}{\partial x_j} + \frac{7}{5} q_i \frac{\partial u_j}{\partial x_j} + \frac{2}{5} q_j \frac{\partial u_j}{\partial x_i} + \frac{7}{5} q_j \frac{\partial u_i}{\partial x_j} + \frac{5}{2} p \frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)$$
$$- \frac{5}{2}\tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{p}{\rho}\right) - p\frac{\partial}{\partial x_j}\left(\frac{\tau_{ij}}{\rho}\right) - \tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{\tau_{jk}}{\rho}\right) = -\frac{1}{\tau} q_i \,.$$

3.4 Recovery of Navier-Stokes Equations

By expressing the 13-moment set in terms of transport equations for the macroscopic moments ρ, u_i, p, τ_{ij}, and q_i, there is a clear distinction between collisional invariants (i.e., conserved quantities associated with ρ, u_i, and p) and quantities that satisfy a weak conservation equation and are relaxing under the action of source terms towards equilibrium conditions due to the inter-particle collisional processes (τ_{ij} and q_i) with a time scale, τ. One can apply a Chapman-Enskog-like perturbative expansion technique to the latter, assuming that the relaxation time, τ, is small (i.e., $\tau \ll 1$).

3.4 Recovery of Navier-Stokes Equations

We will there for consider a perturbative expansion for the unscaled solutions for both τ_{ij} and q_i of the form

$$\tau_{ij} = \tau_{ij}^{(0)} + \tau_{ij}^{(1)} + \tau_{ij}^{(2)} + \tau_{ij}^{(3)} + \cdots \,,$$

$$q_i = q_i^{(0)} + q_i^{(1)} + q_i^{(2)} + q_i^{(3)} + \cdots \,,$$

satisfying the unscaled moment equations

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial}{\partial x_k}\left(u_k \tau_{ij}\right) + \tau_{jk}\frac{\partial u_i}{\partial x_k} + \tau_{ik}\frac{\partial u_j}{\partial x_k} - \delta_{ij}\tau_{kl}\frac{\partial u_k}{\partial x_l} - p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) - \left(\frac{2}{5}\frac{\partial q_i}{\partial x_j} + \frac{2}{5}\frac{\partial q_j}{\partial x_i} - \frac{4}{15}\delta_{ij}\frac{\partial q_l}{\partial x_l}\right) = -\frac{1}{\tau}\tau_{ij} \,,$$

$$\frac{\partial q_i}{\partial t} + u_j\frac{\partial q_i}{\partial x_j} + \frac{7}{5}q_i\frac{\partial u_j}{\partial x_j} + \frac{2}{5}q_j\frac{\partial u_j}{\partial x_i} + \frac{7}{5}q_j\frac{\partial u_i}{\partial x_j} + \frac{5}{2}p\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right) - \frac{5}{2}\tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{p}{\rho}\right) - p\frac{\partial}{\partial x_j}\left(\frac{\tau_{ij}}{\rho}\right) - \tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{\tau_{jk}}{\rho}\right) = -\frac{1}{\tau}q_i \,.$$

3.4 Recovery of Navier-Stokes Equations

Similarly, we will consider scaled perturbative solutions for τ_{ij} and q_i of the form

$$\tau_{ij} = \tau_{ij}^{(0)} + \epsilon\tau_{ij}^{(1)} + \epsilon^2\tau_{ij}^{(2)} + \epsilon^3\tau_{ij}^{(3)} + \cdots\,,$$

$$q_i = q_i^{(0)} + \epsilon q_i^{(1)} + \epsilon^2 q_i^{(2)} + \epsilon^3 q_i^{(3)} + \cdots\,,$$

satisfying the unscaled moment equations

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial}{\partial x_k}(u_k\tau_{ij}) + \tau_{jk}\frac{\partial u_i}{\partial x_k} + \tau_{ik}\frac{\partial u_j}{\partial x_k} - \delta_{ij}\tau_{kl}\frac{\partial u_k}{\partial x_l}$$
$$- p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) - \left(\frac{2}{5}\frac{\partial q_i}{\partial x_j} + \frac{2}{5}\frac{\partial q_j}{\partial x_i} - \frac{4}{15}\delta_{ij}\frac{\partial q_l}{\partial x_l}\right) = -\frac{1}{\epsilon\tau}\tau_{ij}\,,$$

$$\frac{\partial q_i}{\partial t} + u_j\frac{\partial q_i}{\partial x_j} + \frac{7}{5}q_i\frac{\partial u_j}{\partial x_j} + \frac{2}{5}q_j\frac{\partial u_j}{\partial x_i} + \frac{7}{5}q_j\frac{\partial u_i}{\partial x_j} + \frac{5}{2}p\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)$$
$$- \frac{5}{2}\tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{p}{\rho}\right) - p\frac{\partial}{\partial x_j}\left(\frac{\tau_{ij}}{\rho}\right) - \tau_{ij}\frac{\partial}{\partial x_j}\left(\frac{\tau_{jk}}{\rho}\right) = -\frac{1}{\epsilon\tau}q_i\,,$$

for which $\epsilon \ll 1$.

3.4 Recovery of Navier-Stokes Equations

Substition of the scaled solutions for τ_{ij} and q_i into their respective scaled moment equations and then collecting terms of equal order in ϵ will result in the following conditions on the zeroth-order solutions to zeroth-order in ϵ:

$$\tau_{ij}^{(0)} = 0\,,$$

$$q_i^{(0)} = 0\,,$$

which corresponds to the local equilibrium solution for which ρ, u_i, and p satisfy the Euler equations.

3.4 Recovery of Navier-Stokes Equations

Collecting terms to first-order in ϵ will result in the following conditions on the first-order solutions for τ_{ij} and q_i:

$$-p\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right]=-\frac{1}{\tau}\tau_{ij}^{(1)},$$

$$\frac{5}{2}p\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)=-\frac{1}{\tau}q_i^{(1)},$$

or

$$\tau_{ij}^{(1)}=\tau p\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right]=\mu\left[\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right],$$

$$q_i^{(1)}=-\frac{5\tau p}{2}\frac{\partial}{\partial x_i}\left(\frac{p}{\rho}\right)=-\kappa\frac{\partial T}{\partial x_i},$$

which correspond directly to the constitutive relations of the Navier-Stokes equations with $\mu=\tau p$ and $\kappa=5k\tau p/(2m)$. In this sense, it is evident that the Navier-Stokes equations and limit is recovered by the Grad 13-moment system.

3.5 Order of Magnitude Approach

In an attempt to assess the convergence of Grad moment closures to the solution of the Boltzmann equation, the so-called order of magnitude approach was proposed by Struchtrup (2004, 2005, 2006). The order of magnitude approach is a modification of the consistently ordered extended thermodynamics (COET) method of Müller, Reitebuch, and Weiss (2003).

3.5 Order of Magnitude Approach

The order of magnitude approach can be used to determining the order of accuracy of the moment equations in Knudsen number and consists of the following three steps:

- determination of the order of magnitude of the moments;
- construction of the moment set with minimum number of moments for a given accuracy; and
- removal of all terms that contribute higher-order terms to the momentum and energy equations.

A Chapman-Enskog expansion technique is applied to the moments in order to accomplish the first step and the resulting expansions are compared to the results of the Chapman-Enskog method.

3.5 Order of Magnitude Approach

Main Findings:

- The Grad 13-moment closure formally recovers the first-order Chapman-Enskog solution to first-order (i.e., the Navier-Stokes equations); however, it does not recover all of the terms in the second-order solution (i.e., the Burnett equations).
- The so-called regularized 13-moment (R13) closure of Torrilhon and Struchtrup (2004) recovers formally the second-order Chapman-Enskog solution, as does the Grad 26-moment closure. Regularization can also be applied to the 26-moment closure (R26) to recover even greater accuracy within the order of magnitude approach (Gu and Emerson, 2009).

3.6 Assessment/Application of Classical Moment Methods

In order to access the capabilities of classical moment methods and in particular, the Grad moment methods, the following problems will be considered:

- eigenstructure of Grad moment equations;
- stationary one-dimensional planar shock structure; and
- high-frequency sound propagation.

3.6.1 Eigenstructure of Moment Equations

As stated previously, moment closure methods result in a quasi-linear hyperbolic system of non-linear partial-differential equations with relaxation source terms which govern the time evolution and transport of the macroscopic moments of interest. The hyperbolicity of the moment equations is an important consideration.

3.6.1 Eigenstructure of Moment Equations

The moment equations of the Grad closures can all be written in the following form:

$$\frac{\partial \mathbf{W}^{(N)}}{\partial t} + \mathbf{A}^{(N)} \frac{\partial \mathbf{W}^{(N)}}{\partial x} + \mathbf{B}^{(N)} \frac{\partial \mathbf{W}^{N}}{\partial y} + \mathbf{C}^{(N)} \frac{\partial \mathbf{W}^{N}}{\partial z} = \mathbf{S}^{(N)} \,,$$

where $\mathbf{W}^{(N)}$ is the N-component primitive solution vector for the closure and $\mathbf{A}^{(N)}$, $\mathbf{B}^{(N)}$, and $\mathbf{C}^{(N)}$ are $N \times N$ coefficient matrices. The hyperbolicity of the moment equations can be examined by considering the eigenstructure of $\mathbf{A}^{(N)}$, $\mathbf{B}^{(N)}$, and $\mathbf{C}^{(N)}$.

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3.6.1 Eigenstructure of Moment Equations

For one-dimensional flows in the x-direction

- the moment equations are hyperbolic if the eigenvalues of $\mathbf{A}^{(N)}$ are all real;
- the moment equations are strictly hyperbolic if the eigenvalues of $\mathbf{A}^{(N)}$ are all real and distinct;
- the alternative for the latter is a degenerate hyperbolic system.

The eigenstructure is defined by the right and left eigenvalue problems:

$$\mathbf{A}^{(N)}\, \boldsymbol{r} = \lambda \boldsymbol{r} \,, \quad \boldsymbol{l}\, \mathbf{A}^{(N)} = \lambda \boldsymbol{l} \,.$$

where λ is the eigenvalue and $\boldsymbol{r}$ and $\boldsymbol{l}$ are the right and left eigenvectors, respectively.

3.6.1 Eigenstructure of Moment Equations

5-Moment Closure

For the Grad 5-moment equations, the resulting moment equations correspond to the Euler equations and

$$\mathbf{W}^{(5)} = [\rho, u, v, w, p]^{\mathsf{T}} ,$$

and

$$\mathbf{A}^{(5)} = \begin{bmatrix} u & \rho & 0 & 0 & 0 \\ 0 & u & 0 & 0 & \dfrac{1}{\rho} \\ 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & u & 0 \\ 0 & \dfrac{5}{3}p & 0 & 0 & u \end{bmatrix} .$$

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3.6.1 Eigenstructure of Moment Equations

5-Moment Closure

A characteristic analysis reveals that the eigenvalues λ of $\mathbf{A}^{(5)}$ correspond to the roots of the fifth-order polynomial equation

$$\det\left(\mathbf{A}^{(5)} - \lambda\mathbf{I}\right) = \frac{1}{3\rho}(u-\lambda)^3\left(3\rho\lambda^2 - 6\rho u\lambda + 3\rho u^2 - 5p\right)$$
$$= x^3\left(x^2 - \frac{5}{3}\theta^2\right) = 0 ,$$

and are

$$\lambda_1 = u - \sqrt{\frac{5}{3}}\theta ,$$
$$\lambda_2 = \lambda_3 = \lambda_4 = u ,$$
$$\lambda_5 = u + \sqrt{\frac{5}{3}}\theta .$$

where $x = u - \lambda$ and $\theta = \sqrt{p/\rho}$.

3.6.1 Eigenstructure of Moment Equations

5-Moment Closure

The related right eigenvectors, $\boldsymbol{r}$, are

$$\boldsymbol{r}_1 = \left[1,\ -\sqrt{\frac{5}{3}}\frac{\theta}{\rho},\ 0,\ 0,\ \frac{5}{3}\theta^2\right]^{\mathsf{T}},$$

$$\boldsymbol{r}_2 = [1,\ 0,\ 0,\ 0,\ 0]^{\mathsf{T}}, \quad \boldsymbol{r}_3 = [0,\ 0,\ 1,\ 0,\ 0]^{\mathsf{T}}, \quad \boldsymbol{r}_4 = [0,\ 0,\ 0,\ 1,\ 0]^{\mathsf{T}},$$

$$\boldsymbol{r}_5 = \left[1,\ \sqrt{\frac{5}{3}}\frac{\theta}{\rho},\ 0,\ 0,\ \frac{5}{3}\theta^2\right]^{\mathsf{T}}.$$

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3.6.1 Eigenstructure of Moment Equations

5-Moment Closure

The left eigenvectors, $\boldsymbol{l}$, are

$$\boldsymbol{l}_1 = \left[0,\ -\sqrt{\frac{5}{3}}\rho\theta,\ 0,\ 0,\ 1\right],$$

$$\boldsymbol{l}_2 = \left[-\frac{5}{3}\theta^2,\ 0,\ 0,\ 0,\ 1\right], \quad \boldsymbol{l}_3 = [0,\ 0,\ 1,\ 0,\ 0], \quad \boldsymbol{l}_4 = [0,\ 0,\ 0,\ 1,\ 0],$$

$$\boldsymbol{l}_5 = \left[0,\ \sqrt{\frac{5}{3}}\rho\theta,\ 0,\ 0,\ 1\right].$$

The eigenstructures of $\mathbf{B}^{(5)}$ and $\mathbf{C}^{(5)}$ are similar.

3.6.1 Eigenstructure of Moment Equations

5-Moment Closure

The eigenvalues, λ_i are all real for $p > 0$ and $\rho > 0$, and, as the eigevectors are complete and linearly independent, the moment equations of the Grad 5-moment closure are strictly hyperbolic.

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

For the Grad 10-moment equations, have

$$\mathbf{W}^{(10)} = [\rho, u, v, w, P_{xx}, P_{xy}, P_{xz}, P_{yy}, P_{yz}, P_{zz}]^{\mathsf{T}},$$

and

$$\mathbf{A}^{(10)} = \begin{bmatrix} u & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & u & 0 & 0 & \frac{1}{\rho} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 & \frac{1}{\rho} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & u & 0 & 0 & \frac{1}{\rho} & 0 & 0 & 0 \\ 0 & 3P_{xx} & 0 & 0 & u & 0 & 0 & 0 & 0 & 0 \\ 0 & 2P_{xy} & P_{xx} & 0 & 0 & u & 0 & 0 & 0 & 0 \\ 0 & 2P_{xz} & 0 & P_{xx} & 0 & 0 & u & 0 & 0 & 0 \\ 0 & P_{yy} & 2P_{xy} & 0 & 0 & 0 & 0 & u & 0 & 0 \\ 0 & P_{yz} & P_{xz} & P_{xy} & 0 & 0 & 0 & 0 & u & 0 \\ 0 & P_{zz} & 0 & 2P_{xz} & 0 & 0 & 0 & 0 & 0 & u \end{bmatrix}.$$

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

A characteristic analysis reveals that the eigenvalues λ of $\mathbf{A}^{(10)}$ correspond to correspond to the roots of the polynomial equation

$$\begin{aligned}\det\left(\mathbf{A}^{(10)} - \lambda\mathbf{I}\right) &= \frac{1}{\rho^3}(u-\lambda)^4\left(\rho\lambda^2 - 2\rho u\lambda + \rho u^2 - P_{xx}\right)^2 \\ &\quad \left(\rho\lambda^2 - 2\rho u\lambda + \rho u^2 - 3P_{xx}\right) \\ &= x^4\left(x^2-\theta_{xx}^2\right)^2\left(x^2 - 3\theta_{xx}^2\right) = 0\,,\end{aligned}$$

where $x = u - \lambda$ and $\theta_{xx} = \sqrt{P_{xx}/\rho}$.

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

The 10 eigenvalues are the roots of the preceding characteristic polynomial and are

$$\lambda_1 = u - \sqrt{3}\theta_{xx}\,,$$

$$\lambda_2 = \lambda_3 = u - \theta_{xx}\,,$$

$$\lambda_4 = \lambda_5 = \lambda_6 = \lambda_7 = u\,,$$

$$\lambda_8 = \lambda_9 = u + \theta_{xx}\,,$$

$$\lambda_{10} = u + \sqrt{3}\theta_{xx}\,.$$

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

The right eigenvectors, $\boldsymbol{r}$, are

$$\boldsymbol{r}_1 = \left[1,\ -\frac{\sqrt{3}\theta_{xx}}{\rho},\ -\frac{\sqrt{3}\theta_{xx}}{\rho}\frac{P_{xy}}{P_{xx}},\ -\frac{\sqrt{3}\theta_{xx}}{\rho}\frac{P_{xz}}{P_{xx}},\ \frac{3P_{xx}}{\rho},\ \frac{3P_{xy}}{\rho},\ \frac{3P_{xz}}{\rho},\ \frac{1}{\rho P_{xx}}(P_{xx}P_{yy}+2P_{xy}^2),\ \frac{1}{\rho P_{xx}}(P_{xx}P_{yz}+2P_{xy}P_{xz}),\ \frac{1}{\rho P_{xx}}(P_{xx}P_{zz}+2P_{xz}^2)\right]^{\mathsf{T}},$$

$$\boldsymbol{r}_2 = \left[0,\ 0,\ 1,\ 0,\ 0,\ -\rho\theta_{xx},\ 0,\ -\frac{2P_{xy}}{\theta_{xx}},\ -\frac{P_{xz}}{\theta_{xx}},\ 0\right]^{\mathsf{T}},$$

$$\boldsymbol{r}_3 = \left[0,\ 0,\ 0,\ 1,\ 0,\ 0,\ -\rho\theta_{xx},\ 0,\ -\frac{P_{xy}}{\theta_{xx}},\ -\frac{2P_{xz}}{\theta_{xx}}\right]^{\mathsf{T}},$$

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

$$\boldsymbol{r}_4 = [1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0]^{\mathsf{T}},$$

$$\boldsymbol{r}_5 = [0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 0]^{\mathsf{T}},$$

$$\boldsymbol{r}_6 = [0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0]^{\mathsf{T}},$$

$$\boldsymbol{r}_7 = [0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1]^{\mathsf{T}},$$

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

$$\boldsymbol{r}_8 = \left[0,\ 0,\ 1,\ 0,\ 0,\ \rho\theta_{xx}, 0,\ \frac{2P_{xy}}{\theta_{xx}},\ \frac{P_{xz}}{\theta_{xx}},\ 0\right]^{\mathsf{T}},$$

$$\boldsymbol{r}_9 = \left[0,\ 0,\ 0,\ 1,\ 0,\ 0,\ \rho\theta_{xx}, 0,\ \frac{P_{xy}}{\theta_{xx}},\ \frac{2P_{xz}}{\theta_{xx}}\right]^{\mathsf{T}},$$

$$\begin{aligned}\boldsymbol{r}_{10} = & \left[1,\ \frac{\sqrt{3}\theta_{xx}}{\rho},\ \frac{\sqrt{3}\theta_{xx}}{\rho}\frac{P_{xy}}{P_{xx}},\ \frac{\sqrt{3}\theta_{xx}}{\rho}\frac{P_{xz}}{P_{xx}},\ \frac{3P_{xx}}{\rho},\ \frac{3P_{xy}}{\rho},\ \frac{3P_{xz}}{\rho},\right.\\ & \frac{1}{\rho P_{xx}}(P_{xx}P_{yy} + 2P_{xy}^2),\ \frac{1}{\rho P_{xx}}(P_{xx}P_{yz} + 2P_{xy}P_{xz}),\\ & \left.\frac{1}{\rho P_{xx}}(P_{xx}P_{zz} + 2P_{xz}^2)\right]^{\mathsf{T}}.\end{aligned}$$

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3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

The left eigenvectors, $\boldsymbol{l}$, are

$$\boldsymbol{l}_1 = \left[0,\ \sqrt{3}\rho\theta_{xx},\ 0,\ 0,\ -1,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\boldsymbol{l}_2 = \left[0,\ P_{xx}P_{xy},\ -P_{xx}^2,\ 0,\ -P_{xy}\theta_{xx},\ P_{xx}\theta_{xx},\ 0,\ 0,\ 0,\ 0\right],$$

$$\boldsymbol{l}_3 = \left[0,\ P_{xx}P_{xz},\ 0,\ -P_{xx}^2,\ -P_{xz}\theta_{xx},\ 0,\ P_{xx}\theta_{xx},\ 0,\ 0,\ 0\right],$$

$$\boldsymbol{l}_4 = \left[-3\frac{P_{xx}}{\rho},\ 0,\ 0,\ 0,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\boldsymbol{l}_5 = \left[4P_{xy}^2 - P_{xx}P_{yy},\ 0,\ 0,\ 0,\ 0,\ -2\rho P_{xy},\ 0,\ \rho P_{xx},\ 0,\ 0\right],$$

$$\boldsymbol{l}_6 = \left[4P_{xy}P_{xz} - P_{xx}P_{yz},\ 0,\ 0,\ 0,\ 0,\ -\rho P_{xz},\ -\rho P_{xy},\ 0,\ \rho P_{xx}, 0\right],$$

$$\boldsymbol{l}_7 = \left[4P_{xz}^2 - P_{xx}P_{zz},\ 0,\ 0,\ 0,\ 0,\ 0,\ -2\rho P_{xz},\ 0,\ 0,\ \rho P_{xx}\right],$$

3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

$$\boldsymbol{l}_8 = \left[0,\ -P_{xx}P_{xy},\ P_{xx}^2,\ 0,\ -P_{xy}\theta_{xx},\ P_{xx}\theta_{xx},\ 0,\ 0,\ 0,\ 0\right]\,,$$
$$\boldsymbol{l}_9 = \left[0,\ -P_{xx}P_{xz},\ 0,\ P_{xx}^2,\ -P_{xz}\theta_{xx},\ 0,\ P_{xx}\theta_{xx},\ 0,\ 0,\ 0\right]\,,$$
$$\boldsymbol{l}_{10} = \left[0,\ \sqrt{3}\rho\theta_{xx},\ 0,\ 0,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0\right]\,.$$

Again, the eigenstructures of $\mathbf{B}^{(10)}$ and $\mathbf{C}^{(10)}$ are similar to that of $\mathbf{A}^{(10)}$.

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3.6.1 Eigenstructure of Moment Equations

10-Moment Closure

Letting $\Theta_{\alpha\beta} = P_{\alpha\beta}/\rho$, and $\Delta = \det(\boldsymbol{\Theta})$. More specifically,

$$\boldsymbol{\Theta} = \frac{1}{\rho}\begin{bmatrix} P_{xx} & P_{xy} & P_{xz} \\ P_{xy} & P_{yy} & P_{yz} \\ P_{xz} & P_{yz} & P_{zz} \end{bmatrix}\,,$$

$$\boldsymbol{\Theta}^{-1} = \frac{1}{\rho^2\Delta}\begin{bmatrix} P_{yy}P_{zz}-P_{xz}^2 & P_{xz}P_{yz}-P_{xy}P_{zz} & P_{xy}P_{yz}-P_{xz}P_{yy} \\ P_{xz}P_{yz}-P_{xy}P_{zz} & P_{xx}P_{zz}-P_{xz}^2 & P_{xy}P_{xz}-P_{xx}P_{yz} \\ P_{xy}P_{yz}-P_{xz}P_{yy} & P_{xy}P_{xz}-P_{xx}P_{yz} & P_{xx}P_{yy}-P_{xy}^2 \end{bmatrix}\,,$$

$$\Delta = \frac{1}{\rho^3}\left(P_{xx}P_{yy}P_{zz} + 2P_{xy}P_{xz}P_{yz} - P_{xx}P_{yz}^2 - P_{yy}P_{xz}^2 - P_{zz}P_{xy}^2\right)\,,$$

such that $\boldsymbol{\Theta}^{-1}\mathbf{P} = \rho\mathbf{I}$. It can be shown that the moment equations of the 10-moment closure are strictly hyperbolic provided that $\rho > 0$, $\boldsymbol{\Theta}$ is a positive definite, and $\Delta > 0$.

3.6.1 Eigenstructure of Moment Equations

13- and 20-Moment Closures

For the Grad 13- and 20-moment equations, have

$$\mathbf{W}^{(13)} = [\rho, u, v, w, P_{xx}, P_{xy}, P_{xz}, P_{yy}, P_{yz}, P_{zz}, q_x, q_y, q_z]^{\mathsf{T}} \,,$$

and

$$\mathbf{W}^{(20)} = [\rho, u, v, w, P_{xx}, P_{xy}, P_{xz}, P_{yy}, P_{yz}, P_{zz}, \\ Q_{xxx}, Q_{xxy}, Q_{xxz}, Q_{xyy}, Q_{xyz}, Q_{xzz}, Q_{yyy}, Q_{yyz}, Q_{yzz}, Q_{zzz},]^{\mathsf{T}} \,.$$

3.6.1 Eigenstructure of Moment Equations

13- and 20-Moment Closures

Unfortunately, the characteristic polynomials for both $\mathbf{A}^{(13)}$ and $\mathbf{A}^{(20)}$ do not factor and explicit analytical expressions for the eigenvalues of each cannot be obtained (the characteristic polynomials of $\mathbf{A}^{(13)}$ and $\mathbf{A}^{(20)}$ would fill several screens of this presentation!). The eigenstructure can be determined numerically. For near equilibrium conditions, the eigenvalues are all real and the equation sets are hyperbolic. However, experience has shown that the moment equations of the Grad 13- and 20-moment closures do not remain hyperbolic for the full range of physically realizable moments.

3.6.2 Stationary One-Dimensional Planar Shock Structure

The application of the classical Grad moment closures to the prediction of planar shock structure for a monatomic gas is now considered. Shock profile prediction is a challenging problem that features significant departures from local thermodynamic equilibrium (LTE), yet it is unencumbered with difficulties associated with complex geometries and/or boundary condition prescription. For these reasons it is useful for evaluating the capabilities of moment methods. Included in the investigation are results for the Grad 10-, 13- and 20-moment closures with comparisons to the solutions of the Navier-Stokes and Burnett equations. Comparisons are also made with Direct Simulation Monte Carlo (DSMC) results using the method of Bird (1994).

3.6.2 Stationary One-Dimensional Planar Shock Structure

For the shock structure study, so-called ellipsoidal statistical collision operator of Holway (1966) is used to describe collisional processes for monatomic gases. This collision operator, often referred to the ellipsoidal statistical model, preserves much of the simplicity of relaxation-time models, while allowing for a realistic and selectable Prandtl number. For the monatomic gases of interest, it is assumed that $\mathrm{Pr} = 2/3$ and the viscosity is taken to have a power-law dependence on the temperture, T, of the form

$$\mu = \mu_o (T/T_o)^{\omega} ,$$

where μ_o and T_o are reference values and the exponent ω depends on the form for the forces governing inter-particle collisional processes (taken to be $\omega = 1$ for Maxwell molecules here).

3.6.2 Stationary One-Dimensional Planar Shock Structure

The moment equations of the Grad moment closures applied to the prediction of one-dimensional shock-structure flows can be expressed in weak conservation form as

$$\frac{\partial \mathbf{M}^{(N)}}{\partial t} + \frac{\partial \mathbf{F}^{(N)}}{\partial x} = \mathbf{S}^{(N)} ,$$

where $\mathbf{M}^{(N)}$ is the solution vector of N macroscopic velocity moments for the closure, $\mathbf{F}^{(N)}$ is the corresponding moment flux vector, and $\mathbf{S}^{(N)}$ is the source vector describing the time rate of change of the velocity moments produced by collisional processes. A standard Godunov-type finite-volume scheme with piecewise limited linear reconstruction and Riemann-solver-based flux functions is used to solve the moment equations for each closure.

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3.6.2 Stationary One-Dimensional Planar Shock Structure

5-Moment Closure

The most elementary Grad moment closure is the 5-moment Maxwellian model for which $N = 5$. In this approximation, it is assumed that the gas is everywhere in LTE and that the phase-space velocity distribution function is given by the Maxwell-Boltzmann distribution, $\mathcal{M}$, which for the one-dimensional planar flows of interest has the form

$$\mathcal{M} = \frac{\rho}{m\,(2\pi p/\rho)^{3/2}} \exp\left[-\frac{1}{2}\frac{\rho(c_x^2 + 2c_y^2)}{p}\right] .$$

The closure results in the well-known Euler equations of inviscid compressible gas dynamics that describe the time evolution of ρ, u, and p.

3.6.2 Stationary One-Dimensional Planar Shock Structure

5-Moment Closure

The solution vector, $\mathbf{M}^{(5)}$, and source vector, $\mathbf{S}^{(5)}$, of the Euler equations for a monatomic gas can be expressed as

$$\mathbf{M}^{(5)} = \begin{bmatrix} \rho \\ \rho u \\ \frac{1}{2}\rho u^2 + \frac{3}{2}p \end{bmatrix}, \quad \mathbf{S}^{(5)} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Note that the discontinuous solutions for shock wave structure provided by the Euler equations are fully understood (i.e., the Rankine-Hugoniot conditions); however, the Euler equations are used in the shock profile computations to prescribe initial and boundary data.

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3.6.2 Stationary One-Dimensional Planar Shock Structure

20-Moment Closure

For the one-dimensional shock structure flows, the approximate form for the distribution function of the Grad 20-moment closure is given by

$$\begin{aligned} \mathcal{F}^{(20)} = \mathcal{M}\Bigg[1 &- \left(\frac{Q_{xxx}}{2\rho\theta^3} + \frac{Q_{xyy}}{\rho\theta^3}\right)\frac{c_x}{\theta} \\ &+ \frac{(P_{xx} - P_{yy})}{3\rho\theta^2}\left(\frac{c_x^2}{\theta^2} - \frac{c_y^2}{\theta^2}\right) \\ &+ \frac{Q_{xxx}}{6\rho\theta^3}\frac{c_x^3}{\theta^3} + \frac{Q_{xyy}}{\rho\theta^3}\frac{c_x}{\theta}\frac{c_y^2}{\theta^2}\Bigg], \end{aligned}$$

where $\theta = p/\rho$ and the solution and source vectors of the system of moment equations for the six dependent variables ρ, u, P_{xx}, P_{yy}, Q_{xxx}, and Q_{xyy} may be written as

3.6.2 Stationary One-Dimensional Planar Shock Structure

20-Moment Closure

$$\mathbf{M}^{(20)} = \begin{bmatrix} \rho \\ \rho u \\ \rho u^2 + P_{xx} \\ P_{yy} \\ \rho u^3 + 3uP_{xx} + Q_{xxx} \\ uP_{yy} + Q_{xyy} \end{bmatrix},$$

$$\mathbf{S}^{(20)} = \begin{bmatrix} 0 \\ 0 \\ -\frac{2}{3\tau}(P_{xx} - P_{yy}) \\ \frac{1}{3\tau}(P_{xx} - P_{yy}) \\ -\frac{2}{\tau}u(P_{xx} - P_{yy}) - \frac{\Pr}{\tau}Q_{xxx} \\ \frac{1}{3\tau}u(P_{xx} - P_{yy}) - \frac{\Pr}{\tau}Q_{xyy} \end{bmatrix}.$$

3.6.2 Stationary One-Dimensional Planar Shock Structure

13-Moment Closure

The approximate form for the distribution function of the Grad 13-moment closure in the one-dimensional case is given by

$$\mathcal{F}^{(13)} = \mathcal{M}\left[1 - \frac{q_x}{\rho\theta^3}\frac{c_x}{\theta} + \frac{(P_{xx} - P_{yy})}{3\rho\theta^2}\left(\frac{c_x^2}{\theta^2} - \frac{c_y^2}{\theta^2}\right) + \frac{q_x}{5\rho\theta^3}\frac{c_x}{\theta}\left(\frac{c_x^2}{\theta^2} + 2\frac{c_y^2}{\theta^2}\right)\right],$$

where again $\theta = p/\rho$ and the solution and source vectors of the system of moment equations for the five dependent variables ρ, u, P_{xx}, P_{yy}, and q_x can be written as

3.6.2 Stationary One-Dimensional Planar Shock Structure

13-Moment Closure

$$\mathbf{M}^{(13)} = \begin{bmatrix} \rho \\ \rho u \\ \rho u^2 + P_{xx} \\ P_{yy} \\ \frac{1}{2}\rho u^3 + \frac{1}{2} u(3P_{xx} + 2P_{yy}) + q_x \end{bmatrix} .$$

$$\mathbf{S}^{(13)} = \begin{bmatrix} 0 \\ 0 \\ -\frac{2}{3\tau}(P_{xx} - P_{yy}) \\ \frac{1}{3\tau}(P_{xx} - P_{yy}) \\ -\frac{2}{3\tau} u(P_{xx} - P_{yy}) - \frac{\mathrm{Pr}}{\tau} q_x \end{bmatrix} .$$

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3.6.2 Stationary One-Dimensional Planar Shock Structure

10-Moment Closure

Finally, the approximate form for the distribution function of the Grad 10-moment closure in the one-dimensional case is given by

$$\mathcal{F}^{(10)} = \mathcal{M}\left[1 + \frac{(P_{xx} - P_{yy})}{3\rho\theta^2}\left(\frac{c_x^2}{\theta^2} - \frac{c_y^2}{\theta^2}\right)\right] ,$$

with $\theta = p/\rho$ and the solution and source vectors of the system of moment equations for the four dependent variables ρ, u, P_{xx}, and P_{yy} can be written as

3.6.2 Stationary One-Dimensional Planar Shock Structure

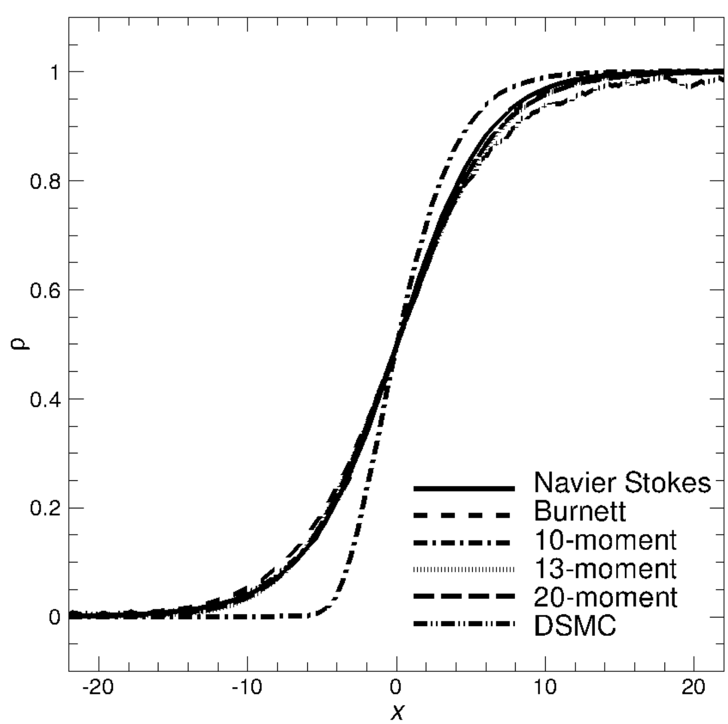
10-Moment Closure

$$\mathbf{M}^{(10)} = \begin{bmatrix} \rho \\ \rho u \\ \rho u^2 + P_{xx} \\ P_{yy} \end{bmatrix},$$

$$\mathbf{S}^{(10)} = \begin{bmatrix} 0 \\ 0 \\ -\dfrac{2}{3\tau}(P_{xx} - P_{yy}) \\ \dfrac{1}{3\tau}(P_{xx} - P_{yy}) \end{bmatrix}.$$

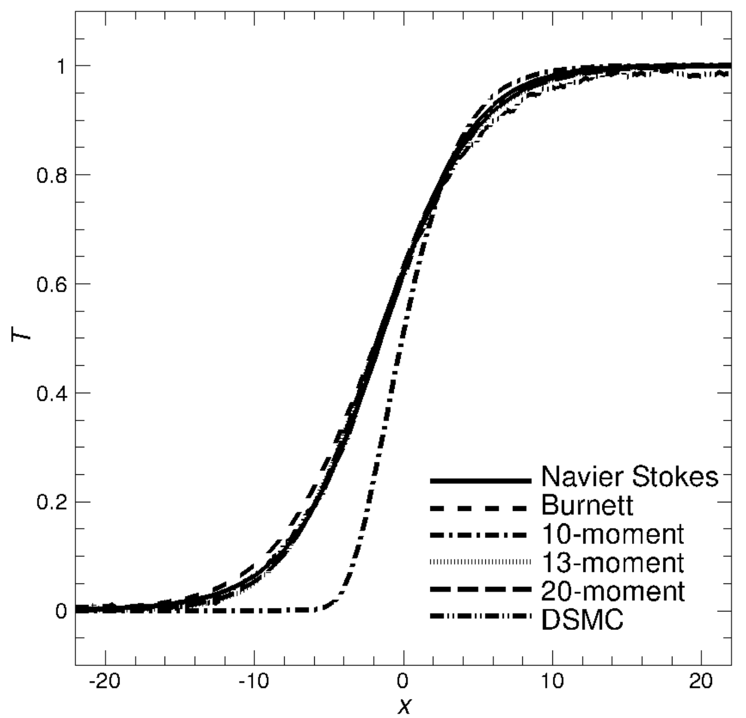
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.25$, Density Profile, ρ



3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.25$, Temperature Profile, T



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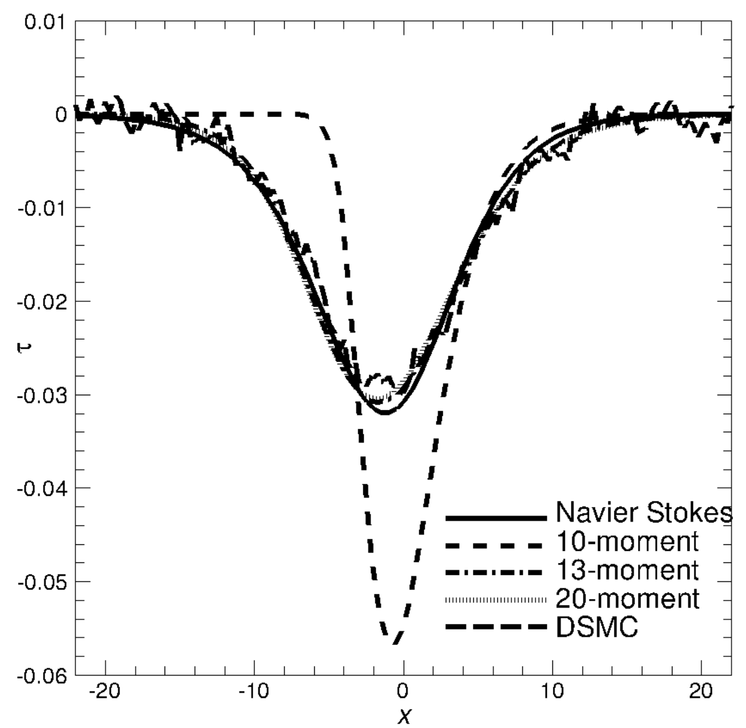
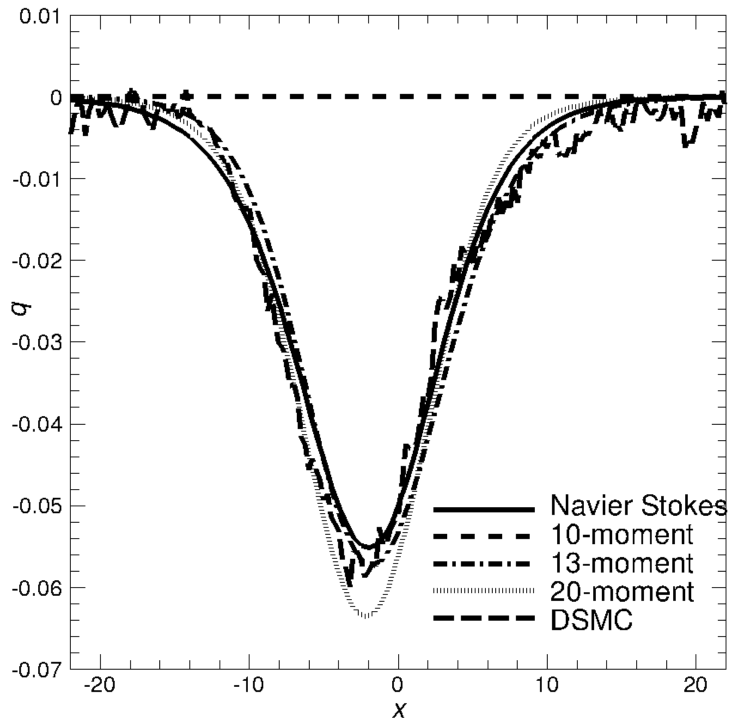
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.25$, Fluid-Stress Profile, $\tau_{xx} = -2(P_{xx} - P_{yy})/3$



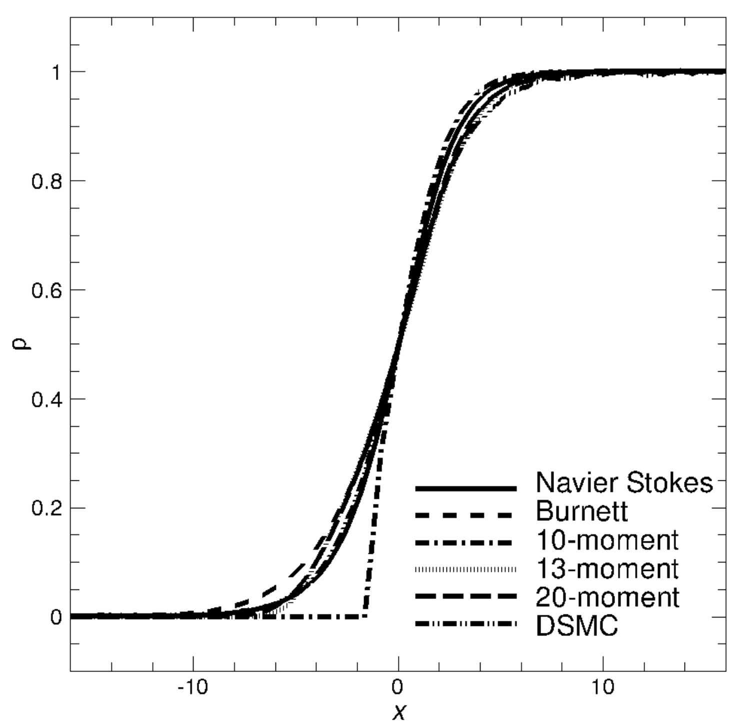
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.25$, Heat-Flux Profile, Q_{xxx}



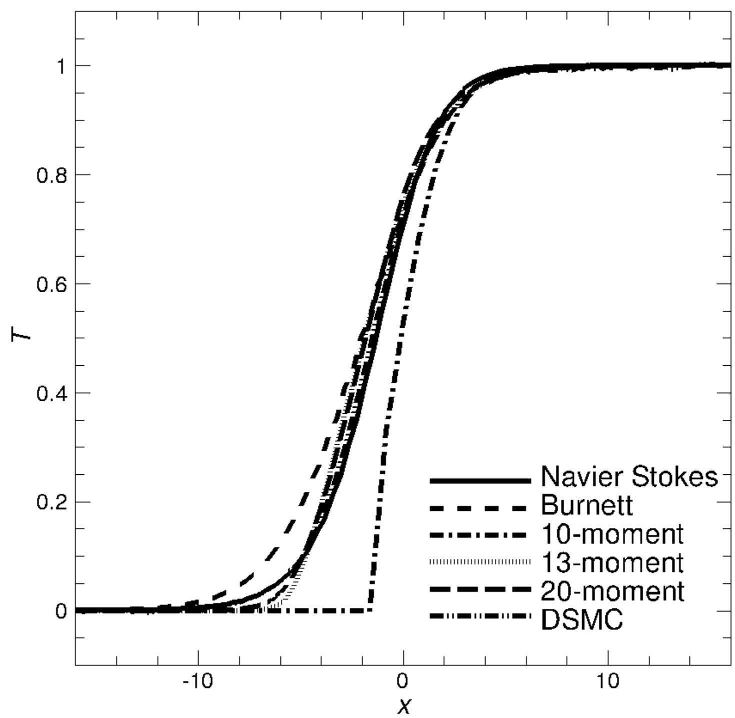
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.55$, Density Profile, ρ



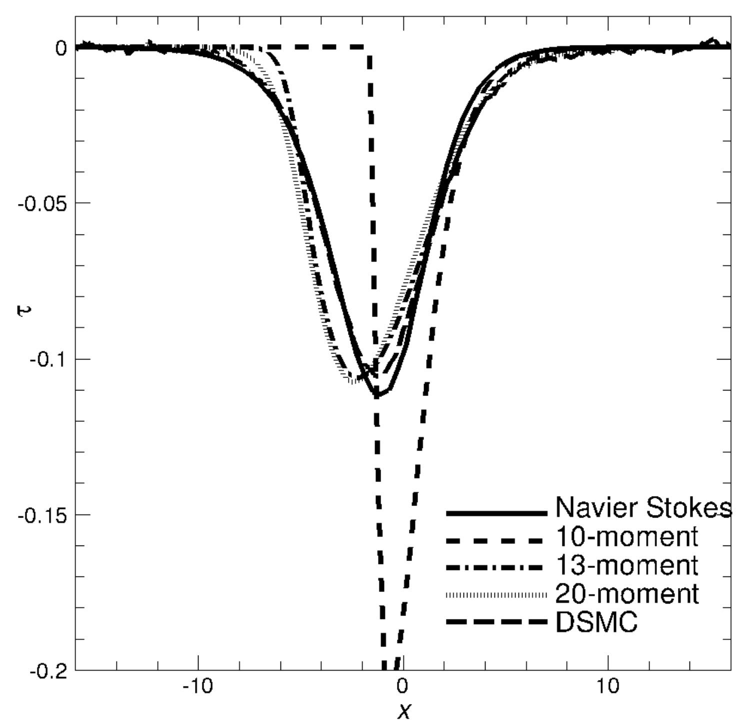
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.55$, Temperature Profile, T



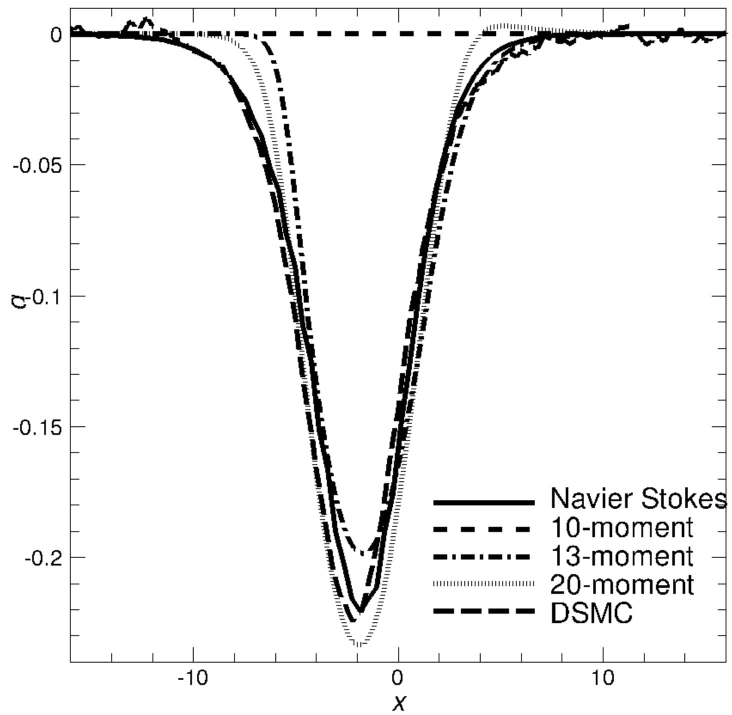
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.55$, Fluid-Stress Profile, $\tau_{xx} = -2(P_{xx} - P_{yy})/3$



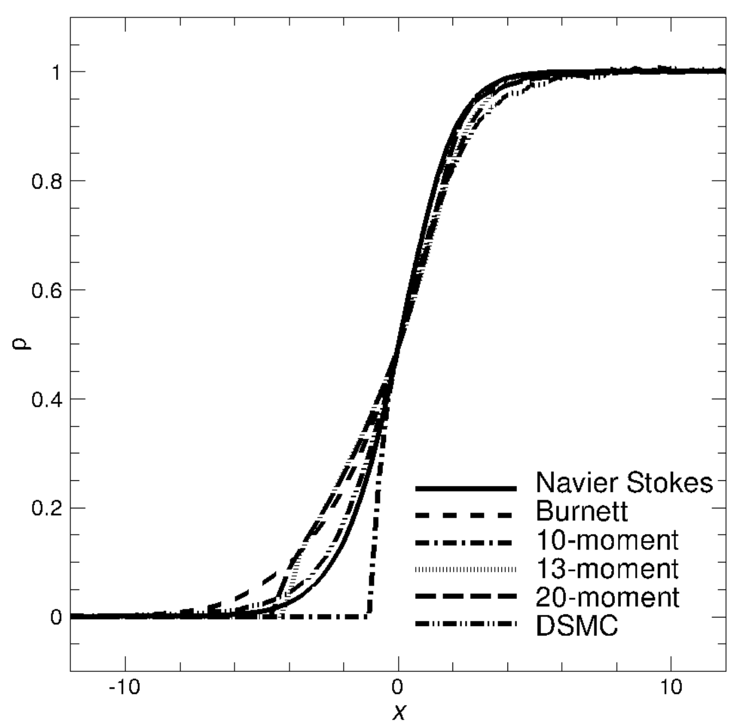
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 1.55$, Heat-Flux Profile, Q_{xxx}



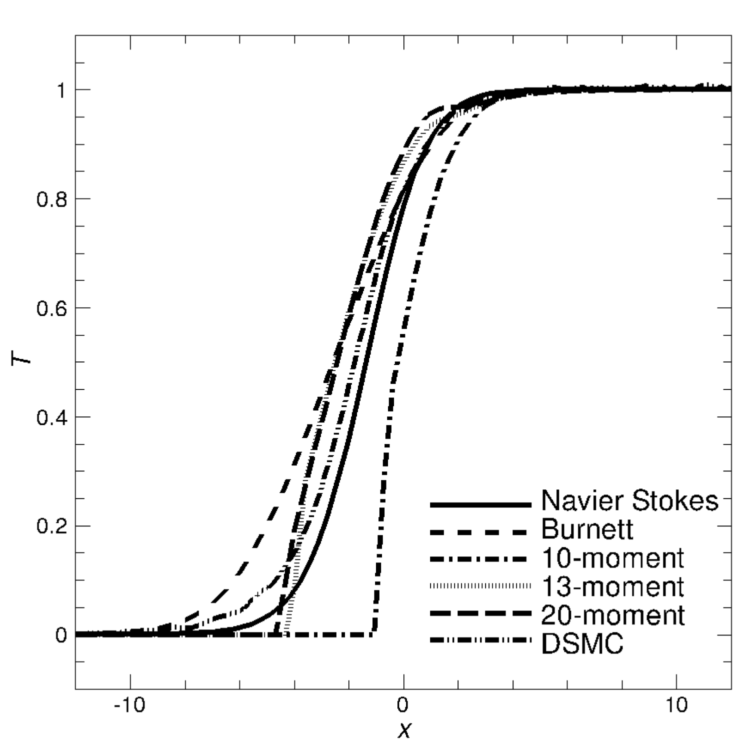
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 2.00$, Density Profile, ρ



3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 2.00$, Temperature Profile, T



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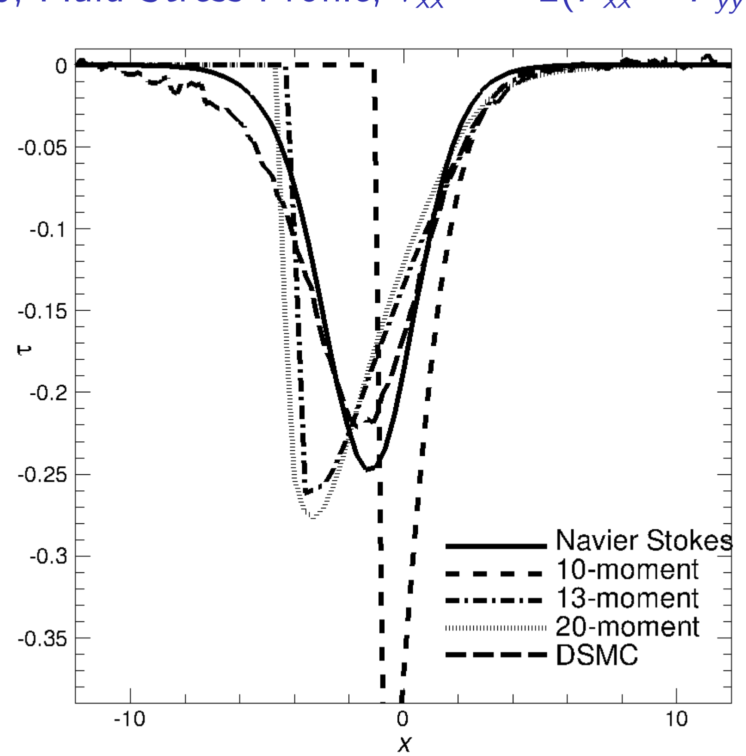
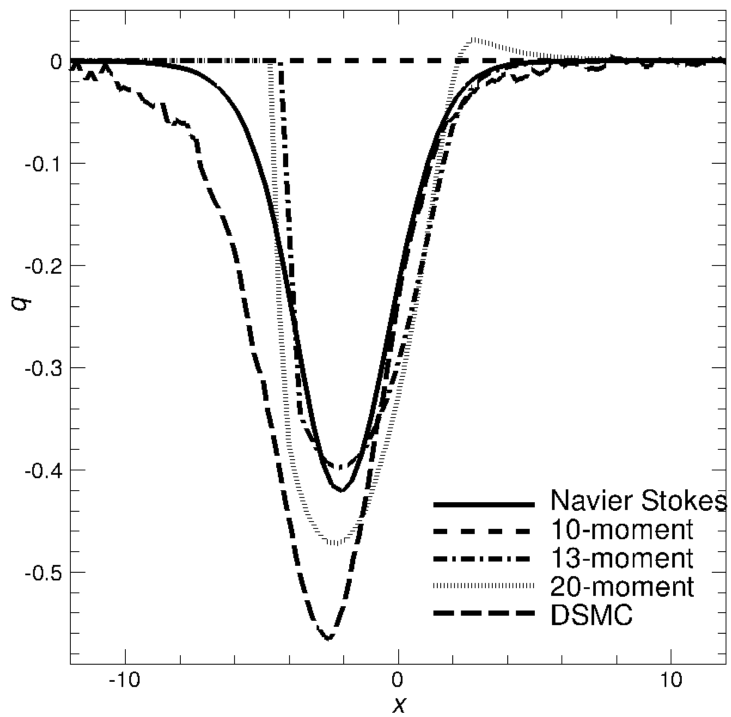
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 2.00$, Fluid-Stress Profile, $\tau_{xx} = -2(P_{xx} - P_{yy})/3$



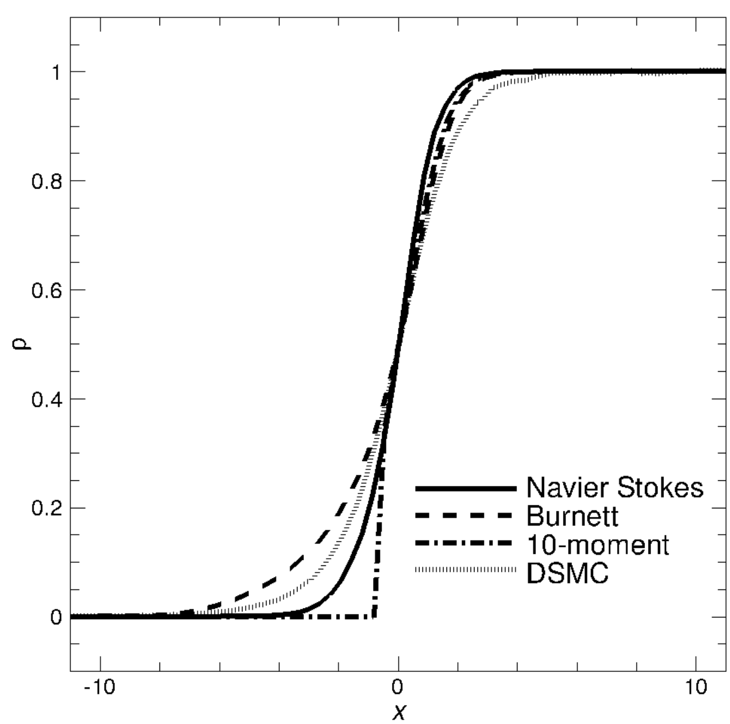
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 2.00$, Heat-Flux Profile, Q_{xxx}



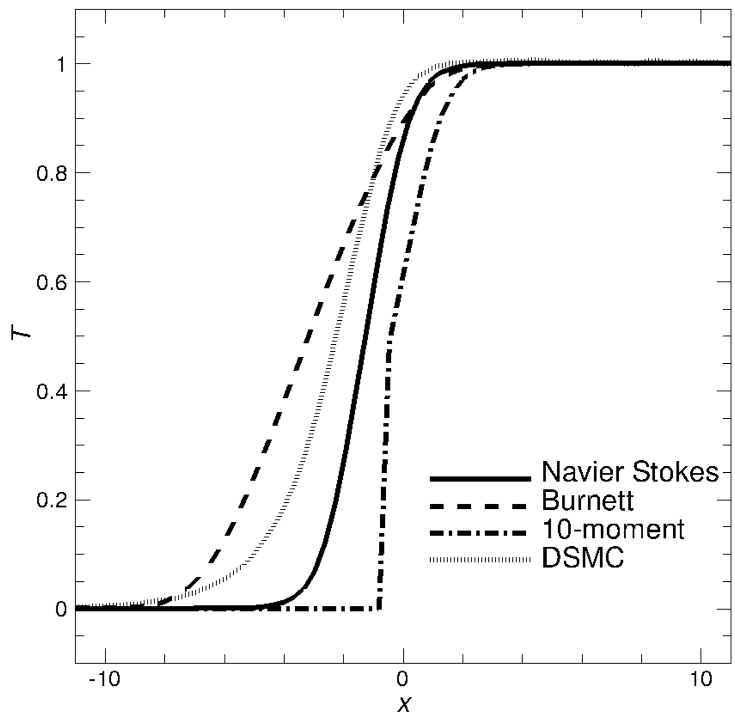
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 3.80$, Density Profile, ρ



3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 3.80$, Temperature Profile, T



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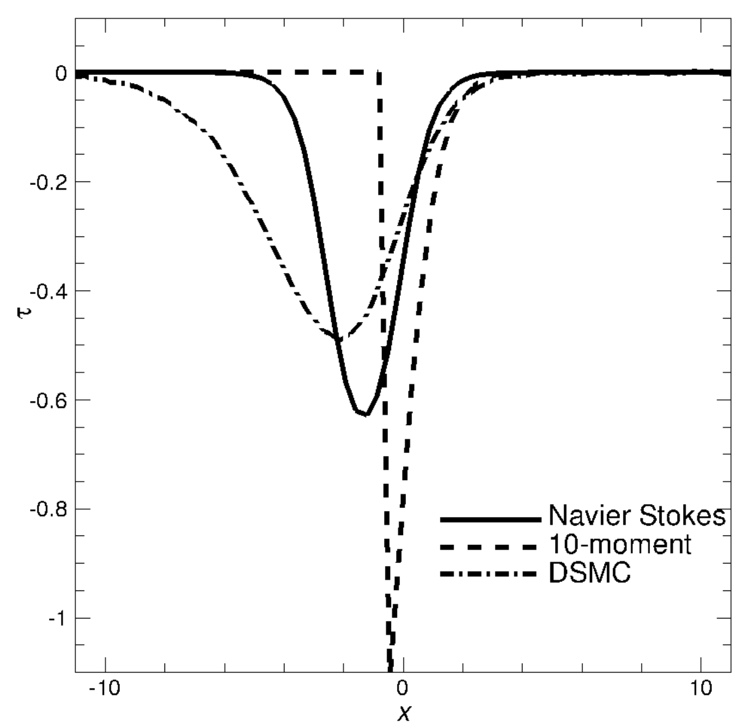
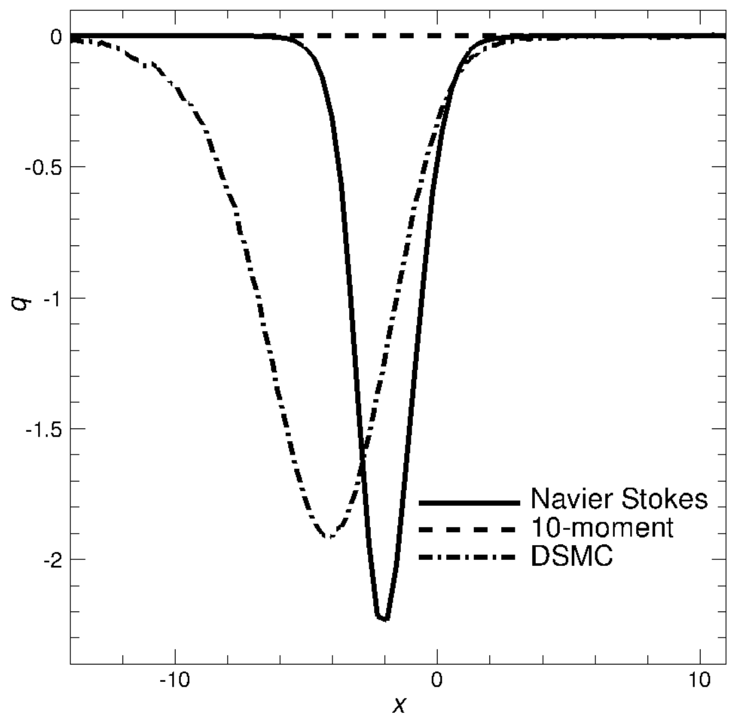
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 3.80$, Fluid-Stress Profile, $\tau_{xx} = -2(P_{xx} - P_{yy})/3$



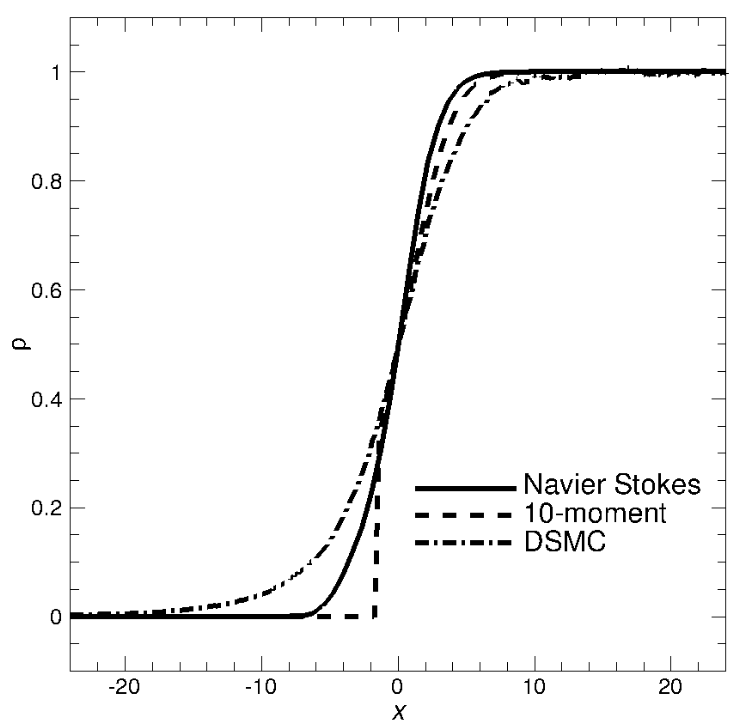
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 3.80$, Heat-Flux Profile, Q_{xxx}



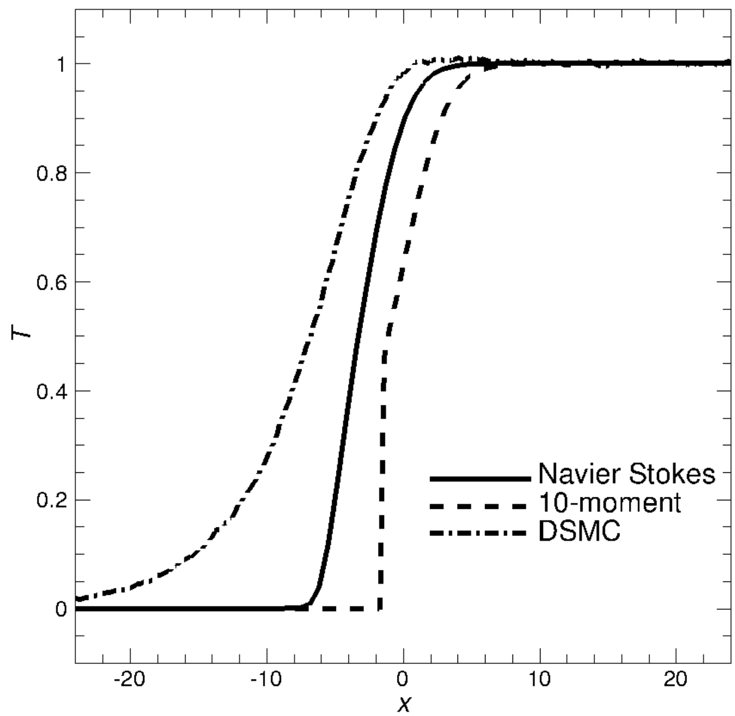
3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 9.00$, Density Profile, ρ



3.6.2 Stationary One-Dimensional Planar Shock Structure

$M_s = 9.00$, Temperature Profile, T



3.6.3 High-Frequency Sound Propagation

The propagation of sound waves can be studied in an acoustic resonator as a function of frequency. The high-frequency (short wave length) limit corresponds to a high-Knudsen number limit. Sound propagation as a function of frequency has been studied experimentally and Müller and Ruggeri (1993) have considered the application of Grad-type moment closures to this problem.

3.6.3 High-Frequency Sound Propagation

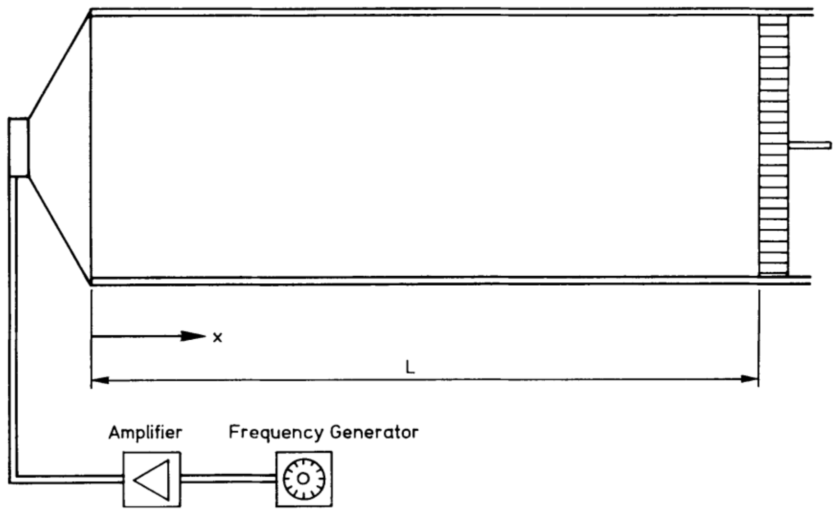


Figure 11.1 Acoustic resonator (schematic)

Schematic of acoustic resonator (taken from Müller and Ruggeri, 1993)

3.6.3 High-Frequency Sound Propagation

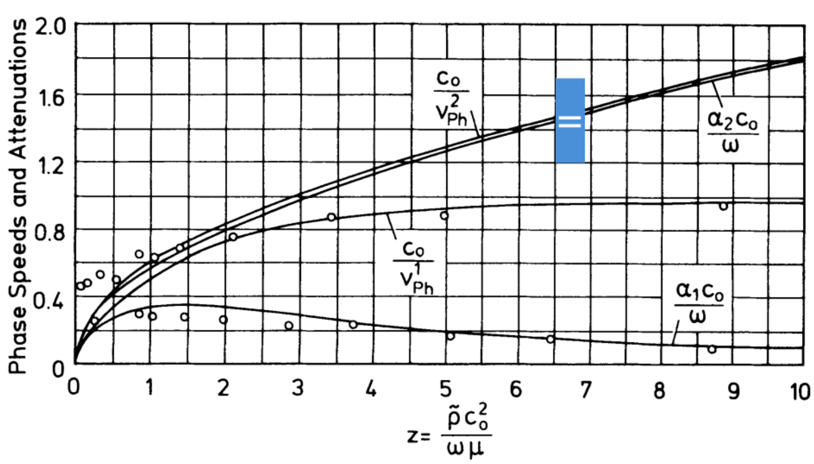


Figure 11.3 Phase speeds and attenuations in the NSF theory. Experimental points by Meyer & Sessler [126]

Navier-Stokes description compared to experiments (taken from Müller and Ruggeri, 1993)

3.6.3 High-Frequency Sound Propagation

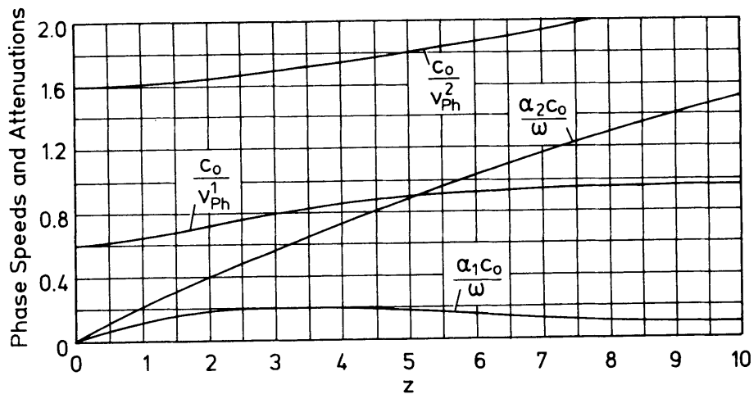


Figure 11.4 Phase speeds and attenuations of extended thermodynamics of 13 variables.

Grad 13-moment description (taken from Müller and Ruggeri, 1993)

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3.6.3 High-Frequency Sound Propagation

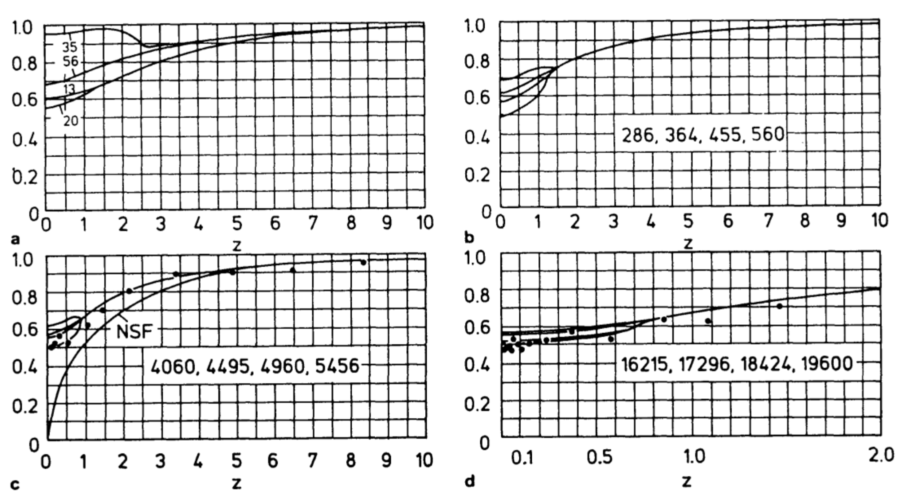

Figure 11.5 Phase speed of the sound mode in theories with more and more moments. (Note the change of scale in Figure 11.5d.)

High-order Grad-type closures compared to experiments (taken from Müller and Ruggeri, 1993)

3.7 Summary of Classical Moment Methods

3.7.1 Difficulties and Challenges with Grad Closures

- Formal convergence of the Grad moment closure approach to the solution of the Boltzmann equation can be assessed via order of magnitude approach
- How many moments should be considered? Which moments should be included in the selected set and is there an optimal set? These questions remain open.
- Approximate form for NDF in Grad moment closures is not strictly positive
- higher-order members of Grad closures suffer from loss of hyperbolicity (as illustrated for shock structure simulations)
- Validity of the Grad closures is therefore questionable for full range of physically realizable moments