Appendix A: Connection between B.G.K., Navier Stokes and Euler equations

Derivations of the Navier-Stokes equations from the Boltzmann equation can be found in Kogan[18], Chapman and Cowling[6] and from the Bhatnagar-Gross-Krook equation in Cercignani[5] for the case of perfect monotonic gases. Here we reconsider the derivation of the Navier-Stokes and Euler equations from the BGK equation, providing from the outset for polyatomic gases.

To derive the Navier-Stokes equations, let \( \tau = \epsilon \hat{\tau} \) where \( \epsilon \) is a small dimensionless quantity, and suppose that \( g \) has a Taylor series expansion about some point \( x_i, t \). Since \( \tau \) depends on the local thermodynamic variables, and since these depend on the moments of \( g \), we may assume that \( \tau \) and consequently \( \hat{\tau} \) can be expanded about the point \( x_i, t \). Now consider the formal solution of the BGK equation for \( f \), supposing that \( g \) is known, and suppose that \( t' > \tau \); i.e. that the initial condition were imposed many relaxation times ago. We can then ignore the initial value of \( f \), and, with negligible error, the difference between \( t' = 0 \) and \( t' = -\infty \) in the integral on the right side of Eq.(2.8). It can be shown from the integral equations(2.10) that the Taylor series expansion of \( \tau \) and \( g \) about \( x_i, t \) may be written as power series in \( \epsilon \), and therefore \( f \) has an expansion in powers of \( \epsilon \). We can find the terms in this expansion from the formal solution for \( f \), or, more easily, by putting

\[
f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \ldots \tag{A.1}
\]

and \( \tau = \epsilon \hat{\tau} \) into the BGK equation directly. Let

\[
D_u = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i},
\tag{A.2}
\]

and write the BGK equation as \( \epsilon \hat{\tau} D_u f + f - g = 0 \). An expansion of this equation in powers of \( \epsilon \) yields

\[
f = g - \epsilon \hat{\tau} D_u g + \epsilon^2 \hat{\tau} D_u (\hat{\tau} D_u g) + \ldots \tag{A.3}
\]
and the compatibility conditions (2.24), after dividing by \( \epsilon \), give

\[
\int \psi_\alpha D_u g d\Xi = \epsilon \int \psi_\alpha D_u (\hat{\nabla} D_u g) d\Xi + O(\epsilon^2) \quad .
\]  \hspace{1cm} (A.4)

We define \( \mathcal{L}_\alpha \) to be the integral on the left side of this equation, and \( \mathcal{R}_\alpha \) to be the integral on the right, so that Eq.(A.4) can be written as

\[
\mathcal{L}_\alpha = \epsilon \mathcal{R}_\alpha + O(\epsilon^2) \quad .
\]  \hspace{1cm} (A.5)

We show that these equations give the Euler equations if we drop the term of \( O(\epsilon) \), and the Navier-Stokes equations if we drop terms of \( O(\epsilon^2) \). To simplify the notation, let

\[
< \psi_\alpha (...) > \equiv \int \psi_\alpha (...) g d\Xi \quad ,
\]  \hspace{1cm} (A.6)

and consider

\[
\mathcal{L}_\alpha \equiv \int \psi_\alpha D_u g d\Xi \\
= \int \psi_\alpha (g,_{t} + u_i g,_{i}) d\Xi \\
= < \psi_\alpha >,_{t} + < \psi_\alpha u_i >,_{i} \quad ,
\]  \hspace{1cm} (A.7)

since \( \psi_\alpha \) is independent of \( x_i \) and \( t \). Now Eq.(A.5) shows that

\[
< \psi_\alpha >,_{t} + < \psi_\alpha u_i >,_{i} = O(\epsilon) \quad .
\]  \hspace{1cm} (A.8)

for all \( \alpha \), and therefore, in reducing \( \mathcal{R}_\alpha \) on the right side of Eq.(A.5), which is already \( O(\epsilon) \), we can drop \( O(\epsilon) \) quantities and their derivatives. Put differently, we first reduce the \( \mathcal{L}_\alpha \) to find that \( \mathcal{L}_\alpha = 0 \) \( (\alpha = 1, 2, ... 5) \) is identical to the Euler equations; then we use the fact that \( \mathcal{L}_\alpha \) is \( O(\epsilon) \) to simplify \( \mathcal{R}_\alpha \) — the result is the Navier-Stokes equations.
The expression for $R_\alpha$ contains time derivatives which must be eliminated. We have, from the definition of $R_\alpha$,

$$R_\alpha = \tilde{\tau}[<\psi_\alpha>,_{tt} + 2<\psi_\alpha u_k>,_{tt} + <\psi_\alpha u_k u_l>,_{lk}]$$

$$+ \tilde{\tau},[<\psi_\alpha>,_{t} + <\psi_\alpha u_l>,_{l}] + \tilde{\tau},[<\psi_\alpha u_k>,_{t} + <\psi_\alpha u_k u_l>,_{l}]. \quad (A.9)$$

According to Eq.(A.8) the coefficient of $\tilde{\tau},$ in this expression is $\mathcal{O}(\epsilon)$, and can therefore be neglected. As for the first term, consider

$$\frac{\partial}{\partial t} [<\psi_\alpha>,_{t} + <\psi_\alpha u_k>,_{k}] = <\psi_\alpha>,_{tt} + <\psi_\alpha u_k>,_{kt}$$

$$= \mathcal{L}_{\alpha, t} = \mathcal{O}(\epsilon) \quad (A.10)$$

Then the first term in Eq.(A.9) is

$$\tilde{\tau} \frac{\partial}{\partial x_k} [<\psi_\alpha u_k>,_{t} + <\psi_\alpha u_k u_l>,_{l}] + \mathcal{O}(\epsilon), \quad (A.11)$$

which can be combined with the third term to give

$$R_\alpha = \frac{\partial}{\partial x_k} \{\tilde{\tau}[<\psi_\alpha u_k>,_{t} + <\psi_\alpha u_k u_l>,_{l}]\} + \mathcal{O}(\epsilon) \quad , \quad (A.12)$$

which eliminates the second time derivatives from $R_\alpha$; the first time derivatives will be removed by using $\mathcal{L}_\alpha \approx 0.$

The Euler equations follow from putting $\mathcal{L}_\alpha = 0.$ To see this, consider

$$\mathcal{L}_1 = <\psi_1>,_{t} + <\psi_1 u_k>,_{k} = \rho,_{t} + (\rho U_k),_{k} \quad , \quad (A.13)$$

since $\psi_1 = 1; \mathcal{L}_1 = \mathcal{O}(\epsilon)$ is the continuity equation if we neglect $\mathcal{O}(\epsilon).$ For $\alpha = 2, 3, 4,$ it is convenient to define $\mathcal{L}_i$ and $R_i$ such that $i = \alpha - 1$ and to let $w_i = u_i - U_i.$ Then

$$\mathcal{L}_i = <u_i>,_{t} + <u_i u_k>,_{k} = (\rho U_i),_{t} + [\rho U_i U_k + <w_i w_k>],_{k} \quad , \quad (A.14)$$
since all moments of \( g \) odd in \( w \) vanish. The pressure tensor is defined by

\[
p_{ik} = \langle w_i w_k \rangle = \pi \delta_{ik}. \tag{A.15}
\]

(The diagonal form of \( p_{ik} \) is obvious from the fact that \( g \) can be written as a function of \( w_k^2 \).) Then

\[
\mathcal{L}_i = (\rho U_i)_t + (\rho U_i U_k + p \delta_{ik})_k \tag{A.16}
\]

and \( \mathcal{L}_i = 0 \) is the Euler equation for the conservation of momentum. For the energy equation we have

\[
\mathcal{L}_5 = \frac{1}{2} \langle u_n^2 + \xi^2 \rangle_k + \frac{1}{2} \langle u_t (u_n^2 + \xi^2) \rangle_t \tag{A.17}
\]

or

\[
\mathcal{L}_5 = \left( \frac{1}{2} \rho U_n^2 + \frac{K}{2} \right)_t + \left( \frac{1}{2} \rho U_k U_n^2 + \frac{K}{2} p U_k \right)_k. \tag{A.18}
\]

Setting \( \mathcal{L}_5 = 0 \) gives the energy equation in the absence of dissipation.

We proceed to eliminate the time derivatives from \( \mathcal{R}_\alpha \) using the fact that \( \mathcal{L}_\alpha = \mathcal{O}(\epsilon) \). For \( \alpha = 1 \), we have

\[
\mathcal{R}_1 = \{ \mathcal{R}[< u_k >_k + < u_k u_t >_k] \}_k \tag{A.19}
\]

The quantity in square brackets is \( \mathcal{L}_k \), which implies that \( \mathcal{R}_1 = \mathcal{O}(\epsilon) \), and \( \mathcal{L}_1 = \epsilon \mathcal{R}_1 = \mathcal{O}(\epsilon^2) \). Hence, to the order we have retained, \( \mathcal{R}_1 = 0 \) and \( \mathcal{L}_1 = 0 \), or

\[
\rho_t + (\rho U_k)_{,k} = 0, \tag{A.20}
\]

which is the continuity equation. We can use the continuity equation to simplify the momentum equations and the energy equation. Multiplying the continuity equation by \( U_i \) and the subtracting the result from \( \mathcal{L}_i \) gives, according to Eq. (A.16),

\[
\mathcal{L}_i = \rho U_{i,t} + \rho U_k U_{i,k} + p_{,i} + \mathcal{O}(\epsilon^2). \tag{A.21}
\]
For $L_5$, we group the terms as follows:

$$
L_5 = \frac{1}{2} U_n^2 (\rho, t + (\rho U_k), k) + \rho U_n U_{n,t} + \rho U_k U_n U_{n,k} + U_k p_{,k}
+ \frac{K + 3}{2} [p, t + U_k p_{,k}] + \frac{K + 5}{2} p U_{k,k}
$$

(A.22)

The first term is $\frac{1}{2} U_n^2 L_1$ which is $O(\epsilon^2)$, and the next three are $U_n L_n$, and are therefore $O(\epsilon)$. Then

$$
L_5 = \frac{K + 3}{2} [p, t + U_k p_{,k}] + \frac{K + 5}{2} p U_{k,k} + U_n L_n.
$$

(A.23)

We can drop the last term in the reduction of $R_\alpha$, but the term $U_n L_n$ must be retained in the reduction of $L_5$ when we finally write $L_5 = \epsilon R_5$ in detail.

For the right sides of the momentum equations, consider $R_j = \langle \hat{\tau} F_j k \rangle_k$, where

$$
F_{jk} = \langle u_j u_k \rangle, t + \langle u_j u_k u_l \rangle, t
$$

(A.24)

or

$$
F_{jk} = U_j [\rho U_k]_{,t} + \rho U_k U_{t,j} + p \delta_{kl}, l
+ \rho U_k U_{j,t} + (\rho U_k U_l + p \delta_{kl}) U_{j,l}
+ (p \delta_{jk})_{,t} + (U_l p \delta_{jk} + U_k p \delta_{jl}), l
$$

(A.25)

using the fact that all moments odd in $w_k$ vanish. The term in square brackets multiplying $U_j$ is $L_k$, i.e. it is $O(\epsilon)$, and can therefore be ignored. Then, after gathering terms with coefficients $U_k$ and $p$, we have

$$
F_{jk} = U_k [\rho U_{j,t} + p U_l U_{j,l} + p_j] + p [U_{k,j} + U_{j,k} + U_{l,j} \delta_{jk}] + \delta_{jk}[p, t + U_l p, l].
$$

(A.26)

The coefficient of $U_k$ is $L_j$, according to Eq.(A.21), and can therefore be neglected.

To eliminate $p_{,t}$ from the last term we use the Eq.(A.23) for $L_5$; this gives

$$
p_{,t} + U_k p_{,k} = -\frac{K + 5}{K + 3} p U_{k,k} + O(\epsilon).
$$

(A.27)
Finally, we decompose the tensor $U_{k,j}$ into its dilation and shear parts in the usual way, which gives

$$F_{jk} = p[ U_{k,j} + U_{j,k} - \frac{2}{3} U_{i,i} \delta_{jk} ] + \frac{2}{3} \left( \frac{K}{K + 3} \right) p U_{i,j} \delta_{jk}. \quad (A.28)$$

The last term is due to bulk viscosity; it vanishes, as it should, for $K = 0$, since the physical mechanism for bulk viscosity involves energy sharing between translational and internal degrees of freedom of the molecules, and $K = 0$ corresponds to a monoatomic ($\gamma = \frac{5}{3}$) gas.

For $\alpha = 5$, we write

$$\mathcal{K}_5 = (\tau N_k)_{,k} \quad (A.29)$$

where

$$N_k \equiv < u_k \frac{u_n^2 + \xi^2}{2} >_{,t} + < u_k u_l \frac{u_n^2 + \xi^2}{2} >_{,l} \quad (A.30)$$

which can be written as $N_k = N_k^{(1)} + N_k^{(2)}$, where

$$N_k^{(1)} = [ U_k < \frac{u_n^2 + \xi^2}{2} > ]_{,t} + [ U_k < u_l \frac{u_n^2 + \xi^2}{2} > ]_{,l} \quad (A.31)$$

and

$$N_k^{(2)} = < w_k \frac{u_n^2 + \xi^2}{2} >_{,t} + < w_k u_l \frac{u_n^2 + \xi^2}{2} >_{,l} \quad (A.32)$$

For $N_k^{(1)}$ we have

$$N_k^{(1)} = U_k \left[ \frac{< u_n^2 + \xi^2 >_{,t}}{2} + \frac{< u_l (u_n^2 + \xi^2) >_{,l}}{2} \right]$$

$$+ \left[ \frac{1}{2} \rho U_n^2 + \frac{K + 3}{2} p \right] U_{k,t} + \frac{1}{2} \rho U_l [ U_n^2 + \frac{(K + 5)p}{\rho} U_{k,l} ]. \quad (A.33)$$

The coefficient of $U_k$ in the equation above is $\mathcal{L}_5$, and can therefore be neglected, and the remaining terms can be rewritten as

$$\left[ \frac{1}{2} \rho U_n^2 + \frac{K + 3}{2} p \right] [ U_{k,t} + U_t U_{k,l} ] + p U_t U_{k,t} \quad (A.34)$$
or, using the fact that $L_k = O(\epsilon)$,

$$N_k^{(1)} = \left[ -\frac{1}{2} U_n^2 + \frac{K + 3}{2} \frac{p}{\rho} \right] p_{,k} + p U_l U_{k,l} .$$  \hspace{1cm} (A.35)$$

For $N_k^{(2)}$, remembering that moments odd in $w_k$ vanish, we have

$$N_k^{(2)} = < U_n w_n w_k >,t + < U_l U_n w_n w_k >,l$$

$$+ \frac{1}{2} < U_n^2 w_k w_l >,l + \frac{1}{2} < w_k w_l (w_n^2 + \xi^2) >,l ,$$  \hspace{1cm} (A.36)

or

$$N_k^{(2)} = (p U_k),t + (p U_k U_l),l + \frac{1}{2} (U_n^2 p),_k + \frac{K + 5}{2} \left( \frac{p^2}{\rho} \right),_k .$$  \hspace{1cm} (A.37)

This result can rewritten as

$$N_k^{(2)} = p [U_k,t + U_l U_{k,l} + U_k U_{l,t} + U_l U_{k,l}]$$

$$+ U_k (p,t + U_l p,l) + \frac{1}{2} U_l^2 p,k + \frac{K + 5}{2} \left( \frac{p^2}{\rho} \right),_k ,$$  \hspace{1cm} (A.38)

and the time derivatives can be removed by using $L_k = O(\epsilon)$, and $L_5 = O(\epsilon)$, neglecting $O(\epsilon)$, since we are evaluating $R_5$. Finally, $N_k^{(1)} + N_k^{(2)}$ can be combined to give (after some algebra)

$$N_k = \frac{K + 5}{2} \frac{p}{\rho},_k + p \left[ -\frac{2}{K + 3} U_k U_{l,t} + U_l (U_{k,l} + U_{l,k}) \right].$$  \hspace{1cm} (A.39)

All time derivatives have now been removed from $R_\alpha$ (for all $\alpha$). The remaining steps in the derivation of the Navier-Stokes equations may be summarized briefly as follows:

1. Drop $O(\epsilon^2)$ in Eq.(A.5).
2. Combine $\epsilon$ and $\tilde{\tau}$ to recover $\tau = \epsilon \tilde{\tau}$.
3. Define the stress tensor

$$\sigma'_{jk} = \eta [U_j,k + U_k,j - \frac{2}{3} U_{l,l} \delta_{jk}] + \zeta U_{l,l} \delta_{jk} ,$$
where
\[ \eta = \tau p \]
and
\[ \zeta = \frac{2}{3} \frac{K}{K + 3} \tau p \]
are the dynamic viscosity and second viscosity coefficients respectively.

4). From Eq.(A.21) for \( \mathcal{L}_j \) and Eq.(A.28) for \( F_{jk} \), it follows that \( \mathcal{L}_j = \epsilon \mathcal{R}_j \) may now be written as
\[ \rho U_{j,t} + \rho U_k U_{j,k} + p,j = \sigma'_{jk,k} \]
which is the Navier-Stokes equation.

5). The energy equation follows from \( \mathcal{L}_5 = \epsilon \mathcal{R}_5 \) by using Eq.(A.23), (A.21) and (A.20) to write \( \mathcal{L}_5 \) in detail, and using Eq.(A.29) and (A.39) for \( \mathcal{R}_5 \). The result is
\[ \frac{K + 5}{2} (p,t + U_k p,k) - \frac{K + 5}{2} p(\rho,t + U_k \rho,k) = (\kappa T,k),k + (U_l \sigma'_{lk}),k \]
where
\[ \kappa = \frac{K + 5}{2} \frac{k}{m} \tau p \]
is the thermal conductivity, \( k \) is the Boltzmann constant, \( m \) is the mass of a molecule and \( T \) is the temperature. The equations can be written in terms of \( \gamma \) instead of \( K \) by using \( K = (5 - 3\gamma)/(\gamma - 1) \) (cf. section(2.2)).
Appendix B: Moments of the Maxwellian Distribution

In this gas kinetic scheme, we need to evaluate many moments of the Maxwellian distribution function with bounded and unbounded integration limits. Derivation of all these moments can be found in many mathematical formula references. Here we will list some general formulas which have been used in our code.

First, we assume the Maxwellian distribution (2-D) to be,

\[ g = A e^{-\lambda((u-U)^2+(v-V)^2+\xi^2)} \]

where \( \xi \) are the internal velocities with \( K \) degrees of freedom. We know the relation between the density and the Maxwellian distribution function, which is

\[ \rho = \int_{-\infty}^{+\infty} g du dv d\xi = A \pi^{(K+2)/2} \lambda^{-(K+2)/2}. \]

In order to simplify the notations, we will use \( \rho \), \( \lambda \), \( U \) and \( V \) as independent variables instead of \( A \), \( \lambda \), \( U \) and \( V \) to describe the Maxwellian. At the same time, we use the following notation for the moments of \( g \),

\[ <...> = \int (...) g du dv d\xi. \]

Thus, the general moment formula is

\[ < u^n v^m \xi^l > = \rho < u^n > < v^m > < \xi^l >, \]

where \( n \) and \( m \) are integers, and \( l \) is an even integer (owing to the symmetrical property of \( \xi \)). The quantities for \( < \xi^l > \) are given as,

\[ < \xi^2 > = \left( \frac{K}{2\lambda} \right) \]

\[ < \xi^4 > = \left( \frac{3K}{4\lambda^2} + \frac{K(K-1)}{4\lambda^2} \right) \]
\[
< \xi^b > = \left( \frac{15K}{8\lambda^3} + \frac{K(K-1)(k-2)}{8\lambda^3} + \frac{9K(K-1)}{8\lambda^3} \right)
\]

The values of \(< u^n >\) and \(< v^m >\) depend on the integration limits. Because they have similar relations, we just show the results for \(< u^n >\). For \(< v^m >\) terms, we change \(U\) to \(V\) in all following equations. If the limits are \(-\infty\) to \(+\infty\), we have

\[
< 1 > = 1
\]

\[
< u > = U
\]

\[
< u^2 > = (U^2 + \frac{1}{2\lambda})
\]

\[
< u^3 > = (U^3 + 1.5 \frac{U}{\lambda})
\]

\[
< u^4 > = (U^4 + \frac{3U^2}{\lambda} + \frac{0.75}{\lambda^2})
\]

\[
< u^5 > = (U^5 + \frac{5U^3}{\lambda} + \frac{3.75U}{\lambda^2})
\]

\[
< u^6 > = (U^6 + 7.5 \frac{U^4}{\lambda} + 11.25 \frac{U^2}{\lambda^2} + \frac{1.875}{\lambda^3})
\]

If the integral is from 0 to \(+\infty\) as \(< ... >_0\) or from \(-\infty\) to 0 as \(< ... >_{<0}\), the solutions are not so obvious and the error functions will be needed. Before that, however we define some quantities (related to the incomplete \(\Gamma\) function),

\[
E_1 = \frac{1}{2} \text{erfc}(\sqrt{\lambda}U)
\]

\[
E_2 = \frac{1}{2} e^{-\frac{U^2}{\lambda^2}}
\]

\[
E_3 = -UE_2 + \frac{1}{2} \frac{E_1}{\lambda}
\]

\[
E_4 = U^2E_2 + \frac{E_2}{\lambda}
\]

\[
E_5 = -U^3E_2 + \frac{3}{2} \frac{E_3}{\lambda}
\]

...
\[ E_n = (-1)^n U^{n-2} E_2 + \frac{(n-2) E_{n-2}}{2} \]

and

\[ G_1 = \frac{1}{2} \text{erfc}(\sqrt{\lambda} U) \]
\[ G_2 = -\frac{1}{2} \frac{e^{-\lambda U^2}}{\sqrt{\pi} \lambda} \]
\[ G_3 = -U G_2 + \frac{1}{2} \frac{G_1}{\lambda} \]
\[ G_4 = U^2 G_2 + \frac{G_2}{\lambda} \]
\[ G_5 = -U^3 G_2 + \frac{3}{2} \frac{G_3}{\lambda} \]
\[ \ldots \]
\[ G_n = (-1)^n U^{n-2} G_2 + \frac{(n-2) G_{n-2}}{2} \frac{1}{\lambda}. \]

From these definitions, the moments for \( u^n \) in the half space are,

\[ < 1 >_{>0} = E_1 \]
\[ < u >_{>0} = (UE_1 + E_2) \]
\[ < u^2 >_{>0} = (U^2 E_1 + 2UE_2 + E_3) \]
\[ < u^3 >_{>0} = (U^3 E_1 + 3U^2 E_2 + 3UE_3 + E_4) \]
\[ \ldots \]
\[ < u^n >_{>0} = (U^n E_1 + C_n^1 U^{n-1} E_2 + C_n^2 U^{n-2} E_3 + \ldots + C_n^n E_{n+1}) \]

In the similar way,

\[ < 1 >_{<0} = G_1 \]
\[ < u >_{<0} = (UG_1 + G_2) \]
\[ < u^2 >_{<0} = (U^2 G_1 + 2UG_2 + G_3) \]
\[<u^3>_0 = (U^2G_1 + 3U^2G_2 + 3UG_3 + G_4)\]

\[\ldots\]

\[<u^n>_0 = (U^nG_1 + C_n^1U^{n-1}G_2 + C_n^2U^{n-2}G_3 + \ldots + C_n^nG_{n+1}),\]

where \(C_n^m\) is the combination \((n(n - 1)\ldots(n - m + 1))/(m(m - 1)\ldots1)\).

In our gas kinetic scheme, there exist a lot of velocity moments. From the above general definitions, all moments can be easily obtained.


