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Expanded analogy between Boltzmann kinetic theory of fluids and turbulence

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We demonstrate that the effects of turbulent fluctuations have a striking resemblance to those of microscale (thermal) fluctuations in laminar flows, even to higher order in the Knudsen number. This suggests that there may be a good basis for understanding turbulence in terms of Boltzmann kinetic theory. If so, turbulence may be better described in terms of 'mixing times' rather than the more classical 'mixing lengths'. Comparisons are made to Reynolds-stress turbulence models.

1. Introduction

The fundamental difference between laminar and turbulent flows is that the latter have fluctuations at scales larger than the microscales of thermal fluctuations. These 'eddy' fluctuations have been known since the work of Saint-Venant (Saint-Venant 1851) in the mid-19th century to enhance the effective viscosity of flows (see also Boussinesq 1870); this enhancement of viscosity has been called 'eddy viscosity' since the work of Reynolds (1894, cf. Lamb 1932, p. 668 who ascribes the specific notion of eddy viscosity to Reynolds in 1886). At about the same time, Lord Kelvin (1887), who appears to have introduced the word 'turbulent' to describe highly irregular flows, emphasized that there was an analogy between Maxwell's (then new) kinetic theory of microscopic thermal fluctuations in gases and eddy transport in turbulence. Eddy viscosity ideas and the analogy between microscopic thermal effects and macroscopic eddy effects have been the pillar of both theoretical and engineering models of turbulence to this day. In this paper, we quantify this analogy to higher order than simple eddy viscosity in order to explore the relationship between higher-order (nonlinear and non-Newtonian) kinetic theory and higher-order turbulence models. In this way, we demonstrate that turbulence modelling has an even firmer basis in kinetic theory than previously thought.

In turbulent flows, eddy effects first appear as the Reynolds stress tensor term, σ_{ij}, in the averaged incompressible (and unit density) Navier–Stokes equation for the mean velocity $\boldsymbol{U}$:

$$(\partial_t + \boldsymbol{U}\cdot\nabla)U_i = -\frac{\partial p}{\partial x_i} + \nu_0\nabla^2 U_i + \frac{\partial \sigma_{ij}}{\partial x_j} \tag{1.1}$$

where the Reynolds stress tensor is an average over the fluctuating velocity $\boldsymbol{u}'$:

$$\sigma_{ij} \equiv -\langle u_i' u_j' \rangle$$

where $\boldsymbol{u}=\boldsymbol{U}+\boldsymbol{u}'$ is the instantaneous velocity at $(\boldsymbol{x}, t)$. One of the major issues in turbulence modelling is to express the Reynolds stress in terms of the mean field and its properties.

The analogy explored in the 19th century between small-scale turbulent eddies and molecular dynamics at a different scale suggested that the deviatoric part of σ_{ij} could be modelled as

$$\sigma_{ij}=2\nu_{turb}S_{ij} \tag{1.2}$$

where ν_{turb} is the eddy viscosity, and

$$S_{ij}\equiv\frac{1}{2}\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)$$

is the rate of strain tensor of the mean flow. This eddy-viscosity hypothesis (1.2) is at best qualitative as it seems to require a definitive separation of scales between the mean and the fluctuating fields. Indeed, simple estimation reveals that the effective mean-free path of eddies (i.e. the Prandtl (1925) mixing length) is at least comparable to the characteristic scales of the mean flow (Wilcox 1993). Nevertheless, eddy viscosity has been the starting point, and to a substantial extent the foundation, of modern turbulence models as well as large-eddy simulations (LES) (Lesieur & Metais 1996; Geurts 2004).

Significant efforts in turbulence modelling have been directed to deriving expressions for ν_{turb} (Launder & Spalding 1974). There have also been attempts to go beyond the eddy-viscosity models in order to better describe turbulence, including secondary flow structures and flows subject to sudden distortions (Yakhot *et al.* 1992). Similar work has been pursued in LES approaches.

Generally speaking, other than the century-old qualitative analogy with molecular dynamics, all eddy-viscosity models are based on various averaging procedures within the (coarse-grained) Navier–Stokes description. Although there have been successes in obtaining good results for various classes of flows, derivations of these models are not satisfactory due to the approximations or assumptions made; they usually contain *ad hoc* parameters which must be specified. Other issues involve mathematical well-posedness and boundary conditions for higher-order closure models. But perhaps most importantly, there is still a lack of clear understanding from these turbulence models of the physical nature of the turbulent fluctuations and their effects on mean flows.

In this paper, we demonstrate that the comparison between turbulent and microscale (thermal) fluctuations can be followed to a deeper level via use of Boltzmann kinetic theory. As a matter of fact, the Boltzmann kinetic theory itself is not constrained to the small mean-free path limit.

2. Boltzmann kinetic theory of turbulent fluctuations

Let us assume that turbulent fluctuations can be likened to isotropic thermal fluctuations in a smooth mean field $\boldsymbol{U}$. For simplicity, we consider low Mach number flows, namely incompressible or nearly incompressible flow. The dynamics of turbulent fluctuations is assumed to be described by a Boltzmann equation for the single-point probability density $f(\boldsymbol{x}, \boldsymbol{v}, t)$ of parcels of fluid in phase $(\boldsymbol{x}, \boldsymbol{v}, t)$ space. This Boltzmann equation is assumed to have a characteristic relaxation time back to a local (slowly varying) equilibrium (Cercignani 1975). In contrast, there are several fundamental differences between turbulent and thermal fluctuations. First, with turbulence, the root-mean-square velocity fluctuations are measured by the (three-dimensional) turbulent kinetic energy $2K/3$, instead of the temperature, θ. Second, the relaxation time is associated with that of intrinsic turbulence time scales. Therefore, we assume that f evolves according to the evolution equation:

$$\partial_t f + \boldsymbol{v} \cdot \nabla f = C_{turb} \tag{2.1}$$

where the collision term is approximated in so-called BGK form (Bhatnagar, Gross & Krook 1954) as

$$C_{turb} = -\frac{1}{\tau_{turb}}(f - f^{eq}) \tag{2.2}$$

which is adequate for the low-Mach-number incompressible limit, in which hydrodynamic modes are transverse (divergence-free). In (2.2), the equilibrium distribution, f^{eq}, can be the usual Maxwell–Boltzmann distribution centred around the mean velocity $\boldsymbol{U}$ with a half-width of $2K/3$. In fact, this is consistent with the experimental observation that one-point fluctuations of the turbulent velocity field are close to Gaussian. Indeed, f^{eq} represents an equilibrium distribution which does not include the non-trivial flow-induced fluctuations that are involved in f; the latter may be non-Gaussian (Frisch 1996).

Based on this kinetic description, we can define all the fundamental fluid properties as moments of the effective Boltzmann distribution (Boltzmann 1872). Specifically, the density ρ, mean velocity $\boldsymbol{U}$, and turbulent kinetic energy K are

$$\rho = \int \mathrm{d}\boldsymbol{v} f,$$

$$\boldsymbol{U} = \langle \boldsymbol{v} \rangle,$$

$$K = \tfrac{1}{2}\langle (\boldsymbol{u}')^2 \rangle \equiv \tfrac{1}{2}\langle (\boldsymbol{v} - \boldsymbol{U})^2 \rangle,$$

where $\langle . \rangle$ is defined by

$$\langle A \rangle \equiv \int \mathrm{d}\boldsymbol{v} A f/\rho.$$

Furthermore, the Reynolds stress is

$$\sigma_{ij} = -\langle u'_i u'_j \rangle \equiv -\langle (\boldsymbol{v} - \boldsymbol{U})_i (\boldsymbol{v} - \boldsymbol{U})_j \rangle. \tag{2.3}$$

This expression for the Reynolds stress tensor does not assume that f is close to a local equilibrium. The Reynolds stress formally contains contributions of all orders in the effective Knudsen number, $\mathscr{K} \sim \tau_{turb}/t_{hydro}$, where t_{hydro} is a representative time scale of the mean field. This is another key point (Chen *et al.* 2003) of the kinetic theory level description.

On the other hand, if $\mathscr{K}$ is treated as a small number, we can use a Chapman–Enskog-like expansion technique (Chapman & Cowling 1990) to obtain deviations from equilibrium at various orders of $\mathscr{K}$:

$$f = f^{(0)} + \mathscr{K} f^{(1)} + \mathscr{K}^2 f^{(2)} + \cdots \tag{2.4}$$

where $f^{(0)} \equiv f^{eq}$. In this way, we can obtain expressions for σ_{ij} at various orders (see the Appendix).

$$\sigma_{ij}^{(0)} = -\tfrac{2}{3} K \delta_{ij} \tag{2.5}$$

which is a diagonal tensor, and

$$\sigma_{ij}^{(1)} = 2\nu_{turb} S_{ij} \tag{2.6}$$

where

$$\nu_{turb} = \tfrac{2}{3} K \tau_{turb}. \tag{2.7}$$

In the above,

$$\sigma_{ij}^{(n)} \equiv - \int \mathrm{d}\boldsymbol{v} (\boldsymbol{v} - \boldsymbol{U})_i (\boldsymbol{v} - \boldsymbol{U})_j f^{(n)} / \rho.$$

Equation (2.7) shows that conventional eddy-viscosity models can be viewed in terms of the choice of τ_{turb}. For example, if we choose τ_{turb} as the large-eddy dissipation time scale in isotropic turbulence, $\tau_{turb} \sim K/\epsilon$, then $\nu_{turb} \sim K^2/\epsilon$, which is standard in the so-called K–ϵ class of turbulence models.

Once again, we emphasize that eddy-viscosity models are only valid if $\mathscr{K}$ is sufficiently small. In order words, there must be a clear separation of time (and space) scales between the mean and the fluctuating velocity fields, so that fluctuations are close to equilibrium and higher-order deviations can be ignored. On the other hand, there is no reason why $\mathscr{K}$ must be small in turbulent flows. The same observation holds for LES which must necessarily deal with turbulent scales close to the grid scale. If $\mathscr{K}$ is not small, the validity of Chapman–Enskog expansions is open to criticism.

Nevertheless, for the purpose of gaining insight, one can formally carry out the Chapman–Enskog expansion to the next order. Fortunately, with the simple BGK form and ignoring contributions due to finite compressibility, the derivation is relatively straightforward; we find (see the Appendix) to second order:

$$\sigma_{ij}^{(2)} = -2\nu_{turb} \frac{\mathrm{D}}{\mathrm{D}t} [\tau_{turb} S_{ij}] - 6 \frac{\nu_{turb}^2}{K} \left[S_{ik} S_{kj} - \tfrac{1}{3} \delta_{ij} S_{kl} S_{kl} \right] + 3 \frac{\nu_{turb}^2}{K} [S_{ik} \Omega_{kj} + S_{jk} \Omega_{ki}] \tag{2.8}$$

where $\mathrm{D}/\mathrm{D}t \equiv \partial_t + \boldsymbol{U} \cdot \nabla$ is the Lagrangian time derivative along the mean velocity field. Here

$$\Omega_{ij} \equiv \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right)$$

is the vorticity tensor of the mean velocity field. It is understood that the summation convention holds.

Equation (2.8) is both interesting and revealing. It provides concrete support for the Boltzmann–kinetic theory based description of turbulent fluctuations (Chen *et al.* 1999; Succi *et al.* 2002; Chen *et al.* 2003; Ansumali, Karlin & Succi 2003). It also reveals two fundamentally new effects. First, a memory effect represented by the first term on the right-handside and, second, additional nonlinear tensorial terms essential to describe some secondary flow structures. Combining the first term with that in (2.6), we find that the effect of a finite τ_{turb} implies that the stress is not simply a function of the local instantaneous rate of strain, but rather a consequence of the rate of strain at an earlier time and an upstream location, namely

$$\sigma_{ij}(\boldsymbol{x}, t) \approx 2\nu_{turb} S_{ij}(\boldsymbol{x} - \tau_{turb} \boldsymbol{U}, t - \tau_{turb}).$$

This non-Newtonian result could be responsible for turbulent phenomena seen in rapid distortion processes. Of course, for flows that are slowly varying in space and time, such effects can be ignored, and we return to a conventional turbulence eddy-viscosity model. It is also worth noting that τ_{turb} can vary on a time scale comparable to that of the mean flow.

The nonlinear terms in (2.8) are also interesting. These terms are responsible for certain observed secondary flow phenomena and can also enhance energy transfer at higher wavenumbers in a way similar to those from the classic closure theories (see Kraichnan 1976; Orszag 1977; Leslie & Quarini 1979; Chollet & Lesieur 1981; Lesieur & Rogallo 1989). Furthermore, the nonlinear terms can be verified to have essentially the same form as those of so-called higher-order turbulence transport models. This may not be surprising considering tensor symmetry arguments. However, the conclusion is made stronger if these higher-order terms are quantitatively compared with some well-known nonlinear turbulence models. For this purpose, we rewrite (2.8) as

$$\sigma_{ij} = \nu_{turb}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] - \nu_{turb}\frac{\mathrm{D}}{\mathrm{D}t}\left[\tau_{turb}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] - \frac{K^3}{\epsilon^2}\left[C_1\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k} + C_2\left(\frac{\partial u_i}{\partial x_k}\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k}\frac{\partial u_k}{\partial x_i}\right) + C_3\frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right] \quad (2.9)$$

where the coefficients C_1, C_2 and C_3 are determined once the turbulent time τ_{turb} is specified. For instance, in order to match the standard K–ϵ model for ν_{turb} at first order (see (2.7)) we choose

$$\tau_{turb} = \frac{3}{2}C_\mu\frac{K}{\epsilon}$$

where $C_\mu \approx 0.09$ so $\nu_{turb} = C_\mu K^2/\epsilon$.

For this choice of τ_{turb}, we find

$$C_1 = 0.024, \quad C_2 = 0.012, \quad C_3 = 0.$$

For comparison, we list the corresponding values from three of the most representative nonlinear turbulence models: the model of Rubinstein & Barton (1990) gives

$$C_1 = 0.034, \quad C_2 = 0.104, \quad C_3 = -0.014;$$

the model of Yoshizawa (1987) gives

$$C_1 = 0.057, \quad C_2 = -0.167, \quad C_3 = -0.0067;$$

while the model of Speziale (1987) gives

$$C_1 = 0.041, \quad C_2 = 0.014, \quad C_3 = -0.014.$$

It is remarkable that the nonlinear terms directly obtained from the simple second-order Chapman–Enskog expansion are quantitatively close to those used in the higher-order turbulence models. This suggests that the analogy between turbulent eddy and thermal fluctuations is deep and there may be a connection between these two seemingly different dynamic processes. We have now seen that the results are quantitatively close at least up to second order in $\mathscr{K}$. As shown above, the key is the proper choice of *two* fundamental measures representing eddy interactions, namely the relaxation time τ_{turb}, and the level of turbulent fluctuations K.

One can argue that such a comparison may be valid for even higher-order terms and to all orders. It is important to note that, by using the Boltzmann kinetic theory description, coefficients of the terms in these high-order models are determined from a few fundamental terms (e.g. τ_{turb} in the kinetic BGK form (2.2)). At higher order, one expects additional memory effects appearing in the nonlinear terms as well as the appearance of higher-order derivative hyperviscous (such as ∇^{2n}) terms. These higher-order effects are similar to effects known from classical analytical turbulence theory. For example, higher-order Knudsen numbers are known to lead to enhanced energy transfer or a 'cusp'-like effective eddy viscosity in wavenumber space near the 'cutoff' length (or time) scale separating the mean and fluctuating components

(Kraichnan 1976; Orszag 1977; Leslie & Quarini 1979; Chollet & Lesieur 1981; Lesieur & Rogallo 1989). The latter effect originates from the order-1 ratio between wavenumbers that lie nearby on opposite sides of the cutoff. As shown by Chollet & Lesieur (1981), these interactions may be expressed as a hyperviscous addition to the real-space eddy viscosity and allow the capture of intermittency effects, typically not described by standard eddy-viscosity models (Lesieur 1997). The incorporation of such hyperviscous effects within LES simulations has been demonstrated to be capable of describing baroclinic jets in the atmosphere (Garnier, Metais & Lesiuer 1998; Lesieur, Metais & Garnier 2000). It should, therefore, be of interest in future work to explore the underlying connections between hyperviscous models and the present kinetic approach.

In fact, moment integration of the Boltzmann distribution naturally includes contributions from all orders in $\mathscr{K}$. The Boltzmann distribution thus serves as a generating function that yields all moments of the fluctuations, such as the Reynolds stress tensor, σ_{ij}. It is known that Boltzmann kinetic theory gives an adequate description of normal fluid flows for both small- and large-$\mathscr{K}$ regimes, as long as microscopic molecule-to-molecule correlations are unimportant (the latter being violated, e.g., at the critical point of a second-order phase transition). We also remark that, e.g., Rosenau (1993) has observed the advantages of formulating generalized ($\mathscr{K} = O(1)$) hydrodynamics in terms of dissipative corrections to hyperbolic equations (like the telegrapher's equation), much in the spirit of the BGK model studied here.

3. Discussion

Based on these results for the Chapman–Enskog expansion up to second order in $\mathscr{K}$, we obtain the following relation for σ_{ij} by combining (2.5), (2.6) and (2.8):

$$\sigma_{ij} \approx -2K/3\delta_{ij} + 2\nu_{turb}S_{ij} - 2\nu_{turb}\frac{\mathrm{D}}{\mathrm{D}t}[\tau_{turb}S_{ij}] - 6\frac{\nu_{turb}^2}{K}\left[S_{ik}S_{kj} - \tfrac{1}{3}\delta_{ij}S_{kl}S_{kl}\right] + 3\frac{\nu_{turb}^2}{K}[S_{ik}\Omega_{kj} + S_{jk}\Omega_{ki}]. \quad (3.1)$$

While (3.1) is formally correct to $O(\mathscr{K}^2)$, another representation of σ_{ij} may be more useful for higher-order Reynolds stress turbulence modelling. Indeed, when $\mathrm{D}/\mathrm{D}t$ is applied to (3.1) and the resulting equation iterated, it is easily seen that the resulting dynamical equation for $\mathrm{D}\sigma_{ij}/\mathrm{D}t$ is

$$(\partial_t + \boldsymbol{U}\cdot\nabla)\sigma_{ij} = -\frac{1}{\tau_{turb}}\left[\sigma_{ij} - 2\nu_{turb}S_{ij} + \tfrac{2}{3}K\delta_{ij}\right] - \left[\sigma_{ik}S_{kj} + \sigma_{jk}S_{ki} - \tfrac{2}{3}\sigma_{kl}S_{kl}\delta_{ij}\right] + [\sigma_{ik}\Omega_{kj} + \sigma_{jk}\Omega_{ki}] - \sigma_{ij}\frac{1}{\tau_{turb}}(\partial_t + \boldsymbol{U}\cdot\nabla)\tau_{turb} \quad (3.2)$$

where $K \equiv -\sigma_{ii}/2$. It is clear from the above that the additional (higher-order) terms are important when there is either a strong time variation or a strong velocity shear in a large-scale turbulent flow. In (3.2), the additional derivative term on the right-hand side that acts on the relaxation time τ_{turb} is unique to turbulence, in contrast with normal high-$\mathscr{K}$ flows. This term could still be significant even if τ_{turb} itself (or $\mathscr{K}$) is small. Since $\tau_{turb} \sim K/\epsilon$ in isotropic turbulence, if necessary we can also use conventional K–ϵ turbulence model equations to express this term. Finally, we observe that diffusion terms, like $\nabla^2\sigma_{ij}$, may arise in (3.2) when the Chapman–Enskog procedure is carried to third or higher order in $\mathscr{K}$.

We comment that to avoid certain unnecessary complications, we have neglected terms that ensure incompressibility of the averaged velocity field; we have assumed the latter to be incompressible without these terms. Strictly speaking, this is not fully self-consistent since we should view the effective Boltzmann representation to be used not only to describe the fluctuating field but also the averaged field. It is known for incompressible flows that the pressure distribution is governed by the mean velocity field according to the constraint

$$-\nabla^2 p = \nabla\nabla : [\rho \boldsymbol{U}\boldsymbol{U}].$$

Incompressibility of the averaged velocity field can be enforced by introducing a corresponding body-force term, $-\nabla p \cdot \nabla_v f$, on the left-hand side of the proposed Boltzmann equation (2.1) (Degond 2002). As a consequence, the resulting equation of state is modified. Furthermore, the equilibrium distribution then also contains a pressure-dependent 'potential energy' (Keizer 1987). It is easy to see that this additional effect does not alter the the first-order (Newtonian) eddy viscosity. On the other hand, it is expected to generate some additional terms in the second (nonlinear) order corresponding to the interactions between the pressure and velocity fields. These interactions can be potentially important for non-trivial (non-Gaussian) behaviour of fluctuations. The kinetic-theory-based approach provides a way to derive all these fully self-consistently. It should be interesting to investigate this in more depth in the future.

In conclusion, we comment that the kinetic approach advocated here suggests that the classical concept of 'mixing lengths', so prevalent in turbulence theory since they were first suggested by Prandtl (1925), may be better described dynamically as 'mixing times', much in accord with Lord Kelvin's (1887) description of the dynamics of turbulence as the 'vitiating re-arrangement' of eddies.

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Appendix. Derivation of the momentum stress via second-order Chapman–Enskog expansion

In this Appendix, we provide a detailed derivation for the analytical expression of the momentum stress tensor (namely (2.8)) via Chapman–Enskog expansion. The Chapman–Enskog procedure has been outlined in the literature (Cercignani 1975; Huang 1987; Chapman & Cowling 1998). On the other hand, because of differences in focus, either the related results are not available or not presented in the relevant forms.

We apply Chapman–Enskog expansion to the Boltzmann equation with a single relaxation parameter, $\tau(\boldsymbol{x}, t)$,

$$(\partial_t + \boldsymbol{v}\cdot\nabla) f(\boldsymbol{x}, \boldsymbol{v}, t) = -\frac{1}{\tau}[f(\boldsymbol{x}, \boldsymbol{v}, t) - f^{eq}[\boldsymbol{x}, \boldsymbol{v}, t)] \tag{A 1}$$

where the equilibrium distribution has the usual Maxwell–Boltzmann form,

$$f^{eq} = \frac{\rho}{(2\pi\theta)^{d/2}} \exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\theta}\right]. \tag{A 2}$$

In the above, d is the 'dimension' of the particle momentum space. The spatial and temporal dependence of f^{eq} is entirely through the hydrodynamic quantities, namely the density $\rho(\boldsymbol{x}, t)$, fluid velocity $\boldsymbol{u}(\boldsymbol{x}, t)$ and temperature $\theta(\boldsymbol{x}, t)$. These quantities are expressed as moments of f:

$$\rho = \int \mathrm{d}\boldsymbol{v} f, \tag{A 3}$$

while

$$\boldsymbol{u} = \langle \boldsymbol{v} \rangle, \quad c_v \theta = \tfrac{1}{2} \langle (\boldsymbol{v} - \boldsymbol{u})^2 \rangle \tag{A 4}$$

where the heat capacity is $c_v \equiv \frac{1}{2} d$. Taking the corresponding hydrodynamic moment of the Boltzmann equation (A 1), we obtain the well-known and exact expressions

$$\left. \begin{aligned} &\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0, \\ &\rho(\partial_t + \boldsymbol{u} \cdot \nabla) \boldsymbol{u} = \nabla \cdot (\rho \boldsymbol{\sigma}), \\ &\rho c_v (\partial_t + \boldsymbol{u} \cdot \nabla) \theta = -\nabla \cdot \boldsymbol{q} + \rho \boldsymbol{\sigma} : \boldsymbol{S}, \end{aligned} \right\} \tag{A 5}$$

where the momentum stress tensor, $\boldsymbol{\sigma}$, heat flux $\boldsymbol{q}$, are, respectively,

$$\sigma_{ij} \equiv -\langle (v_i - u_i)(v_j - u_j) \rangle, \tag{A 6}$$

$$q_i \equiv \tfrac{1}{2} \rho \langle (v_i - u_i)(\boldsymbol{v} - \boldsymbol{u})^2 \rangle, \tag{A 7}$$

while the rate of strain tensor, $\boldsymbol{S}$, is

$$S_{ij} \equiv \frac{1}{2} \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right]. \tag{A 8}$$

The task involved in deriving a macroscopic representation of hydrodynamics is to express the fluxes, σ and $\boldsymbol{q}$ in terms of the fundamental hydrodynamic variables ρ, $\boldsymbol{u}$ and θ, as well as their (spatial and temporal) derivatives. For our purpose here, we only provide the derivation for the momentum stress tensor. If the system is at equilibrium, it is straightforward to show that

$$\sigma_{ij}^{eq} = -\langle (v_i - u_i)(v_j - u_j) \rangle^{eq} = -\theta \delta_{ij}, \tag{A 9}$$

where $\langle A \rangle^{eq} \equiv \int \mathrm{d}\boldsymbol{v} A f^{eq} / \rho$ and δ_{ij} is the Kronecker delta function. Similarly, $\boldsymbol{q}^{eq} = 0$, and $\boldsymbol{\sigma} : \boldsymbol{S} = -\theta \nabla \cdot \boldsymbol{u}$. Equation (A 9) is a familiar result in that the equilibrium stress is a diagonal tensor proportional to temperature (or pressure).

On the other hand, when there exists a flow involving non-trivial (spatial or temporal) inhomogeneities, there will be additional contributions to the stress tensor due to the non-equilibrium part of the distribution function, $f^{neq} \equiv f - f^{eq}$. The Chapman–Enskog method is a systematic procedure to expand the Boltzmann distribution function around its local equilibrium. This is possible if the ratio between the relaxation time τ and the representative advection time scale T of the left-hand side of (A 1), namely when $\mathscr{K}$ is small. Hence we may express the Boltzmann distribution function in terms of a power series in $\mathscr{K}$:

$$f = f^{(0)} + \mathscr{K} f^{(1)} + \mathscr{K}^2 f^{(2)} + \cdots \tag{A 10}$$

where $f^{(0)} = f^{eq}$, and the additional ($n > 0$) terms represent deviations from equilibrium at various orders in $\mathscr{K}$. In this procedure, we assume that the moment integrations over the equilibrium distribution f^{eq} give the same values for the fundamental hydrodynamic quantities (such as ρ, $\boldsymbol{u}$, and θ) as that for the total distribution function f, while all the non-equilibrium corrections make vanishing contributions to these quantities:

$$\int \mathrm{d}\boldsymbol{v}\chi f^{(n)} = 0; \quad \forall n > 0,$$

where $\chi = 1$, $\boldsymbol{v}$, or $\boldsymbol{v}^2$, respectively. However, as shown in the derivation below, these non-equilibrium corrections do contribute to the fluxes. For instance, the momentum stress from the nth-order is given by

$$\sigma_{ij}^{(n)} = -\langle (v_i - u_i)(v_j - u_j)\rangle^{(n)} \equiv -\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j) f^{(n)}/\rho. \tag{A 11}$$

The Chapman–Enskog expansion also requires expansion in time and space accordingly,

$$\partial_t \rightarrow \mathscr{K}\partial_{t_0} + \mathscr{K}^2\partial_{t_1} + \cdots \tag{A 12}$$

and $\nabla \rightarrow \mathscr{K}\nabla$. Consequently the Boltzmann equation (A 1) is turned into an infinite hierarchy of equations according to the order of $\mathscr{K}$,

$$\sum_{k=0}^{n-1} \partial_{t_k} f^{(n-k-1)} + \boldsymbol{v}\cdot\nabla f^{(n-1)} = -\frac{1}{\tau} f^{(n)}, \quad n = 1, 2, \ldots, \infty. \tag{A 13}$$

In particular, we have for the first order ($n = 1$),

$$(\partial_{t_0} + \boldsymbol{v}\cdot\nabla) f^{eq} = -\frac{1}{\tau} f^{(1)}, \tag{A 14}$$

while for the second order ($n = 2$), we have

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{(1)} + \partial_{t_1} f^{eq} = -\frac{1}{\tau} f^{(2)}. \tag{A 15}$$

These can also be conveniently represented as

$$f^{(1)} = -\tau\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{eq}, \tag{A 16}$$

$$f^{(2)} = -\tau\left[\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{(1)} + \partial_{t_1} f^{eq}\right]. \tag{A 17}$$

One of the major differences between the Chapman–Enskog and the so-called Hilbert expansion is that the former also includes an expansion of the differential operators. This has been demonstrated to be essential for avoiding certain serious singularity issues occurring in the Hilbert expansion.

The fastest time derivative ∂_{t_0} corresponding to Euler (inviscid) hydrodynamics is a result of the equilibrium Boltzmann distribution:

$$\left.\begin{aligned} &\partial_{t_0}\rho + \nabla\cdot(\rho\boldsymbol{u}) = 0, \\ &\partial_{t_0}\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \frac{1}{\rho}\nabla(\rho\theta) = 0, \\ &\partial_{t_0}\theta + \boldsymbol{u}\cdot\nabla\theta + \frac{\theta}{c_v}\nabla\cdot\boldsymbol{u} = 0. \end{aligned}\right\} \tag{A 18}$$

Since the space–time dependence in f^{eq} is only through ρ, $\boldsymbol{u}$, and θ, we obtain

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{eq} = \frac{\partial f^{eq}}{\partial\rho}\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)\rho + \frac{\partial f^{eq}}{\partial u_j}\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)u_j + \frac{\partial f^{eq}}{\partial\theta}\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)\theta. \tag{A 19}$$

Using the Maxwell–Boltzmann expression (A 2), it can be directly shown that

$$\left.\begin{aligned} \frac{\partial f^{eq}}{\partial \rho} &= \frac{f^{eq}}{\rho}, \\ \frac{\partial f^{eq}}{\partial u_j} &= \frac{v_j - u_j}{\theta} f^{eq}, \\ \frac{\partial f^{eq}}{\partial \theta} &= \frac{1}{\theta}\left[\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\theta} - \frac{d}{2}\right] f^{eq}. \end{aligned}\right\} \tag{A 20}$$

Combining (A 18)–(A 20), we obtain

$$\begin{aligned} \left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{eq} = f^{eq}\Bigg\{ &\frac{(\boldsymbol{v}-\boldsymbol{u})}{\theta}\cdot\nabla\theta\left[\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\theta} - \frac{d+2}{2}\right] \\ &+ \frac{\nabla \boldsymbol{u}}{\theta} : \left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\Bigg\} \end{aligned} \tag{A 21}$$

where the components of the unity tensor $\boldsymbol{I}$ are δ_{ij}. Substituting (A 21) into (A 16), we arrive at the expression for the first-order correction to the equilibrium distribution function,

$$\begin{aligned} f^{(1)} = -\frac{\tau}{\theta} f^{eq}\Bigg\{ &(\boldsymbol{v}-\boldsymbol{u})\cdot\nabla\theta\left[\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\theta} - \frac{d+2}{2}\right] \\ &+ \boldsymbol{S} : \left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\Bigg\}. \end{aligned} \tag{A 22}$$

Since we are interested in the incompressible limit, we ignore the effects due to variations in density and temperature. Therefore, (A 22) is simplified to

$$f^{(1)} = -\frac{\tau}{\theta} f^{eq}\boldsymbol{S} : \left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]. \tag{A 23}$$

Substituting (A 23) into the stress moment, and after some straightforward algebra, it can be shown that

$$\sigma_{ij}^{(1)} = 2\nu\left[S_{ij} - \frac{1}{d}\delta_{ij}\nabla\cdot\boldsymbol{u}\right] \rightarrow 2\nu S_{ij} \tag{A 24}$$

where the kinematic viscosity is $\nu = \tau\theta$. Equation (A 24) is the usual Newtonian fluid constitutive relation in which the momentum stress is linearly proportional to the instantaneous value of the local rate of strain.

The above results are well known in the literature. What is perhaps not so clearly described are the derivations and the results for higher order. We present a derivation for the second-order Chapman–Enskog expansion in the rest of this Appendix. Using the result of the first-order derivation above, we obtain the hydrodynamic time derivative at the first order. That is,

$$\left.\begin{aligned} &\partial_{t_1}\rho = 0, \\ &\partial_{t_1} u_i = 2\frac{\partial}{\partial x_j}\left[\tau\theta\left(S_{ij} - \frac{1}{d}\delta_{ij}\nabla\cdot\boldsymbol{u}\right)\right], \\ &\partial_{t_1}\theta = \frac{2}{d}\sigma_{ij}^{(1)} S_{ij} = \frac{4\tau\theta}{d}\left(S_{ij} - \frac{1}{d}\delta_{ij}\nabla\cdot\boldsymbol{u}\right) S_{ij}. \end{aligned}\right\} \tag{A 25}$$

It is understood that the conventional (Navier–Stokes) hydrodynamic equation is obtained by combining (A 18) and (A 25). This is a direct result of the Chapman–Enskog expansion up to the first order. Based on (A 17), (A 20) and (A 23), together with

$$\partial_{t_1} f^{eq} = \frac{\partial f^{eq}}{\partial \rho}\partial_{t_1}\rho + \frac{\partial f^{eq}}{\partial u_j}\partial_{t_1}u_j + \frac{\partial f^{eq}}{\partial \theta}\partial_{t_1}\theta \tag{A 26}$$

it is easy to obtain

$$\partial_{t_1} f^{eq} = \frac{2}{\theta} f^{eq}\left\{\frac{2\tau\theta}{d}\left[\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\theta} - \frac{d}{2}\right]\left(S_{ij} - \frac{1}{d}\delta_{ij}\nabla\cdot\boldsymbol{u}\right)S_{ij} + (v_i - u_i)\frac{\partial}{\partial x_j}\left[\tau\theta\left(S_{ij} - \frac{1}{d}\delta_{ij}\nabla\cdot\boldsymbol{u}\right)\right]\right\} \tag{A 27}$$

and

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{(1)} = \left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)\left\{-\frac{\tau}{\theta} f^{eq}\boldsymbol{S}:\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\} \tag{A 28}$$

Performing differentiations term by term, (A 28) can be further written as

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{(1)} \equiv A + B + C \tag{A 29}$$

where the explict expressions for A, B, and C are given by

$$\left.\begin{aligned}
A &\equiv -\left[\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right) f^{eq}\right]\left\{\frac{\tau}{\theta}\boldsymbol{S}:\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\},\\
B &\equiv -\left[\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)(\tau\boldsymbol{S})\right]:\left\{\frac{1}{\theta} f^{eq}\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\},\\
C &\equiv -\left[\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right]:\left\{\frac{\tau}{\theta} f^{eq}\boldsymbol{S}\right\}.
\end{aligned}\right\} \tag{A 30}$$

These can be further organized by using the following relationships:

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)(\tau\boldsymbol{S}) = \left(\partial_{t_0} + \boldsymbol{u}\cdot\nabla\right)(\tau\boldsymbol{S}) + (\boldsymbol{v}-\boldsymbol{u})\cdot\nabla(\tau\boldsymbol{S})$$

and

$$\left(\partial_{t_0} + \boldsymbol{v}\cdot\nabla\right)\boldsymbol{u} = (\boldsymbol{v}-\boldsymbol{u})\cdot\nabla\boldsymbol{u} - \frac{1}{\rho}\nabla(\rho\theta).$$

Hence, we can rewrite (A 30) as

$$\left.\begin{aligned}
A &\equiv -\tau\left\{\frac{1}{\theta}\boldsymbol{S}:\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\}^2 f^{eq},\\
B &\equiv -\left[\left(\partial_{t_0} + \boldsymbol{u}\cdot\nabla\right)(\tau\boldsymbol{S})\right]:\left\{\frac{1}{\theta} f^{eq}\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\}\\
&\quad -[(\boldsymbol{v}-\boldsymbol{u})\cdot(\tau\boldsymbol{S})]:\left\{\frac{1}{\theta} f^{eq}\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}) - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})^2\right]\right\},\\
C &\equiv 2\frac{\tau}{\theta} f^{eq}\boldsymbol{S}:\left[(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u})\cdot\nabla\boldsymbol{u} - \frac{1}{d}\boldsymbol{I}(\boldsymbol{v}-\boldsymbol{u})(\boldsymbol{v}-\boldsymbol{u}):\nabla\boldsymbol{u}\right].
\end{aligned}\right\} \tag{A 31}$$

The second-order non-equilibrium distribution $f^{(2)}$ is determined by substituting the expressions for (A 27) and (A 28), together with (A 29) and (A 31), into (A 17).

The derivation of $\sigma_{ij}^{(2)}$ proceeds using a set of straightforward Gaussian integrals,

$$\frac{1}{(2\pi\theta)^{d/2}}\int \mathrm{d}\boldsymbol{v}\, v_{i_1}v_{i_2}v_{i_3}\cdots v_{i_n}\exp\left[-\frac{\boldsymbol{v}^2}{2\theta}\right] = \theta^{n/2}\delta^{(n)}_{i_1 i_2\cdots i_n}, \quad n = 2, 4, 6, \ldots, \tag{A 32}$$

where $\delta^{(n)}$ is the so-called n-dimensional delta function that is a summation of a product of $n/2$ simple Kronecker delta functions $\delta_{i_1 i_2} \cdots \delta_{i_{n-1} i_n}$ and those from permutations of its sub-indices (involving $(n-1)(n-3)\cdots 3\cdot 1$ total number of terms). Specifically, $\delta^{(2)}_{ij} = \delta_{ij}$, and

$$\delta^{(4)}_{ijkl} = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk},$$

$$\delta^{(6)}_{ijklmn} = \delta_{ij}\delta^{(4)}_{klmn} + \delta_{ik}\delta^{(4)}_{jlmn} + \delta_{il}\delta^{(4)}_{jkmn} + \delta_{im}\delta^{(4)}_{jkln} + \delta_{in}\delta^{(4)}_{jklm}.$$

Using these basic properties of the Gaussian integrals, we can directly calculate term-by-term the expression for $\sigma^{(2)}_{ij}$:

$$\sigma^{(2)}_{ij} = -\frac{1}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j) f^{(2)} = \frac{\tau}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j)\left[\partial_{t_1} f^{eq} + A + B + C\right] \tag{A 33}$$

where $\partial_{t_1} f^{eq}$, A, B, and C are given by (A 27) and (A 31). We provide the analytical result of the integration for each term, as shown below:

$$\frac{\tau}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j)\partial_{t_1} f^{eq} = \frac{4\tau^2\theta}{d}\delta_{ij} S_{kl} S_{kl} \tag{A 34}$$

where we have ignored terms proportional to $\nabla\cdot\boldsymbol{u}$. The remainder of the integrations give

$$\frac{\tau}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j)A = -2\tau^2\theta[\delta_{ij} S_{kl} S_{kl} + 4 S_{ik} S_{kj}], \tag{A 35}$$

$$\frac{\tau}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j)B = -2\tau\theta(\partial_t + \boldsymbol{u}\cdot\nabla)(\tau S_{ij}), \tag{A 36}$$

$$\frac{\tau}{\rho}\int \mathrm{d}\boldsymbol{v}(v_i - u_i)(v_j - u_j)C = 2\tau^2\theta\left[\delta_{ij} S_{kl} S_{kl} + S_{ik}\frac{\partial u_k}{\partial x_j} + S_{jk}\frac{\partial u_k}{\partial x_i}\right], \tag{A 37}$$

where we have safely omitted the sub-index '0' in the time derivative. Combining the results of (A 34)–(A 37) into (A 33), we obtain, after some final reorganization, the second–order momentum stress tensor:

$$\sigma^{(2)}_{ij} = -2\tau\theta(\partial_t + \boldsymbol{u}\cdot\nabla)(\tau S_{ij}) - 4\tau^2\theta\left[S_{ik}S_{kj} - \frac{1}{d}\delta_{ij} S_{kl} S_{kl}\right] + 2\tau^2\theta[S_{ik}\Omega_{kj} + S_{jk}\Omega_{ki}] \tag{A 38}$$

where the vorticity tensor is defined as

$$\Omega_{ij} \equiv \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right].$$

Ignoring terms proportional to $\nabla\rho$, $\nabla\theta$, and $\nabla\cdot\boldsymbol{u}$ in the incompressible limit, the analytical expression for the momentum stress tensor up to the second order is

$$\begin{aligned}\sigma_{ij} &\approx \sigma^{(0)}_{ij} + \sigma^{(1)}_{ij} + \sigma^{(2)}_{ij} \\ &= -\theta\delta_{ij} + 2\nu[S_{ij} - (\partial_t + \boldsymbol{u}\cdot\nabla)(\tau S_{ij})] \\ &\quad - 4\frac{\nu^2}{\theta}\left[S_{ik}S_{kj} - \frac{1}{d}\delta_{ij} S_{kl} S_{kl}\right] + 2\frac{\nu^2}{\theta}[S_{ik}\Omega_{kj} + S_{jk}\Omega_{ki}]\end{aligned} \tag{A 39}$$

where $\nu \equiv \tau\theta$.

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