From Boltzmann Kinetics to the Navier-Stokes Equations without a Chapman-Enskog Expansion

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(Dated: March 14, 2018)

Abstract

It is well known that the Navier-Stokes equations can be derived from the Boltzmann Equation, which governs the kinetic theory of gases, upon (i) assuming the Bhatnagar-Gross-Krook collision formulation (a simple relaxation toward an equilibrium distribution), (ii) assuming the Maxwell-Boltzmann form of this equilibrium distribution, and (iii) performing the so-called Chapman-Enskog perturbation expansion under the assumption of a short relaxation time. Herein, we demonstrate that there is an alternate path from Boltzmann to Navier-Stokes (in lieu of the Chapman-Enskog expansion) and that the particular form of the equilibrium distribution is inconsequential, as long as it meets some basic properties such as isotropy in velocity space and integrability of several moments. The essential ingredients are the relaxation formulation of the collision term and the assumption of a short relaxation time. This analysis provides new insights into the connections between kinetic theory and continuum mechanics, and it suggests new possibilities for fluid flow modeling using kinetic theory.

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6 I. INTRODUCTION

Boltzmann kinetic theory describes the microscopic evolution of a large number of colliding particles, such as in a monoatomic ideal gas. This theory has become accepted as a valid representation of fluid mechanics since it was shown that the microscopic description of Boltzmann kinetics produces the Navier-Stokes equations at the macroscopic level [1]. This strong connection between Boltzmann and Navier-Stokes has subsequently justified numerical simulation of continuum fluid flows based on the *Boltzmann Equation* (which governs kinetic theory); in particular, the *lattice-Boltzmann method* (LBM) has enjoyed great success due to the ease of coding, ease of accommodating complex moving boundaries, and computational efficiency [2–4]. Today, the LBM is used across a very wide array of applications from improving vehicle aerodynamics [5, 6] to flow through porous media [7].

Historically, the link between microscopic Boltzmann kinetics and macroscopic fluid mechanics was made through the so-called Chapman-Enskog perturbation expansion [1, 8–10]. The expansion is based on the assumption that the mean free time τ between successive collisions is very short compared to the time scale of evolution of the fluid flow L/V, where L and V are characteristic length and velocity scales of the macroscopic flow. In other words, the fluid flow is assumed to evolve only slightly over a great many particle collisions. This short-time assumption is consistent with assuming a very small $Knudsen\ number\ \epsilon \equiv \lambda/L = U\tau/L \ll 1$, where $\lambda \equiv U\tau$ is the mean free path, U is the thermal speed, and it is assumed that $V \leq \mathcal{O}(U)$. Based on the smallness of the Knudsen number, the particle mass probability distribution function f (i.e. the probability of finding mass moving at a certain velocity at a certain location; SI units: kg/[(m/s)³· m³]) can be formally expanded:

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots$$
 (1)

²⁸ with time likewise split into multiple time variables, each one evolving more slowly than the previous one:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots$$
 (2)

³⁰ Upon inserting (1) and (2) into the Boltzmann Equation, the Navier-Stokes equations can be ³¹ derived. The procedure is systematic and straightforward, although the algebra is tedious.

Although the Chapman-Enskog procedure is beyond debate, it is worth exploring other connections between the Boltzmann and Navier-Stokes equations, because these connections could
provide a fresh perspective on turbulence modeling [11–14]. In this paper we show that there
is an alternate path from the Boltzmann Equation to the Navier-Stokes equations that does not
involve the Chapman-Enskog expansion. Instead, a formal solution for the distribution f is first
established, and then using this solution the constitutive relations for the stress and energy flux
are obtained. The assumption of a short relaxation time (equivalent to a small Knudsen number)
simplifies the expressions by means of Taylor series expansions, and the Navier-Stokes equations
emerge. This theoretically-minded paper provides a crucial step towards establishing new perspectives on turbulence modeling via Boltzmann kinetics, although such turbulence modeling efforts

⁴² are beyond the scope of this contribution. What follows instead is a detailed derivation of the ⁴³ continuum mass, momentum, and energy conservation equations from the Boltzmann Equation in ⁴⁴ a novel way that does not involve the Chapman-Enskog expansion.

45 II. FROM BOLTZMANN KINETICS TO CONTINUUM MECHANICS

46 A. Boltzmann Kinetics

Our premise is Boltzmann kinetic theory, which governs the evolution of a mass probability distribution $f(t,\mathbf{x},\mathbf{u})$. The quantity $f(t,\mathbf{x},\mathbf{u}) d\mathbf{x} d\mathbf{u}$ represents the mass of fluid particles that, at time t, are located within volume $d\mathbf{x} = dx_1 dx_2 dx_3$ surrounding position $\mathbf{x} = [x_1, x_2, x_3]$ and endowed with velocity within the range $d\mathbf{u} = du_1 du_2 du_3$ surrounding $\mathbf{u} = [u_1, u_2, u_3]$. Like the particle positions \mathbf{x} , the particle velocities \mathbf{u} are independent variables, and the ensemble-averaged hydrodynamic variables are derived from $f(t, \mathbf{x}, \mathbf{u})$ via integrals over all possible velocities [3, 15]:

density:
$$\rho(t, \mathbf{x}) \equiv \iiint f(t, \mathbf{x}, \mathbf{u}) \ d\mathbf{u}$$
 (3)

velocity:
$$\bar{u}_i(t,\mathbf{x}) \equiv \frac{1}{\rho} \iiint u_i \ f(t,\mathbf{x},\mathbf{u}) \ d\mathbf{u}$$
 (4)

internal energy:¹
$$\frac{3}{2}U^{2}(t,\mathbf{x}) \equiv \frac{1}{\rho} \iiint \frac{1}{2} |\mathbf{u} - \bar{\mathbf{u}}(t,\mathbf{x})|^{2} f(t,\mathbf{x},\mathbf{u}) d\mathbf{u}$$
 (5)

total energy:
$$\check{e}(t,\mathbf{x}) \equiv \frac{1}{\rho} \iiint \frac{1}{2} |\mathbf{u}|^2 f(t,\mathbf{x},\mathbf{u}) d\mathbf{u} = \frac{1}{2} |\bar{\mathbf{u}}(t,\mathbf{x})|^2 + \frac{3}{2} U^2(t,\mathbf{x})$$
 (6)

stress:
$$\sigma_{ij}(t,\mathbf{x}) \equiv -\iiint (u_i - \bar{u}_i(t,\mathbf{x}))(u_j - \bar{u}_j(t,\mathbf{x})) f(t,\mathbf{x},\mathbf{u}) d\mathbf{u}$$
 (7)

energy flux:
$$q_i(t,\mathbf{x}) \equiv \iiint_{\frac{1}{2}} |\mathbf{u} - \bar{\mathbf{u}}(t,\mathbf{x})|^2 (u_i - \bar{u}_i(t,\mathbf{x})) f(t,\mathbf{x},\mathbf{u}) d\mathbf{u} , \qquad (8)$$

47 in which $\iiint(\ldots) d\mathbf{u}$ is shorthand for the definite integral $\iiint_{-\infty}^{\infty}(\ldots) du_1 du_2 du_3$. For convenience, 48 we will hereafter use index notation for vectors (and tensors) and adopt the convention of implicit 49 summation over repeated indices.

The velocity U of the internal energy (5) can be understood as the thermal agitation velocity; that is, the average velocity of Brownian motions of particles between collisions. The right hand set side of equation (6) follows from (4) and (5) and the fact that $|\mathbf{u} - \bar{\mathbf{u}}|^2 = |\mathbf{u}|^2 - 2\mathbf{u} \cdot \bar{\mathbf{u}} + |\bar{\mathbf{u}}|^2$.

The evolution of the mass probability distribution is governed by the *Boltzmann Equation* [3] (written here with gravity as the sole external force):

$$\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} - g \frac{\partial f}{\partial u_3} = \mathcal{C}(f) , \qquad (9)$$

55 in which -g is the downward gravitational acceleration (with x_3 directed upward). This evolution 56 equation states that mass distribution function f is advected in physical space by the particle 57 velocities, altered in velocity space by the gravitational acceleration, and redistributed by collisions. 58 The collision term C(f) may be expressed in a variety of ways depending on assumptions made 59 about individual collisions [3, 16], but for the purpose of the recovery of the Navier-Stokes Equa-60 tions, it turns out that a fairly simple form is sufficient: It is assumed that the accumulated

² The factor $\frac{3}{2}$ in front of U^2 is reflective of the three dimensions of the physical space. This factor becomes $\frac{2}{2}$ in two dimensions and $\frac{1}{2}$ in one dimension.

61 effect of collisions is merely to relax the distribution f toward an equilibrium distribution f^{eq} via 62 $C(f) = \frac{1}{\tau}(f^{eq} - f)$. This is the so-called BGK formulation [17], with a relaxation time τ that can be 63 interpreted as the averaged time between successive collisions. This formulation leads to rewriting 64 Equation (9) as the *Boltzmann-BGK equation*:

$$\left[\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} = \frac{1}{\tau} (f^{eq} - f) + g \frac{\partial f}{\partial u_3} \right]. \tag{10}$$

65 The form of the equilibrium distribution f^{eq} is discussed next.

66 B. Form of the Equilibrium Distribution

Since Ludwig Boltzmann [18] considered gas particles animated by Brownian motions, it has been traditional to adopt for f^{eq} the Maxwell-Boltzmann distribution:

$$f^{eq}(t,\mathbf{x},\mathbf{u}) = \frac{\rho(t,\mathbf{x})}{(2\pi)^{3/2} U^{3}(t,\mathbf{x})} \exp\left(-\frac{|\mathbf{u} - \bar{\mathbf{u}}(t,\mathbf{x})|^{2}}{2U^{2}(t,\mathbf{x})}\right) , \qquad (11)$$

69 which is a Gaussian distribution of velocities u_i centered on their averages \bar{u}_i and with standard 70 deviation U.

Alternative distributions are worth considering, especially Lévy α -stable distributions [14]. So, 72 we will proceed using a generic distribution of the form

$$f^{eq}(t,\mathbf{x},\mathbf{u}) = \frac{\rho(t,\mathbf{x})}{U^3(t,\mathbf{x})} F(\Delta(t,\mathbf{x},\mathbf{u})) \quad \text{with} \quad \Delta(t,\mathbf{x},\mathbf{u}) = \frac{|\mathbf{u} - \bar{\mathbf{u}}(t,\mathbf{x})|^2}{U^2(t,\mathbf{x})} . \tag{12}$$

To ensure that the collision term $(f^{eq} - f)/\tau$ on the right hand side of (10) conserves mass, momentum, and energy, f^{eq} is required to obey equations (3), (4), and (5) [3]. Clearly, this is the case for the Maxwell-Boltzmann distribution (11). For the generic distribution (12), condition (4) is automatically satisfied by symmetry, whereas satisfaction of (3) and (5) imposes respectively:

$$I_1 \equiv \int_0^\infty \Delta^{\frac{1}{2}} F(\Delta) \ d\Delta = \frac{1}{2\pi} \ , \tag{13}$$

$$I_3 \equiv \int_0^\infty \Delta^{\frac{3}{2}} F(\Delta) \ d\Delta = \frac{3}{2\pi} \ . \tag{14}$$

⁷⁷ Equations (13) and (14) are obtained by inserting (12) into (3) and (5), passing to spherical coordinates, and evaluating the angular integrals. Equations (13) and (14) impose two constraints on the moments of $F(\Delta)$. Not only must they be finite, but but they must take on these specific values in order to conserve mass and energy during collisions. If $F(\Delta)$ corresponds to Maxwell-Boltzmann, these constraints are satisfied naturally. If $F(\Delta)$ has a heavy tail (as in a Lévy α -stable distribution with $\alpha < 2$), then a truncation and renormalization are required.

C. Continuum Governing Equations as Moments

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The governing equations of continuum mechanics can be derived by taking moments of the Boltzmann-BGK Equation (10). In particular, the zeroth, first and second moments of (10) result

86 in the continuum equations for conservation of mass, momentum, and energy. This development is 87 well known, but it is reviewed here both for completeness and to contextualize the novel solution 88 presented in §III.

89 1. Mass

Mass conservation is obtained by the zeroth moment of Equation (10), which is simply its integration over the velocity space:

$$\iiint \left\{ \frac{\partial f}{\partial t} + u_i \, \frac{\partial f}{\partial x_i} \right\} d\mathbf{u} = \iiint \left\{ \frac{1}{\tau} (f^{eq} - f) + g \, \frac{\partial f}{\partial u_3} \right\} d\mathbf{u} \,. \tag{15}$$

The temporal and spatial derivatives commute with the velocity integrations because they are independent variables. The gravity term vanishes because $f \to 0$ as $u_3 \to \pm \infty$. The $f^{eq} - f$ term vanishes because collisions conserve mass (i.e. both distributions satisfy (3)). Then, with definitions (3) and (4), Equation (15) reduces to the continuity equation:

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho \bar{u}_i) = 0} \ . \tag{16}$$

96 2. Momentum

The momentum equations are obtained by the first-order moments of (10):

$$\iiint u_j \left\{ \frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} \right\} d\mathbf{u} = \iiint u_j \left\{ \frac{1}{\tau} (f^{eq} - f) + g \frac{\partial f}{\partial u_3} \right\} d\mathbf{u} . \tag{17}$$

98 Upon expansion of $u_i u_j = (u_i - \bar{u}_i)(u_j - \bar{u}_j) + u_i \bar{u}_j + u_j \bar{u}_i - \bar{u}_i \bar{u}_j$, the advective term in (17) 99 evaluates to

$$\frac{\partial}{\partial x_i} \iiint u_i u_j \ f \ d\mathbf{u} = \frac{\partial}{\partial x_i} \iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) f \ d\mathbf{u} + \frac{\partial}{\partial x_i} \iiint (u_i \bar{u}_j + u_j \bar{u}_i - \bar{u}_i \bar{u}_j) f \ d\mathbf{u}}_{\equiv -\sigma_{ij} \text{ via (7)}} + \frac{\partial}{\partial x_i} \iiint (u_i \bar{u}_j + u_j \bar{u}_i - \bar{u}_i \bar{u}_j) f \ d\mathbf{u}}_{=\rho \bar{u}_i \bar{u}_j} \tag{18}$$

The gravity term is evaluated by making use of $u_3 \frac{\partial f}{\partial u_3} = \frac{\partial (u_3 f)}{\partial u_3} - f$ and the fact that $u_3 f \to 0$ 101 as $u_3 \to \pm \infty$. The $f^{eq} - f$ term vanishes because collisions conserve momentum (i.e. both 102 distributions satisfy (4)). Thus, (17) with (18) simplifies to the Cauchy momentum equation:

$$\frac{\partial}{\partial t}(\rho \bar{u}_j) + \frac{\partial}{\partial x_i}(\rho \bar{u}_i \bar{u}_j) = \frac{\partial \sigma_{ij}}{\partial x_i} - \rho g \delta_{j3} \quad .$$
(19)

At this point, we note that if the stress (7) can be reduced to the Newtonian constitutive equation, then continuity equation (16) and momentum equation (19) would together become the Navier-Stokes equations.

106 3. Energy

The total energy equation is obtained as (half of) the second moment of (10)

$$\iiint \frac{1}{2} u_i u_i \left\{ \frac{\partial f}{\partial t} + u_j \frac{\partial f}{\partial x_j} \right\} d\mathbf{u} = \iiint \frac{1}{2} u_i u_i \left\{ \frac{1}{\tau} (f^{eq} - f) + g \frac{\partial f}{\partial u_3} \right\} d\mathbf{u} . \tag{20}$$

The unsteady term readily evaluates to $\frac{\partial}{\partial t}(\frac{3}{2}\rho U^2 + \frac{1}{2}\rho\bar{u}_i\bar{u}_i)$ by definition (6). The collision term integrates to zero because collisions conserve energy (i.e. both distributions satisfy (6)). The gravitational term integrates by parts to $-\rho g\bar{u}_3$, assuming $u_3^2 f \to 0$ as $u_3 \to \pm \infty$.

The advective term can be partitioned via $u_i = (u_i - \bar{u}_i) + \bar{u}_i$ to obtain:

$$\iiint_{\frac{1}{2}} u_{i} u_{i} u_{j} f d\mathbf{u} = \iiint_{\frac{1}{2}} (u_{i} - \bar{u}_{i})(u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j}) f d\mathbf{u} + \bar{u}_{i} \iiint_{\frac{1}{2}} (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j}) f d\mathbf{u} \\
+ \bar{u}_{j} \iiint_{\frac{1}{2}} (u_{i} - \bar{u}_{i})(u_{i} - \bar{u}_{i}) f d\mathbf{u} + \left(\frac{1}{2} \bar{u}_{i} \bar{u}_{i}\right) \bar{u}_{j} \iiint_{\frac{1}{2}} f d\mathbf{u} \\
= \frac{3}{2} \rho U^{2} \text{ via (5)} \\
= q_{j} - \bar{u}_{i} \sigma_{ij} + \left(\frac{3}{2} \rho U^{2} + \frac{1}{2} \rho \bar{u}_{i} \bar{u}_{i}\right) \bar{u}_{j} . \tag{21}$$

112 With this expression, the total energy budget (20) becomes:

$$\frac{\partial}{\partial t} \left(\frac{3}{2} \rho U^2 + \frac{1}{2} \rho \bar{u}_i \bar{u}_i \right) + \frac{\partial}{\partial x_j} \left[\left(\frac{3}{2} \rho U^2 + \frac{1}{2} \rho \bar{u}_i \bar{u}_i \right) \ \bar{u}_j \right] = \frac{\partial}{\partial x_j} (\bar{u}_i \sigma_{ij}) - \rho g \bar{u}_3 - \frac{\partial q_j}{\partial x_j} \ . \tag{22}$$

Equation (22) can be simplified by making use of the earlier momentum equation (19) to eliminate the mean kinetic energy. Upon switching the i and j indices in (19), multiplying by \bar{u}_i , and then using (16) we obtain the kinetic energy evolution equation:

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho \bar{u}_i \bar{u}_i \right) + \frac{\partial}{\partial x_j} \left(\frac{1}{2} \rho \bar{u}_i \bar{u}_i \bar{u}_j \right) = \bar{u}_i \frac{\partial \sigma_{ij}}{\partial x_j} - \rho g \bar{u}_3 . \tag{23}$$

116 Then subtracting (23) from (22) yields the equation for the evolution of only the internal energy:

$$\left| \frac{\partial}{\partial t} \left(\frac{3}{2} \rho U^2 \right) + \frac{\partial}{\partial x_j} \left(\frac{3}{2} \rho U^2 \bar{u}_j \right) = \sigma_{ij} \left| \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j} \right|. \tag{24}$$

Equations (16), (19) and (24) provide a set of three equations for the three hydrodynamic variables ρ , \bar{u}_i , and U^2 . The key is to be able to express the stress tensor σ_{ij} and energy flux vector q_j in terms of only the same hydrodynamic variables in order to have a closed set of governing equations.

121 III. CONSTITUTIVE EQUATIONS FOR THE STRESS AND ENERGY FLUX

With the development presented in the preceding section, the Chapman-Enskog expansion could then be used to derive the constitutive relations for the stress and energy flux. Herein, we present a novel route towards deriving these constitutive relations. The end result of the present derivation 125 is the same: Assuming the equilibrium distribution f^{eq} is the Maxwell-Boltzmann distribution, the 126 derivation leads to the constitutive relations consistent with a compressible Newtonian fluid that 127 behaves as an ideal gas. The present derivation, however, lays a framework for considering other 128 equilibrium distributions (such as the $L\acute{e}vy$ α -stable distributions [14]), although such considerations 129 are beyond the current scope.

130 A. General Solution of the Boltzmann-BGK Equation

Our derivation begins with the realization that the Boltzmann-BGK equation (10) is linear in unknown f. Therefore, the closed form solution is immediate:

$$f(t, x_i, u_i) = \frac{1}{\tau} \int_{-\infty}^{t} f^{eq} \left(t', x_i - u_i \left(t - t' \right) - \delta_{i3} \frac{1}{2} g \left(t - t' \right)^2, u_i + \delta_{i3} g \left(t - t' \right) \right) e^{-\frac{t - t'}{\tau}} dt', \quad (25)$$

where δ_{ij} stands for the Kronecker delta (the identity tensor). Note that the equilibrium distribuwithin the integrand is shifted in time, space, and velocity to an earlier time t', corresponding upstream position, and corresponding vertical velocity $u_3 + g(t - t')$. This earlier time t' varies from long ago $-\infty$ to the present time t. The exponential decay indicates that contributions from more remote times are attenuated compared to more recent times and is attributable to memory loss caused by collisions.³

A more compact expression of (25) can be obtained by switching from the earlier time t' to the dimensionless elapsed time $s \equiv (t - t')/\tau$, which runs from 0 to $+\infty$. We further introduce the tilde notation to indicate a variable with space-time shift

$$\tilde{f}^{eq} \equiv f^{eq} \left(t - s\tau, x_i - u_i s\tau - \delta_{i3} \frac{1}{2} g s^2 \tau^2, u_i + \delta_{i3} g s\tau \right) , \qquad (27)$$

142 so that (25) becomes

$$f = \int_0^\infty \tilde{f}^{eq} e^{-s} ds$$
 (28)

The spatial domain is taken as infinite so as to avoid the complications of boundary conditions.

B. General Form of the Stress and Energy Flux

The stress tensor σ_{ij} and the energy flux vector q_j were defined in equations (7) and (8), respectively. Inserting the general solution (28) into (7) and (8), we can write

$$\sigma_{ij} = -\iiint_{0}^{\infty} (u_i - \bar{u}_i)(u_j - \bar{u}_j) \ \tilde{f}^{eq} \ e^{-s} \ ds \ d\mathbf{u}$$
 (29)

$$q_{j} = \iiint_{0}^{\infty} \frac{1}{2} |\mathbf{u} - \bar{\mathbf{u}}|^{2} (u_{j} - \bar{u}_{j}) \ \tilde{f}^{eq} \ e^{-s} \ ds \ d\mathbf{u} \ . \tag{30}$$

$$f(t, x_i, u_i) = \frac{1}{\tau} \int_0^t f^{eq} \left(t', x_i - u_i (t - t') - \delta_{i3} \frac{1}{2} g (t - t')^2, u_i + \delta_{i3} g (t - t') \right) e^{-\frac{t - t'}{\tau}} dt'$$

$$+ f_0 \left(x_i - u_i t - \delta_{i3} \frac{1}{2} g t^2, u_i + \delta_{i3} g t \right) e^{-\frac{t}{\tau}},$$
(26)

in which $f_0(x_i, u_i)$ is the initial distribution. Note how its contribution is fading with time.

³ If one is uneasy about going back in time forever (t' starting at $-\infty$), one can write the solution in terms of an initial condition (with time t' now starting from 0):

These integrals (over ds and $d\mathbf{u}$) would be straightforward to calculate if it were not for the spacetime shift in \tilde{f}^{eq} . Indeed, without the space-time shift, \tilde{f}^{eq} would be replaced by f^{eq} , the integrals would decouple, and $\int_0^\infty e^{-s} ds = 1$. Denoting the resulting stress and energy flux as $\sigma_{ij}^{(0)}$ and $\sigma_{ij}^{(0)}$ we have

$$\sigma_{ij}^{(0)} = -\iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) \ f^{eq} \ d\mathbf{u} = -\rho U^2 \delta_{ij}$$
 (31)

$$q_j^{(0)} = \iiint_{\frac{1}{2}} |\mathbf{u} - \bar{\mathbf{u}}|^2 (u_j - \bar{u}_j) \ f^{eq} \ d\mathbf{u} = 0 \ , \tag{32}$$

Note that the diagonal elements of the stress are equal to one another because f^{eq} is isotropic in velocity space, and the off-diagonal elements vanish because f^{eq} is symmetric in $(u_i - \bar{u}_i)$. We recognize here the pressure component of the stress tensor, with pressure defined as $p = \rho U^2$. The stress tensor can thus be decomposed as follows:

$$\sigma_{ij} = -p \,\delta_{ij} + \tau_{ij} \,\,, \tag{33}$$

155 with the deviatoric component au_{ij} corresponding to the space-time shift in $ilde{f}^{eq}$.

The conclusion at this point is that, if the space-time shift is ignored, the non-dissipative Euler equations are recovered. Put another way, the space-time shift is what introduces viscosity in the momentum equation and diffusion in the energy equation.

The integral expressions of the deviatoric stress tensor and energy flux vector are:

$$\tau_{ij} = -\int_0^\infty e^{-s} ds \iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) (\tilde{f}^{eq} - f^{eq}) d\mathbf{u}$$
 (34)

$$q_{j} = \int_{0}^{\infty} e^{-s} ds \iiint_{\frac{1}{2}} |\mathbf{u} - \bar{\mathbf{u}}|^{2} (u_{j} - \bar{u}_{j}) \left(\tilde{f}^{eq} - f^{eq} \right) d\mathbf{u}, \tag{35}$$

160 in which we recall that the tilde indicates a time shift by $-s\tau$, space shift by $-u_i s\tau$, and velocity 161 shift by $\delta_{i3} gs\tau$, so the integrals are coupled. The problem is to find a way to express the integrals 162 in (34) and (35) in terms of only ρ , \bar{u}_i and U. We shall proceed by considering the deviatoric stress 163 (34) in §III C and the energy flux (35) in §III D.

C. Deviatoric stress

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In this subsection, we evaluate the deviatoric stress (34). To start, we invoke the assumption of a short relaxation time. In the spirit of Chapman-Enskog, we assume τ is so short compared to the time scale over which the overall system evolves that only short time shifts $t - t' = s\tau$ need to be considered, because the time exponential in (34) vanishes rapidly. This means that the space-time shift in \tilde{f}^{eq} is relatively small, and a Taylor expansion of \tilde{f}^{eq} may be performed with respect to $s\tau$. Recalling that the space-time shift occurs inside the hydrodynamic variables ρ , \bar{u}_i and U on which f^{eq} depends, we apply the chain rule to $f^{eq} = f^{eq}(\rho(t,x_i),\bar{u}_i(t,x_i),U^2(t,x_i),u_i)$:

$$\tilde{f}^{eq} = f^{eq} + \frac{\partial f^{eq}}{\partial \rho} \left(\tilde{\rho} - \rho \right) + \frac{\partial f^{eq}}{\partial \bar{u}_m} \left(\tilde{u}_m - \bar{u}_m \right) + \frac{\partial f^{eq}}{\partial (U)^2} \left(\tilde{U}^2 - U^2 \right) + \frac{\partial f^{eq}}{\partial u_3} gs\tau + O(s^2 \tau^2)$$
 (36)

and then expand the shifted hydrodynamic variables (e.g. $\tilde{\rho} = \rho(t-s\tau,x_i-u_is\tau-\delta_{i3}\frac{1}{2}gs^2\tau^2)$):

$$\tilde{\rho} = \rho + \left(\frac{\partial \rho}{\partial t} + u_n \frac{\partial \rho}{\partial x_n}\right) (-s\tau) + O(s^2\tau^2)$$
(37)

$$\tilde{\bar{u}}_m = \bar{u}_m + \left(\frac{\partial \bar{u}_m}{\partial t} + u_n \frac{\partial \bar{u}_m}{\partial x_n}\right) (-s\tau) + O(s^2\tau^2)$$
(38)

$$\tilde{U}^2 = U^2 + \left(\frac{\partial(U^2)}{\partial t} + u_n \frac{\partial(U^2)}{\partial x_n}\right) (-s\tau) + O(s^2\tau^2) . \tag{39}$$

Using (36)–(39), the deviatoric stress (34) becomes

$$\tau_{ij} = +\tau \underbrace{\int_{0}^{\infty} s \ e^{-s} \ ds}_{=1} \iiint (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j})$$

$$\left[\frac{\partial f^{eq}}{\partial \rho} \left(\frac{\partial \rho}{\partial t} + u_{n} \frac{\partial \rho}{\partial x_{n}}\right) + \frac{\partial f^{eq}}{\partial \bar{u}_{m}} \left(\frac{\partial \bar{u}_{m}}{\partial t} + u_{n} \frac{\partial \bar{u}_{m}}{\partial x_{n}}\right) + \frac{\partial f^{eq}}{\partial (U^{2})} \left(\frac{\partial (U^{2})}{\partial t} + u_{n} \frac{\partial (U^{2})}{\partial x_{n}}\right) - g \frac{\partial f^{eq}}{\partial u_{3}}\right] d\mathbf{u}$$

$$(40)$$

The u_n terms within the square bracket are evaluated with the aid of $u_n = (u_n - \bar{u}_n) + \bar{u}_n$ and the following arguments: Since f^{eq} is required to be isotropic in the velocity space according to (12), it must be an even function of $(u_m - \bar{u}_m)$, and its derivatives with respect to \bar{u}_m and u_3 are odd. However, the derivatives $\partial f^{eq}/\partial \rho$ and $\partial f^{eq}/\partial (U^2)$ remain even functions of their argument. These symmetries and anti-symmetries lead to the cancellation of numerous integrals in (40), including that with gravity. The integral over s, which now stands alone, can be readily evaluated (= 1). After this series of simplifications, (40) becomes

$$\tau_{ij} = \tau \left(\frac{\partial \rho}{\partial t} + \bar{u}_n \frac{\partial \rho}{\partial x_n} \right) \iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) \frac{\partial f^{eq}}{\partial \rho} d\mathbf{u}$$

$$+ \tau \frac{\partial \bar{u}_m}{\partial x_n} \iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j)(u_n - \bar{u}_n) \frac{\partial f^{eq}}{\partial \bar{u}_m} d\mathbf{u}$$

$$+ \tau \left(\frac{\partial (U^2)}{\partial t} + \bar{u}_n \frac{\partial (U^2)}{\partial x_n} \right) \iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) \frac{\partial f^{eq}}{\partial (U^2)} d\mathbf{u} .$$

$$(41)$$

For the generic equilibrium distribution f^{eq} given in (12), its derivatives with respect to ρ , \bar{u}_m and u_{182} U^2 are:

$$\frac{\partial f^{eq}}{\partial \rho} = \frac{1}{U^3} F(\Delta) \tag{42}$$

$$\frac{\partial f^{eq}}{\partial \bar{u}_m} = -\frac{2\rho}{U^5} \left(u_m - \bar{u}_m \right) F'(\Delta) \tag{43}$$

$$\frac{\partial f^{eq}}{\partial (U^2)} = -\frac{3\rho}{2U^5} F(\Delta) - \frac{\rho}{U^5} \Delta F'(\Delta), \tag{44}$$

and the expression (41) for τ_{ij} becomes:

$$\tau_{ij} = \frac{\tau}{U^{3}} \left(\frac{\partial \rho}{\partial t} + \bar{u}_{n} \frac{\partial \rho}{\partial x_{n}} \right) \iiint (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j}) F(\Delta) d\mathbf{u}$$

$$- \frac{2\rho\tau}{U^{5}} \frac{\partial \bar{u}_{m}}{\partial x_{n}} \iiint (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j})(u_{m} - \bar{u}_{m})(u_{n} - \bar{u}_{n}) F'(\Delta) d\mathbf{u}$$

$$- \frac{3\rho\tau}{2U^{5}} \left(\frac{\partial (U^{2})}{\partial t} + \bar{u}_{n} \frac{\partial (U^{2})}{\partial x_{n}} \right) \iiint (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j}) F(\Delta) d\mathbf{u}$$

$$- \frac{\rho\tau}{U^{5}} \left(\frac{\partial (U^{2})}{\partial t} + \bar{u}_{n} \frac{\partial (U^{2})}{\partial x_{n}} \right) \iiint (u_{i} - \bar{u}_{i})(u_{j} - \bar{u}_{j}) \Delta F'(\Delta) d\mathbf{u}.$$

$$(45)$$

Using spherical coordinates in velocity space (r, θ, ϕ) with $(u_1 - \bar{u}_1, u_2 - \bar{u}_2, u_3 - \bar{u}_3) = (r \sin \phi \cos \theta, 185 r \sin \phi \sin \theta, r \cos \phi)$, such that $d(u_1 - \bar{u}_1) d(u_2 - \bar{u}_2) d(u_3 - \bar{u}_3) = r^2 \sin \phi d\phi d\theta dr$, and $(0 \le \phi \le \pi, 186 0 \le \theta \le 2\pi, \Delta = r^2/U^2)$, the preceding integrals (some after integration by parts) can be expressed 187 in more compact forms and then evaluated using (14):

$$\iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) F(\Delta) d\mathbf{u} = +\frac{2\pi}{3} U^5 \left(\int_0^\infty \Delta^{\frac{3}{2}} F(\Delta) d\Delta \right) \delta_{ij} = U^5 \delta_{ij}$$

$$\iiint (u_i - \bar{u}_i)(u_j - \bar{u}_j) \Delta F'(\Delta) d\mathbf{u} = -\frac{5\pi}{3} U^5 \left(\int_0^\infty \Delta^{\frac{3}{2}} F(\Delta) d\Delta \right) \delta_{ij} = -\frac{5}{2} U^5 \delta_{ij}$$
 (47)

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$$\int (u_i - \bar{u}_i)(u_j - \bar{u}_j)(u_m - \bar{u}_m)(u_n - \bar{u}_n) F'(\Delta) du$$

$$= \begin{cases}
-\pi U^7 \left(\int_0^\infty \Delta^{\frac{3}{2}} F(\Delta) d\Delta \right) = -\frac{3}{2} U^7 & \text{if all indices are equal} \\
-\frac{\pi}{3} U^7 \left(\int_0^\infty \Delta^{\frac{3}{2}} F(\Delta) d\Delta \right) = -\frac{1}{2} U^7 & \text{if indices make two pairs} \\
0 & \text{if at least one index is unique} \\
= -\frac{1}{2} U^7 \left(\delta_{ij} \delta_{mn} + \delta_{im} \delta_{jn} + \delta_{in} \delta_{jm} \right).$$
(48)

in which the combination $(\delta_{ij}\delta_{mn} + \delta_{im}\delta_{jn} + \delta_{in}\delta_{jm})$ equals 3 if i = j = n = m, equals 1 if the set 190 (i, j, m, n) consists of two pairs, and equals 0 otherwise. Upon inserting (46)–(48) into (45), the 191 deviatoric stress tensor is found to be:

$$\tau_{ij} = \tau \left[\frac{\partial}{\partial t} (\rho U^2) + \bar{u}_n \frac{\partial}{\partial x_n} (\rho U^2) \right] \delta_{ij} + \rho \tau U^2 \frac{\partial \bar{u}_m}{\partial x_n} (\delta_{ij} \delta_{mn} + \delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}), \tag{49}$$

This expression can be further simplified by making use of the continuity equation (16) and internal energy equation (24). Taking the energy equation (24) at leading order in $s\tau$ (i.e. with taken as $\sigma_{ij}^{(0)} = -\rho U^2 \delta_{ij}$ and q_j taken as $q_j^{(0)} = 0$, which is sufficient at this order of $s\tau$), we arrive at the final expression for the deviatoric stress tensor:

$$\tau_{ij} = \rho \tau U^2 \left[\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \left(\frac{\partial \bar{u}_m}{\partial x_m} \right) \delta_{ij} \right]. \tag{50}$$

196 Equation (50) represents the constitutive equation for a compressible Newtonian fluid with viscosity

$$\mu = \rho \tau U^2 = \rho U \lambda \ . \tag{51}$$

197 It is important to note that this value is independent of the particular form of the equilibrium 198 distribution, so long as it is isotropic and satisfies the constraints (13) and (14).

Upon inserting (50) and (51) into the momentum equation (19), we recover the compressible flow Navier-Stokes equation. Thus we have derived the Navier-Stokes momentum equation from both Boltzmann Equation without a Chapman-Enskog expansion.

D. Energy flux

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We now proceed likewise to obtain the energy flux vector so as to complete the closure of the hydrodynamic equations. Our starting point is expression (35), which is repeated here for convenience:

$$q_{j} = \int_{0}^{\infty} e^{-s} ds \iiint_{\frac{1}{2}} |\mathbf{u} - \bar{\mathbf{u}}|^{2} (u_{j} - \bar{u}_{j}) \left(\tilde{f}^{eq} - f^{eq} \right) d\mathbf{u} .$$
 (52)

Note that because (52) contains all scales of \mathbf{u} , the quantity q_j represents both the flux of both heat and kinetic energy due to velocity departures from the mean. Thus, we expect q_j to be related to the heat flux (as in Fourier's law) and may possibly contain an additional term to account for a kinetic energy flux.

We again make use of the Taylor expansion of \tilde{f}^{eq} performed in (36)–(39). With the time integral now decoupled, it evaluates readily: $\int_0^\infty s \ e^{-s} ds = 1$. Using $|\mathbf{u} - \bar{\mathbf{u}}|^2 = U^2 \Delta$ by virtue of 212 (12), Equation (52) turns into:

$$q_{j} = -\frac{\tau U^{2}}{2} \iiint (u_{j} - \bar{u}_{j}) \Delta \left[\frac{\partial f^{eq}}{\partial \rho} \left(\frac{\partial \rho}{\partial t} + u_{n} \frac{\partial \rho}{\partial x_{n}} \right) + \frac{\partial f^{eq}}{\partial \bar{u}_{m}} \left(\frac{\partial \bar{u}_{m}}{\partial t} + u_{n} \frac{\partial \bar{u}_{m}}{\partial x_{n}} \right) + \frac{\partial f^{eq}}{\partial (U^{2})} \left(\frac{\partial (U^{2})}{\partial t} + u_{n} \frac{\partial (U^{2})}{\partial x_{n}} \right) - g \frac{\partial f^{eq}}{\partial u_{3}} \right] d\mathbf{u}.$$

$$(53)$$

Using again the set (42)–(44), to which we add

$$\frac{\partial f^{eq}}{\partial u_3} = \frac{2\rho}{U^5} (u_3 - \bar{u}_3) F'(\Delta), \tag{54}$$

214 replacing u_n by $(u_n - \bar{u}_n) + \bar{u}_n$, and observing that many integrals vanish by symmetry, we obtain:

$$q_{j} = -\frac{\tau}{2U} \frac{\partial \rho}{\partial x_{n}} \iiint (u_{j} - \bar{u}_{j})(u_{n} - \bar{u}_{n}) \Delta F(\Delta) d\mathbf{u}$$

$$+ \frac{\rho \tau}{U^{3}} \left(\frac{\partial \bar{u}_{m}}{\partial t} + \bar{u}_{n} \frac{\partial \bar{u}_{m}}{\partial x_{n}} \right) \iiint (u_{j} - \bar{u}_{j})(u_{m} - \bar{u}_{m}) \Delta F'(\Delta) d\mathbf{u}$$

$$+ \frac{3\rho \tau}{4U^{3}} \frac{\partial (U^{2})}{\partial x_{n}} \iiint (u_{j} - \bar{u}_{j})(u_{n} - \bar{u}_{n}) \Delta F(\Delta) d\mathbf{u}$$

$$+ \frac{\rho \tau}{2U^{3}} \frac{\partial (U^{2})}{\partial x_{n}} \iiint (u_{j} - \bar{u}_{j})(u_{n} - \bar{u}_{n}) \Delta^{2} F'(\Delta) d\mathbf{u}$$

$$+ \frac{\rho g \tau}{U^{3}} \iiint (u_{j} - \bar{u}_{j})(u_{3} - \bar{u}_{3}) \Delta F'(\Delta) d\mathbf{u} .$$

$$(55)$$

Clearly, the remaining integrals vanish unless j equals one of m, n, or 3. The non-zero integrals can be evaluated by passing to spherical coordinates in velocity space:

$$\iiint (u_j - \bar{u}_j)(u_n - \bar{u}_n) \ \Delta \ F(\Delta) \ d\mathbf{u} = \frac{2\pi}{3} \ U^5 I_5 \ \delta_{jn}$$
 (56)

$$\iiint (u_j - \bar{u}_j)(u_m - \bar{u}_m) \Delta F'(\Delta) d\mathbf{u} = -\frac{5\pi}{3} U^5 I_3 \delta_{jm}$$

$$(57)$$

$$\iiint (u_j - \bar{u}_j)(u_n - \bar{u}_n) \ \Delta^2 \ F'(\Delta) \ d\mathbf{u} = -\frac{7\pi}{3} \ U^5 I_5 \ \delta_{jn}$$
 (58)

215 in which I_3 was defined in (14) and I_5 is defined as:⁴

$$I_5 \equiv \int_0^\infty \Delta^{\frac{5}{2}} F(\Delta) \ d\Delta \ . \tag{59}$$

216 Upon inserting (56)–(58) into (55), we obtain for the energy flux:

$$q_{j} = -\frac{\pi}{3} I_{5} \tau U^{4} \frac{\partial \rho}{\partial x_{j}} - \frac{5\pi}{3} I_{3} \rho \tau U^{2} \left(\frac{\partial \bar{u}_{j}}{\partial t} + \bar{u}_{n} \frac{\partial \bar{u}_{j}}{\partial x_{n}} + g \delta_{j3} \right) - \frac{2\pi}{3} I_{5} \rho \tau U^{2} \frac{\partial (U^{2})}{\partial x_{j}} . \tag{60}$$

This expression can be simplified by making use of the momentum equation (19) taken at leading order in τ (which reads $\frac{\partial \bar{u}_j}{\partial t} + \bar{u}_n \frac{\partial \bar{u}_j}{\partial x_n} + g \delta_{j3} = \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_i} = -\frac{1}{\rho} \frac{\partial (\rho U^2)}{\partial x_j}$):

$$q_{j} = -\frac{\pi}{3} I_{5} \rho \tau U^{2} \frac{\partial (U^{2})}{\partial x_{j}} - \frac{\pi}{3} (I_{5} - 5I_{3}) \tau U^{2} \frac{\partial (\rho U^{2})}{\partial x_{j}}.$$
 (61)

The first term in Equation (61) constitutes the heat flux in the classical sense. In the context of classical Boltzmann kinetic theory, the equilibrium distribution is restricted to be the Maxwell-Boltzmann distribution, for which $I_5 = \frac{15}{2\pi} = 5I_3$. This leads to the cancellation of the second term in (61), leaving $q_j = -\frac{5}{2}\rho\tau U^2 \frac{\partial(U^2)}{\partial x_j}$. The classical theory relates the thermal speed U to the absolute temperature by $U^2 = \frac{k_B}{m}T$, where $k_B = 1.381 \times 10^{-23}$ J/K is the Boltzmann constant and is the mass of a particle. Then (61) is equivalent to

$$q_j = -k \frac{\partial T}{\partial x_j}$$
, with $k = \frac{5}{2}nk_BU^2\tau$, (62)

where k is the thermal conductivity (W/m·K) and $n = \rho/m$ is the number of particles per volume. Thus, with f^{eq} taken as the Maxwell-Boltzmann distribution and the preceding relation between thermal speed and absolute temperature, we have recovered Fourier's Law of heat conduction without performing a Chapman-Enskog expansion.

But when the equilibrium distribution is other than Maxwell-Boltzmann, the difference $I_5 - 5I_3$ does not necessarily vanish, and the second energy flux term of (61) may remain. The presence of this term can be rationalized with the following analogy: The Reynolds-average equation⁵ for the turbulent kinetic energy $tke \equiv \frac{1}{2}\rho \overline{u_i'u_i'}$ is:

$$\frac{\partial (tke)}{\partial t} + \frac{\partial (tke \ \bar{u}_j)}{\partial x_j} = -\rho \ \overline{u_i'u_j'} \ \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{1}{2}\rho \ \overline{u_i'u_j'u_j'} + \overline{u_j'p'} - \mu \ \overline{u_i's_{ij}} \right) - 2\mu \ \overline{S_{ij}'S_{ij}'} \ . \tag{63}$$

⁴ Using the Schwartz inequality, it can be shown that $I_1I_5 \ge I_3^2$, and thus $I_5 \ge 9/2\pi$ for all distributions.

⁵ The form given here is for incompressible flow in the absence of gravity (Pope, 2000, page 125) in order to make the argument as brief as possible. Primed quantities denote turbulent fluctuations, in accord with the classical Reynolds decomposition.

where $S'_{ij} \equiv \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}$ is the fluctuating strain rate. The analogy is not perfect, and it suffices to 234 ignore the viscous terms in (63). Mapping the non-viscous terms in (63) onto the energy budget 235 (24) of Boltzmann kinetic theory, the analogy yields:

$$\frac{3}{2}\rho U^2 = \frac{1}{2}\rho \,\overline{u_i'u_i'} \equiv tke \tag{64}$$

$$\sigma_{ij} \frac{\partial \bar{u}_i}{\partial x_j} = -\rho \, \overline{u'_i u'_j} \, \frac{\partial \bar{u}_i}{\partial x_j} \tag{65}$$

$$q_j = \frac{1}{2}\rho \, \overline{u_i' u_i' u_j'} + \overline{u_j' p'} \,, \tag{66}$$

The equivalence expressed in (64) is obvious from the form of (5), but now interpreting U as the rms velocity fluctuation rather than the thermal speed. Likewise, the mapping (65) is clear from the definition of the stress tensor (7). This leaves Equation (66) to be matched with (61). With $p = \rho U^2$ according to (33), the natural partitioning is:

$$-\frac{\pi}{3}I_5 \rho \tau U^2 \frac{\partial(U^2)}{\partial x_j} = \frac{1}{2}\rho \overline{u_i' u_i' u_j'}$$

$$\tag{67}$$

$$-\frac{\pi}{3}(I_5 - 5I_3) \tau U^2 \frac{\partial p}{\partial x_j} = \overline{u_j' p'}$$

$$\tag{68}$$

²⁴⁰ with correlations expressed as down-gradient fluxes, as it could be expected. From this consider-²⁴¹ ation, the second term of (61) represents redistribution of kinetic energy by pressure fluctuations ²⁴² (modeled as a gradient of the mean pressure). What is rather unexpected is that this term vanishes ²⁴³ when the equilibrium distribution happens to be Gaussian.

244 IV. CONCLUSIONS

The preceding analysis leads to three important conclusions: First, the Chapman-Enskog expansion is not the only path to obtain the Navier-Stokes equations from the Boltzmann Equation. Second, the alternative path followed here shows that the particular form of the equilibrium distribution is rather inconsequential as long as it obeys a few basic properties, chiefly isotropy in velocity space and integrability. The two essential ingredients in the Boltzmann Equation are the BGK formulation for the collision term and the smallness of its relaxation time. Third, there is a new term in the expression for energy flux when the equilibrium distribution f^{eq} is not Gaussian, which is found to be similar to the pressure redistribution flux of the Reynolds-average equation for the turbulent kinetic energy.

254 ACKNOWLEDGMENTS

The authors are grateful to Dr. Hudong Chen for valuable insight and discussions that helped shape this article.

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