COARSE-GRAINED TRANSPORT OF A TURBULENT FLOW VIA MOMENTS OF THE REYNOLDS-AVERAGED BOLTZMANN EQUATION

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Abstract. Here we introduce new coarse-grained variables for a turbulent flow in the form of moments of its Reynolds-averaged Boltzmann equation. With the exception of the collision moments, the transport equations for the new variables are identical to the usual moment equations, and thus naturally lend themselves to the variety of already existing closure methods. Under the anelastic turbulence approximation, we derive equations for the Reynolds-averaged turbulent fluctuations around the coarse-grained state. We show that the global relative entropy of the coarse-grained state is bounded from above by the Reynolds average of the fine-grained global relative entropy, and thus obeys the time decay bound of Desvillettes and Villani. This is similar to what is observed in the rarefied gas dynamics, which makes the Grad moment closure a good candidate for truncating the hierarchy of the coarse-grained moment equations. We also show that, under additional assumptions on the form of the coarse-grained collision terms, one arrives at the Navier-Stokes closure, which can be naturally extended to the Burnett and super-Burnett orders. Finally, we suggest crude parameterizations of the coarse-grained collision terms for use as starting points in numerical simulation and modeling.

1. Introduction

A common principle in turbulence modeling involves the averaging of the well-known Navier-Stokes equations to filter out the rapid small-scale turbulent fluctuations from their solutions to reduce computational cost. This is usually done via the Reynolds averaging of the Navier-Stokes equations [25,26,29,38], which produces additional nonlinear terms in the equations. These additional terms are often modeled via the turbulent eddy viscosity assumption, which was suggested back in 1877 by Boussinesq [5], and which generally provides good agreement with experiments in near-wall boundary layers.

However, for the fully developed three-dimensional turbulence it was observed that the concept of the turbulent eddy viscosity fails [19]. Girimaji [12] argued that the reason why the turbulent viscosity approximation could be invalid for the averaged Navier-Stokes equations was that the latter required that the corresponding solution of the Boltzmann equation [6,7,13,21] was near its Maxwellian equilibrium, while the corresponding averaged solution did not have to be near equilibrium. As an alternative to the Reynolds averaging of the Navier-Stokes equations, Girimaji [12] proposed the direct filtering of the solution of the Boltzmann equation instead, and then solve the filtered equation using the lattice Boltzmann method (LBM).
However, Girimaji’s approach had a few drawbacks. First, the Reynolds stress closure problem was not eliminated in [12], and the Reynolds stress was modeled by the standard Smagorinsky-Lilly closure [33], the assumptions of which can be traced back to the Boussinesq approximation [5]. Second, the Bhatnagar-Gross-Krook (BGK) approximation of the collision terms [4], which was used in [12], sets the Prandtl number of the flow strictly to 1, whereas it is known that the Prandtl number of a fluid is generally different from 1; for example, for a monatomic ideal gas it equals 2/3, and its value for the air is around 0.7-0.8 (there are, however, improved BGK collision parameterizations with non-unitary Prandtl numbers [1, 2]). Third, the lattice Boltzmann method usually involves more computational variables than the standard fluid dynamics methods, which may limit its use in some applications.

In this work we propose a new coarse-graining approach were the Reynolds averaging is used directly on the Boltzmann equation like in [12], however, we further convert the resulting Reynolds-averaged Boltzmann equation into the hierarchy of the coarse-grained moment equations. While the new coarse-grained moments are different from the usual Reynolds averages of moment variables used in conventional transport methods, the resulting hierarchy of the transport equations for the coarse-grained moments is identical to the usual moment transport hierarchy, with the exception of the nonlinear collision terms. We show that the global relative entropy of the Reynolds-averaged Boltzmann equation is bounded from above by the Reynolds average of the global relative entropy of the usual Boltzmann equation, and, therefore, obeys the same bound on the decay rate as established by Desvillettes and Villani [10] for the usual Boltzmann equation. This justifies the same closure methodologies as are used to truncate the moment transport equations for the rarefied gas dynamics [8], in particular the Grad [14,15] closure.

For the modeling of statistical properties of the turbulent fluctuations, we derive the equation for the transport of the turbulent kinetic energy under the approximation of the anelastic turbulence, as well as the appropriate relations for the turbulent components of the stress and heat flux. There remain three unspecified dissipation terms: the turbulent energy dissipation rate, and the two collision moments for the coarse-grained stress and heat flux. The reason why the coarse-grained collision terms remain unspecified is because they originate from the Reynolds average of the nonlinear collision operator of the Boltzmann equation, and thus require additional information about the structure of the statistical ensemble (and, therefore, the physics of the flow). We suggest crude approximations for these remaining nonlinear terms, based on a dimensional reasoning.

The manuscript is organized as follows. In Section 2 we discuss the Boltzmann equation and its conventional closures: the Euler, Navier-Stokes and Grad equations. In Section 3 we introduce the Reynolds averaging operator, define the new coarse-grained variables, and show that the transport equations for the new coarse-grained variables have the same hierarchy as those for the conventional fine-grained variables, with different collision terms. In Section 4 we parameterize the turbulent fluctuations of the stress and heat flux, and derive the transport equation for the turbulent energy. In Section 5 we describe the Grad and Navier-Stokes moment closures for the new coarse-grained transport equations, as well as mention how to extend the latter to the Burnett and
super-Burnett orders. In Section 6 we discuss basic approaches to the modeling of the coarse-grained collision terms and the turbulent energy dissipation rate. In Section 7 we summarize the results and discuss future work.

2. Conventional moment closures of the Boltzmann equation

In the absence of external forces, the Boltzmann equation for a 3-dimensional fluid is given by [6, 7]

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = C(f).
\]

Here, \(t\) and \(x\) are the time and space coordinates, \(v\) is the velocity of a fluid particle, and \(f(t, x, v)\) is the statistical velocity distribution of the fluid particles, at the location \(x\) and time \(t\). The left-hand side contains the transport terms for \(f\), while the right-hand side contains the nonlinear collision term, which generally has the effect of dissipation. In many applications, \(C(f)\) is assumed to be bilinear in \(f\), as the situations where three or more particles collide at once rarely occur.

Let the angle brackets denote the average over the fluid particles \(v\):

\[
\langle b \rangle_f(t, x) = \int b(v)f(t, x, v) \, dv,
\]

\[
\langle b \rangle_{C(f)}(t, x) = \int b(v)C(f(t, x, v)) \, dv.
\]

for an integrable function \(b(v)\). Then, one can apply these averages onto the Boltzmann equation in (2.1) and obtain the corresponding moment transport equation:

\[
\frac{\partial}{\partial t} \langle b \rangle_f + \text{div}_x \langle bv \rangle_f = \langle b \rangle_{C(f)}.
\]

The nonlinear collision term \(C(f)\) has the requirement of the mass, momentum, and energy conservation:

\[
\langle 1 \rangle_{C(f)} = 0, \quad \langle v \rangle_{C(f)} = 0, \quad \langle \|v\|^2 \rangle_{C(f)} = 0.
\]

The last identity also signifies that there is no “internal energy” in the fluid – all energy that the fluid carries is confined to the velocity of its particles. This transport-collision model applies, for example, to a monatomic ideal gas. Here we adopt this model for the sake of simplicity of illustration, as the presence of “hidden” energy-accumulating degrees of freedom in the fluid particles requires a different, more complicated treatment of the Boltzmann equation, which will be presented elsewhere.

In order to obtain the conventional moment closures from the moment transport equation (2.3), we first introduce the following conventional velocity moments of \(f\):

\[
\rho = \langle 1 \rangle_f, \quad \text{density},
\]

\[
\rho u = \langle v \rangle_f, \quad \text{momentum},
\]

\[
p = \frac{1}{3} \langle \|v - u\|^2 \rangle_f, \quad \text{pressure},
\]
\[ S = \langle (v - u) \otimes (v - u) \rangle_f - pI, \] stress,

\[ q = \frac{1}{2} \langle \|v - u\|^2(v - u) \rangle_f, \] heat flux,

where \( \otimes \) denotes the outer product of two vectors. Rearranging the averages \( (2.5c) - (2.5e) \) above, one writes the identities

\[ \langle \|v\|^2 \rangle_f = 3p + \rho \|u\|^2, \] (2.6a)

\[ \langle v \otimes v \rangle_f = S + pI + \rho u \otimes u, \] (2.6b)

\[ \frac{1}{2} \langle \|v\|^2 v \rangle_f = q + Su + \frac{5}{2}pI + \frac{1}{2}\rho \|u\|^2u. \] (2.6c)

Now, writing the moment transport equation in \( (2.3) \) for the velocity moments in \( (2.5a), (2.5b), (2.6a) - (2.6c) \), expressing those moments in terms of \( \rho, u, p, S \) and \( q \) using the identities above, and taking into account the mass, momentum, and energy conservation laws in \( (2.4) \), one arrives at the following system of equations:

\[ \frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0, \] (2.7a)

\[ \frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u \otimes u + pI + S) = 0, \] (2.7b)

\[ \frac{\partial p}{\partial t} + \text{div}(pu) + \frac{2}{3}(p \text{div}u + S : (\nabla \otimes u) + \text{div}q) = 0, \] (2.7c)

\[ \frac{\partial S}{\partial t} + (u \cdot \nabla)S + \text{div}(u)S + 2[S(\nabla \otimes u)]_{TS} + \text{div}Q - \frac{2}{3}(\text{div}q)I + 2p[\nabla \otimes u]_{TS} = C_S, \] (2.7d)

\[ \frac{\partial q}{\partial t} + \text{div}(q \otimes u) + (q \cdot \nabla)u - \frac{1}{\rho} \left( \frac{5}{2}pI + S \right) \text{div}(pI + S) + Q : (\nabla \otimes u) + \text{div}R = c_q, \] (2.7e)

where

\[ C_S = \langle v \otimes v \rangle_{C(f)}, \quad c_q = \frac{1}{2} \langle (\|v\|^2 - 2u \cdot v)v \rangle_{C(f)}, \]

the symbol \( : \) denotes the Frobenius product of two matrices, and \( [A]_{TS} \) denotes the traceless symmetrization of a \( 3 \times 3 \) matrix \( A \):

\[ [A]_{TS} = \frac{1}{2} \left( A + A^T \right) - \frac{1}{3} \text{Tr}(A)I. \] (2.9)

Above in \( (2.7) \), \( Q \) and \( R \) are the unknown higher-order moments,

\[ Q = \langle (v - u) \otimes (v - u) \otimes (v - u) \rangle_f \]

being the full 3-rank skewness tensor, and

\[ R = \frac{1}{2} \langle \|v - u\|^2(v - u) \otimes (v - u) \rangle_f \] (2.10b)
being the matrix of the contracted 4th-order moment. Both $Q$ and $R$ obey their own transport equations, which, in turn, obviously include moments of yet higher orders, and so forth.

In order to understand how to close the moment equations above, we turn to the well-known Boltzmann’s $H$-theorem for ideal gases. We state Boltzmann’s $H$-theorem in the same form as in Golse [13]:

**Proposition 1 (Boltzmann’s $H$-theorem).** The following inequality holds for the collision term:

$$
\langle \ln f \rangle_{C(f)} \leq 0.
$$

Moreover, the following three conditions are equivalent:

1. $\langle \ln f \rangle_{C(f)} = 0$,
2. $C(f) = 0$ for all $v \in \mathbb{R}^3$,
3. $f$ is the local Maxwellian distribution,

$$
f_M(v) = \frac{\rho}{(2\pi \theta)^{3/2}} \exp \left(-\frac{\|v - u\|^2}{2\theta}\right),
$$

where $\theta$ denotes the temperature

$$
\theta = \frac{p}{\rho}.
$$

In order to make use of this theorem, one introduces the local and global entropy functionals as follows. The local entropy $S_l[f](t, x)$ is given by the functional

$$
S_l[f](t, x) = -\int f \ln f \, dv = -\langle \ln f \rangle_f.
$$

The global entropy $S_g[f](t)$ is further given by

$$
S_g[f](t) = \int S_l[f] \, dx = -\int \langle \ln f \rangle_f \, dx.
$$

Now, we can look at the evolution equation for $\langle \ln f \rangle_f$, which is given by

$$
\frac{\partial}{\partial t} \langle \ln f \rangle_f = \int (\ln f + 1) \frac{\partial f}{\partial t} \, dv = \int (\ln f + 1) (\nabla f + C(f)) \, dv.
$$

Observing the mass conservation law in (2.4), we further derive

$$
\frac{\partial}{\partial t} \langle \ln f \rangle_f + \nabla_x \langle v \ln f \rangle_f = \langle \ln f \rangle_C(f).
$$

Assuming that one can omit the effect of the spatial boundaries when integrating, we obtain for the global entropy

$$
\frac{d}{dt} S_g[f] = -\int \langle \ln f \rangle_C(f) \, dx.
$$

Qualitatively, the equations in (2.17) and (2.18) do, roughly, the following:
(1) The equation for the local entropy in (2.17) tends to increase the local entropy $S_l[f]$, unless $f$ is already the local Maxwellian state in (2.12), in which case $S_l[f]$ is already at its maximum for given local constraints $\rho$, $\mu$ and $\theta$ (or, equivalently, $p$). The rate of convergence towards the local maximum entropy state here is usually very rapid, however, the presence of advection prevents $S_l[f]$ from reaching its local maximum at (2.12).

(2) The equation for the global entropy in (2.18) tends to increase $S_g[f]$, unless $f$ is the global Maxwellian distribution of the form

$$f_g^M(v) = \frac{\rho_0}{(2\pi \theta_0)^{3/2}} \exp\left(-\frac{\|v - u_0\|^2}{2\theta_0}\right),$$

where $\rho_0$, $u_0$ and $\theta_0$ are constants throughout the spatial domain, specified by the total mass, momentum and energy constraints in the system. This process is unaffected by advection, and the time rate of convergence to the global maximum state is $O(t^{-\infty})$ (Desvillettes and Villani [10]), that is, rather slow.

These two processes are, in a certain sense, “mutually exclusive”, that is, the closer the $S_l[f](t, x)$ is to its local maximums at each $x$, the slower the rate with which $S_g[f](t)$ approaches its global maximum. This relation between the two processes can be quantified more systematically by introducing the relative entropy (Kullback-Leibler distance, [20]) $H[f|g]$ between two distributions $f$ and $g$ as

$$H[f|g](t) = \int f \ln(f/g) \, dv \, dx.$$

It is easy to show that $H[f|g]$ is always non-negative, and is zero if and only if $f = g$. Now we denote the local and global relative entropies as

$$H_l[f] = H[f|f_M], \quad H_g[f] = H[f|f_g^M],$$

respectively. Then, $H_l[f]$ and $H_g[f]$ measure the information-theoretic distance between $f$ and (2.12) or (2.19), respectively, becoming quantitative indicators of the relation between the local and global entropy processes, described above. The “mutually exclusive” behavior (slow decrease rate of $H_g$ for small values of $H_l$, and, vice-versa, rapid decrease of $H_g$ for large values of $H_l$) can be observed in Figure 5 of [10], and also in Figures 8 and 9 of Filbet, Mouhot and Pareschi [11], where the time series of the local and global Kullback-Leibler distance between $f$ and both (2.12) and (2.19) are displayed for a direct numerical simulation with a Boltzmann equation. In Figure 1 we show an example of such time series, adapted from Figure 8 of [11]. In fact, if, in a hypothetical situation, $S_l[f]$ is always at its maximum at all points $x$ (which amounts to strictly zero $H_l[f]$), then $S_g[f]$ must be constant in time even if it is below its global possible maximum (or, equivalently, $H_g[f]$ must be constant in time even if nonzero). This assumption is, of course, unrealistic in practice, however, it is used in the Euler closure of the moment equations as we show below.

Different assumptions about the time-scale separation between the local and global entropy processes lead to three different conventional moment closures of the moment transport equations in (2.7).
2.1. The Euler closure. In the Euler closure, it is assumed that time-scale separation between the local and global entropy processes is infinite. Namely, it is assumed that the local entropy $S_l[f]$ always instantaneously jumps to its maximum for given $\rho$, $u$ and $\theta$, and $f(t, x, v)$ is permanently the Maxwellian state in (2.12). The global entropy $S_g[f]$ is, therefore, fixed at its initial value, irrespective of its maximum state for the present total mass, momentum and energy constraints. This assumption allows to set the stress $S$ and heat flux $q$ identically to zeros everywhere, since their corresponding velocity moments are indeed zeros for the Maxwellian distribution in (2.12). The resulting famous Euler equations are given by

\begin{align}
(2.22a) & \quad \frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0, \\
(2.22b) & \quad \frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u \otimes u) + \nabla p = 0, \\
(2.22c) & \quad \frac{\partial p}{\partial t} + \text{div}(pu) + \frac{2}{3} p \text{div}u = 0.
\end{align}

The practical application of the Euler equations is somewhat limited due to the lack of any kind of diffusion.
2.2. The Navier-Stokes closure. The Navier-Stokes closure is more sophisticated than the Euler closure in the sense that it recognizes the finiteness of the time scale of the local entropy dissipation process, as well as takes into account the correction in the local entropy process due to advection. As a result, dissipation of the global entropy is present on the long time scale, which is more physically realistic than the constant global entropy in the Euler closure.

As a result of statistical analysis of collisions of large numbers of ideal spheres (which ideal gas is modeled upon), one arrives at the following first-order linear approximations of the stress and heat flux collision operators in the equations for the stress (2.7d) and heat flux (2.7e):

\begin{equation}
C_S \approx -\frac{p}{\mu} S, \quad c_q \approx -\frac{5}{2} \frac{p}{\kappa} q,
\end{equation}

where the coefficients \(\mu\) and \(\kappa\) are the viscosity and heat conductivity of the fluid, respectively (for more details, see, for example, [13, 14]). Both \(\mu\) and \(\kappa\) are defined largely by the physical properties of colliding spheres, and for ideal gases they also weakly depend on the temperature \(\theta\). The ratio of the heat flux over stress dissipation rates is known as the Prandtl number,

\begin{equation}
Pr = \frac{\text{heat flux dissipation rate}}{\text{stress dissipation rate}} = \frac{5 \mu}{2 \kappa},
\end{equation}

which for monatomic gases equals precisely 2/3 [14].

In what follows, we prefer to keep both the viscosity \(\mu\) and heat conductivity \(\kappa\) as unrelated parameters, in order to distinguish between the terms related to the stress, and those related to the heat flux. However, it must be noted that, strictly put, all derivations below are only valid when \(15\mu = 4\kappa\), since this is what the monatomic gas model inherently implies.

Both \(\mu\) and \(\kappa\) are proportional to the masses of colliding spheres, which, in the case of molecules, renders both \(\mu\) and \(\kappa\) very small. As a result, the time scale of local entropy dissipation is \(\sim \mu/p\) (or, equivalently, \(\sim \kappa/p\)), and if \(p\) is not too small, both the stress \(S\) and heat flux \(q\) are very rapidly damped by their collision operators towards their Maxwellian values (that is, zeros). This allows to simplify the transport equations for the stress (2.7d) and heat flux (2.7e) into

\begin{equation}
\frac{\partial S}{\partial t} + 2p\left[\nabla \otimes u\right]_{TS} \approx -\frac{p}{\mu} S,
\end{equation}

\begin{equation}
\frac{\partial q}{\partial t} + \frac{5}{2} p \nabla \left( \frac{p}{\rho} \right) \approx -\frac{5}{2} \frac{p}{\kappa} q,
\end{equation}

where the advection terms with \(S\), \(q\) and \(Q\) were dropped, and the contracted fourth-order moment \(R\) was replaced with its Maxwellian value

\begin{equation}
R \approx \frac{5}{2} \frac{p^2}{\rho} I.
\end{equation}
Now, assuming that $\mu$ and $\kappa$ are small enough so that $S$ and $q$ decay on a much shorter time scale than the evolution of $\rho$, $u$ and $p$, one then approximates the stress and heat flux by their approximate steady states:

\begin{align}
(2.27a) \quad S &= -2\mu[\nabla \otimes u]_{TS}, \\
(2.27b) \quad q &= -\kappa \nabla (p/\rho).
\end{align}

A similar procedure is described by Grad [14], pp. 371–372, and by Struchtrup and Torrilhon [35].

The important consequence here is that the attracting states for $S$ and $q$ are not zeros (as opposed to the Euler closure) due to the effect of advection, which was taken into account. Lastly, substitution of the approximate states in (2.27) into the transport equations (2.7a)–(2.7c) yields the famous Navier-Stokes equations:

\begin{align}
(2.28a) \quad \frac{\partial \rho}{\partial t} + \text{div}(\rho u) &= 0, \\
(2.28b) \quad \frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u \otimes u) + \nabla p &= 2 \text{div} \left( \mu [\nabla \otimes u]_{TS} \right), \\
(2.28c) \quad \frac{\partial p}{\partial t} + \text{div}(pu) + \frac{2}{3}p \text{div} u &= \frac{4}{3}\mu \left\| [\nabla \otimes u]_{TS} \right\|^2 + \frac{2}{3} \text{div} (\kappa \nabla (p/\rho)).
\end{align}

Observe that now the Laplace diffusion is present in both the momentum and pressure equations, on the characteristic time scale of $\sim \mu^{-1}$ (or, equivalently, $\sim \kappa^{-1}$). This Laplace dissipation has the effect of “smoothing out” the velocity and pressure fields, which tends to slowly increase the global entropy $S_g[f]$ (or, alternatively, decrease the global relative entropy $H_g[f]$), making the process more consistent with the findings of Desvillettes and Villani [10]. The term with $\mu$ in the pressure equation is “ill-posed” (in the sense that it tends to increase the pressure, without any counter-balancing), and thus is often dropped.

In what follows, we assume that the Navier-Stokes relations (2.27) are valid approximations for the fine-grained stress $S$ and heat flux $q$ at all times.

### 2.3. The Grad closure.

Under certain conditions, the pressure $p$ becomes so small that the characteristic time scales $\sim \mu/p$ and $\sim \mu^{-1}$ become comparable. This happens when the fluid is “rarefied”, that is, the fluid particles are so spread out in space that the collisions rarely happen [8]. In this situation, the local entropy $S_l[f]$ and the global entropy $S_g[f]$ may exhibit comparable time scales of evolution, and the Navier-Stokes (let alone Euler’s) closure becomes inapplicable. In particular, one can no longer assume that the solution $f$ of the Boltzmann equation in (2.1) is a local Maxwellian (2.12), or anywhere near it.

An appropriate closure for this situation was suggested by Grad [14, 15]. The Grad approximation is based on the Hilbert expansion of the distribution function $f$ in the Boltzmann equation around its local Maxwellian state (2.12), such that it has the prescribed stress and heat flux, in addition to the density, momentum and pressure. The
resulting distribution approximates the statistical state of the fluid away from the local thermodynamic equilibrium and is given by

\( f_G(v) = f_M(v) \left[ 1 + \frac{\rho}{p^2} \left( \frac{\|v - u\|^2}{5p/\rho} - 1 \right) q \cdot (v - u) + \frac{\rho}{2p^2} S : ((v - u) \otimes (v - u)) \right], \)

where \( f_M \) is the corresponding Maxwellian distribution (2.12). As a result, the full skewness tensor \( Q \) and the contracted flatness matrix \( R \) are approximated by their values provided by (2.29), which can be computed explicitly as:

\[
(Q)_{ijk} = \frac{2}{5} \left( (q)_i \delta_{jk} + (q)_j \delta_{ik} + (q)_k \delta_{ij} \right),
\]

\[
R = \left( \frac{5p^2}{2\rho} I + \frac{7p^2}{2\rho} S \right).
\]

In particular, this means

\[
\text{div} Q = \frac{4}{5} [\nabla \otimes q]_{TS} + \frac{2}{3} (\text{div} q) I,
\]

\[
Q : (\nabla \otimes u) = \frac{2}{5} ((\text{div} u) q + (q \cdot \nabla) u + (\nabla \otimes u) q).
\]

Substituting these Grad approximations into the transport equations (2.7), we obtain the full set of closed transport equations for the coarse-grained variables \( \rho, u, p, S, q \):

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0,
\]

\[
\frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u \otimes u + p I + S) = 0,
\]

\[
\frac{\partial p}{\partial t} + \text{div}(pu) + \frac{2}{3} (p \text{div} u + S : (\nabla \otimes u) + \text{div} q) = 0,
\]

\[
\frac{\partial S}{\partial t} + (u \cdot \nabla) S + \text{div}(u) S + 2[S(\nabla \otimes u)]_{TS} + \frac{4}{5} [\nabla \otimes q]_{TS} + 2p[\nabla \otimes u]_{TS} = C_S,
\]

\[
\frac{\partial q}{\partial t} + \frac{7}{5} (\text{div} (q \otimes u) + (q \cdot \nabla) u) + \frac{2}{5} ((\nabla \otimes u) q - (u \cdot \nabla) q) -
\]

\[
- \frac{1}{\rho} \left( \frac{5p^2}{2\rho} I + \frac{7p^2}{2\rho} S \right) \text{div}(p I + S) + \text{div} \left( \frac{5p^2}{2\rho} I + \frac{7p^2}{2\rho} S \right) = c_q.
\]

Observe that the collision terms \( C_S \) and \( c_q \) retain their general form, while before in the Navier-Stokes closure they were approximated by the linear damping terms. Although the equations in (2.32) are known to develop shock waves at high Mach numbers [14,15], a suitable regularization have already been developed by Struchtrup and Torrilhon [34,35,37], by applying a similar type of closure as in (2.25)–(2.27), but to the higher-order transport equations for \( Q \) and \( R \), which produced additional diffusion terms in the equations for the stress and heat flux.
2.4. **Higher-order moment closures.** Obviously, one does not have to close the hierarchy in (2.7) at the equations for the stress $S$ and heat flux $q$, and instead choose to include the transport equations for $Q$, $R$ and higher-order moments \[3, 18, 27, 28, 31\]. However, for the clarity of presentation, we restrict ourselves here to the relatively simple closures presented above.

### 3. The moments of the Reynolds-averaged Boltzmann equation

In a turbulent flow, the quantities $\rho$, $u$, $p$, etc usually exhibit rapid small-scale oscillations in both space and time (that is, they are “noisy”), which often renders the direct numerical simulation of such flow computationally intractable, due to the need of extremely fine space and time discretization. Instead, one resorts to solving a different system of transport equations, which resolves the large scale features of the flow while forgoing the small scale oscillations in favor of a more smooth (and, of course, approximate) solution, in order to afford a more coarse computational discretization. Below, we refer to such approximate “smoothed out” variables as the coarse-grained variables, superscripted by asterisks.

Historically, such coarse-grained flow equations where obtained by applying the operation of “averaging” onto the turbulent Navier-Stokes equations, which was purported to smooth out small scale rapid oscillations. Reynolds \[29\] pioneered the use of such averaging operators back in 1895, and they became therefore named after him. Throughout the twentieth century, multiple different interpretations of the Reynolds averaging operator were developed, including time averaging for steady coarse-grained flows, running time-average for unsteady flows, scale-dependent spatial averaging (which later evolved into the large eddy simulation method \[30\], or LES), and so forth. Eventually, the idea of statistical Reynolds averaging was adopted (see \[25, 26\] and references therein), due to its convenient mathematical properties.

In the current work, we formally assume that the Reynolds averaging operator is a linear operator, conventionally denoted by an overbar, with the following properties:

1. **Linearity:** for two variables $h_1$ and $h_2$, and two numbers $a_1$ and $a_2$,

\[
\overline{a_1 h_1 + a_2 h_2} = a_1 \overline{h_1} + a_2 \overline{h_2}.
\]

Additionally, $\overline{a} = a$ if $a$ is a number.

2. **Commutativity with respect to differentiation and integration:**

\[
\overline{\partial h} = \overline{\partial h}, \quad \int \overline{h} = \int \overline{h}.
\]

3. **The Reynolds property:**

\[
\overline{h_1 h_2} = \overline{h_1} \overline{h_2}.
\]

We also formally assume that the Reynolds-averaged quantities $\overline{\rho}$, $\overline{u}$, $\overline{p}$, as well as their Reynolds-averaged products (such as $\overline{p u}$, for example) are sufficiently smooth at small scales to be computationally tractable. However, due to inherent nonlinearity in the velocity variable $u$, the transport equations for these Reynolds-averaged variables involve
new unresolved variables which are the Reynolds averages of products of turbulent fluctuations between the fine-grained and averaged variables. For example, the averaged momentum equation involves the Reynolds-averaged outer product of the turbulent velocity fluctuations, called the “Reynolds stress”, for which a closure is usually sought in the form of the Boussinesq approximation \[5\]. In this work we present a different approach, which produces the equations for the coarse-grained variables with a better closure potential.

Here we formally apply the Reynolds operator, described above, to the Boltzmann equation in (2.1) (rather than the Navier-Stokes equations), as was done previously by Girimaji \[12\]. The main novelty of our work is that, unlike \[12\], we further rebuild the hierarchy of the transport equations like the one in (2.7) for the moments of the Reynolds-averaged Boltzmann distribution. The resulting coarse-grained moment variables are different from the usual Reynolds averages of conventional moments in (2.5), and we provide suitable formulas to relate the new coarse-grained moment variables to the Reynolds averages of the conventional moments. The key advantage of our approach is that the transport equations for the new coarse-grained moments are identical to the conventional moment transport equations in (2.7) (collision terms being an exception), and, therefore, naturally lend themselves to the variety of previously developed closures for (2.7). The only unspecified closure parameters originate from the nonlinear collision term of the Boltzmann equation, which is not explicitly tractable by a linear averaging operator.

We define the new coarse-grained variables \(\rho^*, u^*, p^*, S^*, q^*, Q^*, R^*\) as follows:

\[
\begin{align*}
(3.4a) \quad & \rho^* = \langle 1 \rangle, \quad \text{coarse-grained density}, \\
(3.4b) \quad & \rho^* u^* = \langle v \rangle, \quad \text{coarse-grained momentum}, \\
(3.4c) \quad & p^* = \frac{1}{3} \langle \|v - u^*\|^2 \rangle, \quad \text{coarse-grained pressure}, \\
(3.4d) \quad & S^* = \langle (v - u^*) \otimes (v - u^*) \rangle - p^* I, \quad \text{coarse-grained stress}, \\
(3.4e) \quad & q^* = \frac{1}{2} \langle \|v - u^*\|^2 (v - u^*) \rangle, \quad \text{coarse-grained heat flux}, \\
(3.4f) \quad & Q^* = \langle (v - u^*) \otimes (v - u^*) \otimes (v - u^*) \rangle, \quad \text{coarse-grained skewness}, \\
(3.4g) \quad & R^* = \frac{1}{2} \langle \|v - u^*\|^2 (v - u^*) \otimes (v - u^*) \rangle, \quad \text{coarse-grained contracted flatness}.
\end{align*}
\]

Then, the following straightforward result follows.

**Proposition 2** (Coarse-grained transport equations). *The new coarse-grained variables are related to the Reynolds averages of the fine-grained variables as follows:*

\[
\begin{align*}
(3.5a) \quad & \rho^* = \bar{\rho}, \\
(3.5b) \quad & \rho^* u^* = \bar{\rho} \bar{u}, \quad u' = u - u^*.
\end{align*}
\]
(3.5c) \[ p^* = \bar{p} + \frac{1}{3}\rho \|u'\|^2, \]

(3.5d) \[ S^* = \bar{S} + \rho u' \otimes u' - \frac{1}{3}\rho \|u'\|^2 I, \]

(3.5e) \[ q^* = \bar{q} + \bar{S} u' + \frac{5}{2} \rho u' + \frac{1}{2} \rho \|u'\|^2 w', \]

(3.5f) \[ Q^* = \bar{Q} + (pI + S) \otimes u' + (pI + S) \otimes u'^T + (pI + S) \otimes u'^{TT} + \rho u' \otimes u' \otimes u', \]

(3.5g) \[ R^* = \bar{R} + \bar{Q} u' + (Su' + q) \otimes u' + u' \otimes (Su' + q) + \frac{7}{2} \rho u' \otimes u' + \frac{1}{2} \rho \|u'\|^2 (pI + S) + \frac{1}{2} \rho \|u'\|^2 u' \otimes u'. \]

Above, \( A^T \) and \( A^{TT} \) denote two possible transpositions of a 3-rank tensor \( A \). The transport equations for the coarse-grained variables in (3.5) are of the same form as the moment transport equations in (2.7), namely

(3.6a) \[ \frac{\partial \rho^*}{\partial t} + \text{div}(\rho^* u^*) = 0, \]

(3.6b) \[ \frac{\partial (\rho^* u^*)}{\partial t} + \text{div}(\rho^* u^* \otimes u^* + p^* I + S^*) = 0, \]

(3.6c) \[ \frac{\partial p^*}{\partial t} + \text{div}(p^* u^*) + \frac{2}{3} [p^* \text{div} u^* + S^* : (\nabla \otimes u^*) + \text{div} q^*] = 0, \]

(3.6d) \[ \frac{\partial S^*}{\partial t} + (u^* \cdot \nabla) S^* + \text{div}(u^*) S^* + 2 [S^* (\nabla \otimes u^*)]_{TS} + \text{div} Q^* - \frac{2}{3} (\text{div} q^*) I + 2 p^* [\nabla \otimes u^*]_{TS} = C^*_S, \]

(3.6e) \[ \frac{\partial q^*}{\partial t} + \text{div}(q^* \otimes u^*) + (q^* \cdot \nabla) u^* - \frac{1}{\rho^*} \left( \frac{5}{2} p^* I + S^* \right) \text{div}(p^* I + S^*) + Q^* : (\nabla \otimes u^*) + \text{div} R^* = c^*_q, \]

where the coarse-grained collision terms are given by the Reynolds averages

(3.7) \[ C^*_S = \bar{C}_S, \quad c^*_q = \bar{c}_q + \bar{C}_S u'. \]

**Proof.** The transport part of (3.6) is identical to that of (2.7) since the transport parts of the underlying Boltzmann’s equations for \( f \) and \( \bar{f} \) are identical. To derive the formulas in (3.5), first observe the following relations:

(3.8a) \[ \rho^* = \langle 1 \rangle \bar{f} = \langle 1 \rangle f = \bar{\rho}, \]

(3.8b) \[ \rho^* u^* = \langle v \rangle \bar{f} = \langle v \rangle f = \bar{\rho} u, \]
\begin{align}
(3.8c) \quad p^* + \frac{1}{3}\rho^* \|u^*\|^2 &= \frac{1}{3}\langle \|v\|^2 \rangle_f = \frac{1}{3}\langle \|v\|^2 \rangle_f = p + \frac{1}{3}\rho \|u\|^2, \\
(3.8d) \quad S^* + p^* I + \rho^* u^* \otimes u^* &= \langle v \otimes v \rangle_f = \langle v \otimes v \rangle_f = \mathcal{S} + \rho I + \rho u \otimes u, \\
(3.8e) \quad q^* + S^* u^* + \frac{5}{2} p^* u^* + \frac{1}{2} \rho^* \|u^*\|^2 u^* &= \frac{1}{2}\langle \|v\|^2 v \rangle_f = \mathcal{Q}, \\
(3.8f) \quad Q^* + (p^* I + S^*) \otimes u^* + ((p^* I + S^*) \otimes u^*)^T + ((p^* I + S^*) \otimes u^*)^T + p^* u^* \otimes u^* + (p I + S) \otimes u + ((p I + S) \otimes u)^T + ((p I + S) \otimes u)^T + p u \otimes u \otimes u,
\end{align}

Rearranging the above relations and noting that \(\bar{\rho}u^t = 0\), one obtains the definitions for the coarse-grained variables in \((3.5)\). Lastly, let us derive the formulas for the coarse-grained collision terms. The Reynolds-averaged moment transport equation in \((2.3)\) is given by

\begin{align}
(3.9) \quad \frac{\partial}{\partial t} \langle b \rangle_f + \operatorname{div}_x \langle bv \rangle_f = \langle b \rangle_{\mathcal{C}f},
\end{align}

In particular, for the stress matrix it is given by

\begin{align}
(3.10) \quad \frac{\partial}{\partial t} \langle v \otimes v \rangle_f + \operatorname{div}_x \langle v \otimes v \otimes v \rangle_f = \mathcal{C}_s,
\end{align}

where the collision term is unchanged, since the combinations of equations, added to the stress equation, have no collision terms. Now, subtracting the same combinations of the transport equations for the coarse-grained variables (which also do not have collision terms) in reverse order, we obtain the coarse-grained stress equation with the same averaged collision term. For the heat flux equation the situation is slightly different, as it is given by

\begin{align}
(3.11) \quad \frac{1}{2} \frac{\partial}{\partial t} \langle \|v\|^2 v \rangle_f + \frac{1}{2} \operatorname{div}_x \langle \|v\|^2 v \otimes v \rangle_f = \mathcal{C}_{q} + \mathcal{C}_s u,
\end{align}

as the derivation of the moment equation above requires adding the stress equation, multiplied by \(u\), to the heat flux equation. Now, the derivation of the coarse-grained
heat flux equation from the equation above requires subtracting the coarse-grained stress equation, accordingly multiplied by the coarse-grained velocity \( u^* \). This results in the coarse-grained collision terms of the form (3.7).

Unfortunately, there appears to be little we can do about the Reynolds-averaged collision terms in the context of turbulence transport. While the transport part of the Boltzmann equation is linear and thus is “transparent” to the Reynolds averaging, the same is not true for the collision terms. Without more information about the properties of the statistical ensemble (and, therefore, statistical physics of the fluid under consideration), we can only conclude that the coarse-grained collision terms \( C_S^* \) and \( c_q^* \) have a general dissipative effect towards the global maximum entropy state under the total mass, momentum and energy constraints. Below in Section 6 we suggest crude parameterizations of \( C_S^* \) and \( c_q^* \) based on dimensional arguments.

4. The Transport of Turbulent Energy under the Anelastic Turbulence Approximation

In the previous section we derived a hierarchy of the coarse-grained equations (3.6), which does not seem to require anything other than a suitable closure to become computationally tractable. However, observe that the new coarse-grained variables in (3.5) are not exactly what one would naturally need to model. For example, a meteorologist would likely need to model, among other variables, the Reynolds average of the pressure \( \bar{p} \) (as the closest computable alternative to the pressure \( p \) itself), yet observe that the coarse-grained variable \( p^* \) is not \( \bar{p} \), but rather \( \bar{p} + \rho \| u' \|^2 / 3 \) (see (3.5c)), where the additional term is not zero!

Therefore, we need to provide a means to recover the Reynolds averages of the fine-grained variables from the computed coarse-grained variables. In order to do this, we make an additional simplifying approximation about the nature of the small-scale turbulent fluctuations, which absolves us of the need to address the Reynolds averages of the density and velocity variables, leaving only the pressure, stress and heat flux to work with. Above, in the derivation of the equations for the coarse-grained variables, we assumed the most general form of turbulence, were the turbulent fluctuations were present in all fluid variables, and thus the Reynolds averages of fluid variables were generally never identity operators in the presence of turbulence. However, in many applications it is known that the density \( \rho \) is weakly affected by the small-scale turbulent fluctuations, and varies only on the coarse-grained “resolved” scale, while the higher order moments, such as the velocity \( u \), pressure \( p \), etc are still affected by the turbulence. Thus, here we assume the identity \( \rho = \rho^* \), and, therefore, \( \rho \) can be factored out of the Reynolds averages. As a result, the turbulent velocity component \( u' = u - u^* \) becomes anelastic:

\[
(4.1) \quad \text{div}(\rho u') = 0.
\]

Indeed, observe that subtracting the coarse-grained density equation (3.6a) from the fine-grained density equation (2.7a) results in

\[
(4.2) \quad \frac{\partial}{\partial t} (\rho - \rho^*) = \text{div}(\rho u - \rho^* u^*).
\]
Setting \( \rho^* = \rho \) above yields (4.1).

The anelastic turbulence approximation does not change the form of the coarse-grained transport equations in (3.6), but instead simplifies the definitions of the coarse-grained variables in (3.5) to some extent. For the Reynolds averages of the anelastic turbulent fluctuations

\[
\begin{align*}
  u' &= u - u^*, \\
p' &= p - p^*, \\
  S' &= S - S^*, \\
  q' &= q - q^*,
\end{align*}
\]

we obtain directly

\[
\begin{align*}
  (4.4a) & \quad \overline{u'} = 0, \\
  (4.4b) & \quad \overline{p'} = -\frac{1}{3} \rho \|u'\|^2, \\
  (4.4c) & \quad \overline{S'} = -\rho \left( u' \otimes u' - \frac{1}{3} \|u'\|^2 I \right), \\
  (4.4d) & \quad \overline{q'} = -\left( \overline{S'u'} + \frac{5}{2} \overline{p'u'} + \frac{1}{2} \rho \|u'\|^2 u' \right).
\end{align*}
\]

Obviously, computing \( \overline{p'} \), \( \overline{S'} \) and \( \overline{q'} \) in addition to the coarse-grained variables in (3.5) allows to connect back to the Reynolds averages of the original variables. Here we are going to start with \( \overline{p'} \), which requires its own separate equation.

To derive the transport equation for the Reynolds-averaged turbulent pressure \( \overline{p'} \), we subtract the coarse-grained pressure equation (3.6c) from the fine-grained pressure equation (2.7c) and obtain

\[
\begin{align*}
  (4.5) & \quad \frac{\partial \overline{p'}}{\partial t} + \text{div} \left( \overline{p'u'} + \rho' \text{div} u' \right) + \frac{2}{3} \left( \rho' \text{div} u' + \text{div} u^* + \text{div} u' \right) + \\
  & \quad + \frac{2}{3} \left( S : (\nabla \otimes u) - S^* : (\nabla \otimes u^*) \right) + \frac{2}{3} \text{div} \overline{q'} = 0.
\end{align*}
\]

Applying the Reynolds average to the equation above results in

\[
(4.6) \quad \frac{\partial \overline{p'}}{\partial t} + \text{div} \left( \overline{p'u'} \right) + \frac{2}{3} \overline{p' \text{div} u^*} + \text{div} \left( \overline{p'u'} \right) + \frac{2}{3} \overline{p' \text{div} u'} + \\
  + \frac{2}{3} \left( S : (\nabla \otimes u) - S^* : (\nabla \otimes u^*) \right) + \frac{2}{3} \text{div} \overline{q'} = 0.
\]

We now observe that

\[
\begin{align*}
  (4.7a) & \quad p' \text{div} u' = \frac{p'}{\rho} \text{div} u' = \frac{p'}{\rho} \left( \text{div}(\rho u') - u' \cdot \nabla \rho \right) = -p' u' \cdot \frac{\nabla \rho}{\rho}, \\
  (4.7b) & \quad S : (\nabla \otimes u) - S^* : (\nabla \otimes u^*) = \overline{S'} : (\nabla \otimes u^*) + \overline{S'} : (\nabla \otimes u'),
\end{align*}
\]
which further results in

\[
\frac{\partial \overline{p'}}{\partial t} + \text{div} \left( \overline{p' u^*} \right) + \frac{2}{3} \overline{p'} \text{div} u^* + \text{div} \left( \overline{p' u'} \right) - \frac{2}{3} \frac{\nabla \rho}{\rho} \cdot \overline{p' u'} + \\
\quad + \frac{2}{3} \left( \overline{S'} : (\nabla \otimes u^*) + \overline{S'} : (\nabla \otimes u') + \text{div} q' \right) = 0.
\]

The turbulent pressure \( \overline{p'} \) is not a convenient measure of turbulence from a physicist’s perspective, since, according to (4.4b), it cannot be positive. Thus, it is more convenient to replace it with a nonnegative quantity, and here we choose the kinetic energy of turbulent velocity fluctuations \([25, 26]\) for this purpose:

\[
E_t = -\frac{3}{2} \overline{p'} = \frac{1}{2} \rho \| u' \|^2.
\]

For the turbulent energy in (4.9), the transport equation becomes

\[
\frac{\partial E_t}{\partial t} + \text{div} \left( E_t u^* \right) + \frac{2}{3} E_t \text{div} u^* - \frac{3}{2} \text{div} \left( \overline{p' u'} \right) + \frac{\nabla \rho}{\rho} \cdot \overline{p' u'} - \\
\quad - \overline{S'} : (\nabla \otimes u^*) - \overline{S'} : (\nabla \otimes u') - \text{div} q' = 0.
\]

The term \( \overline{S'} : (\nabla \otimes u') \) in the equation above can be rearranged as follows. We assume that the microscale viscosity \( \mu \) can be factored out of the Reynolds average (that is, replacing \( \mu \) with its own Reynolds average is an acceptable simplification). Then, one writes

\[
\overline{S'} : (\nabla \otimes u') = \overline{S} : (\nabla \otimes u') = -2\mu \left[ \nabla \otimes u' \right]_{TS} : (\nabla \otimes u') = \\
\quad = -2\mu \left[ \nabla \otimes u' \right]_{TS} : (\nabla \otimes u') = \frac{2}{3} \mu (\text{div} u')^2 - \mu (\nabla \otimes u') : (\nabla \otimes u')^T - \mu \| \nabla \otimes u' \|^2,
\]

where we replaced the fine-grained stress \( S \) with its Navier-Stokes approximation \([2.27a]\). For the first term in the right-hand side of (4.11) we use the anelastic turbulence approximation (4.1) and obtain

\[
(\text{div} u')^2 = \frac{1}{\rho^2} (\text{div} u')^2 = \frac{1}{\rho^2} (\rho \text{div} u' - \nabla \rho \cdot u')^2 = \frac{1}{\rho^2} (\nabla \rho \otimes \nabla \rho) : (u' \otimes u') = \\
\quad = -\left( \overline{S'} + \overline{p'I} \right) : \frac{1}{\rho^2} (\nabla \rho \otimes \nabla \rho) = \frac{2}{3} \frac{\| \nabla \rho \|^2}{\rho^3} - E_t - \frac{1}{\rho^3} (\nabla \rho \otimes \nabla \rho) : \overline{S'},
\]
where we used (4.4c) and (4.9) in the last equality. For the second term in the right-hand side of (4.11) we obtain

\[ (4.13) \quad (\nabla \otimes \mathbf{u}^e)^T = (\nabla \otimes \nabla) : (\mathbf{u}^e \otimes \mathbf{u}^e) + 2 \text{div} \left( \frac{\mathbf{u}^e \otimes \mathbf{u}^e}{\rho} \right) + \]

\[ + \frac{1}{\rho^2} (\nabla \rho \otimes \nabla \rho) : (\mathbf{u}^e \otimes \mathbf{u}^e) = (\nabla \otimes \nabla) : \left( \frac{2}{3 \rho} \mathbf{E}_t - \frac{1}{3} \mathbf{S} \right) + 2 \text{div} \left( \frac{2}{3 \rho} \mathbf{E}_t \nabla \rho - \frac{1}{3} \mathbf{S} \nabla \rho \right) + \]

\[ + \frac{1}{\rho^2} (\nabla \rho \otimes \nabla \rho) : \left( \frac{2}{3 \rho} \mathbf{E}_t - \frac{1}{3} \mathbf{S} \right) = \frac{2}{3} \Delta \left( \frac{\mathbf{E}_t}{\rho} \right) + \frac{4}{3} \text{div} \left( \frac{\mathbf{E}_t \nabla \rho}{\rho^2} \right) + \frac{2}{3} \frac{\| \nabla \rho \|^2}{\rho^2} \mathbf{E}_t - \]

\[ - (\nabla \otimes \nabla) : \left( \frac{\mathbf{S}}{\rho} \right) - 2 \text{div} \left( \frac{\mathbf{S} \nabla \rho}{\rho^2} \right) - \frac{1}{\rho} (\nabla \otimes \nabla) : \mathbf{S} - \frac{1}{\rho^2} ((\nabla \otimes \nabla) \rho) : \mathbf{S} + \frac{2}{3} \frac{\Delta \mathbf{E}_t}{\rho} - \]

\[ - \frac{2}{3} \frac{\| \nabla \rho \|^2}{\rho^3} \mathbf{E}_t - \frac{1}{\rho} (\nabla \otimes \nabla) : \mathbf{S} - \frac{1}{\rho^3} ((\nabla \otimes \nabla) \rho) : \mathbf{S} + \frac{1}{\rho^3} (\nabla \rho \otimes \nabla \rho) : \mathbf{S}. \]

Now, we denote the last term in the right-hand side of (4.11) as the turbulent energy dissipation rate \[25, 26, 38],

\[ (4.14) \quad \rho \varepsilon_t = \mu \| \nabla \otimes \mathbf{u}^e \|^2, \]

as it cannot be expressed in terms of the Reynolds averages of the turbulent fluctuations that we already defined. This leads to

\[ (4.15) \quad \mathbf{S} : (\nabla \otimes \mathbf{u}^e) = - \frac{2}{3} \frac{\Delta \mathbf{E}_t}{\rho} + \frac{2}{3} \frac{\mu}{\rho} \left( \frac{5}{3} \frac{\| \nabla \rho \|^2}{\rho^2} - \frac{\Delta \rho}{\rho} \right) \mathbf{E}_t + \]

\[ + \frac{\mu}{\rho} ((\nabla \otimes \nabla) : \mathbf{S} + \frac{\mu}{\rho^2} ((\nabla \otimes \nabla) \rho) : \mathbf{S} - \frac{5}{3} \frac{\mu}{\rho^3} (\nabla \rho \otimes \nabla \rho) : \mathbf{S} - \rho \varepsilon_t, \]

and, consequently,

\[ (4.16) \quad \frac{\partial \mathbf{E}_t}{\partial t} + \text{div} (\mathbf{E}_t \mathbf{u}^e) + \frac{2}{3} \left( \text{div} \mathbf{u}^e + \frac{\mu}{\rho} \Delta + \frac{\mu}{\rho^2} - \frac{5}{3} \frac{\mu}{\rho^3} \| \nabla \rho \|^2 \right) \mathbf{E}_t - \]

\[ - \left( \nabla \otimes \mathbf{u}^e + \frac{\mu}{\rho} (\nabla \otimes \nabla) + \frac{\mu}{\rho^2} ((\nabla \otimes \nabla) \rho) - \frac{5}{3} \frac{\mu}{\rho^3} (\nabla \rho \otimes \nabla \rho) \right) : \mathbf{S} - \]

\[ - \text{div} \mathbf{q} - \frac{3}{2} \text{div} (p' \mathbf{u}^e) + \frac{\nabla \rho}{\rho} : p' \mathbf{u}^e + \rho \varepsilon_t = 0. \]

Observe that the equation for the turbulent energy above depends on the Reynolds-averaged turbulent stress \[\mathbf{S}'\), heat flux \[\mathbf{q}'\], the quantity \[p' \mathbf{u}^e\], as well as the turbulent energy dissipation rate \[\rho \varepsilon_t\].

### 4.1. Isotropic turbulence assumption and its limitations

As a special case of the turbulent flow, here we consider a hypothetical situation where the turbulent velocity fluctuations \[\mathbf{u}'\] at each spatial point are statistically decorrelated and isotropic. This implies
the following conditions for statistical averages of turbulent quantities:

\[(4.17) \quad \overline{u' \otimes u'} = \frac{1}{3} \|u'\|^2 I, \quad \overline{S'} = 0, \quad \overline{p'u'} = \overline{q'} = 0.\]

The first equality above is due to the fact that the cross-correlations between different components of the turbulent velocity are zeros, while self-correlations are equal. The second equality follows immediately from the first one by using (4.4c). The third equality is due to the fact that, because of isotropy, for each instance of \(u', p'\) and \(q'\), there must be another with \(-u', p'\) and \(-q'\), and with the same statistical weight. This is, of course, an idealized assumption, which is unlikely to hold exactly in practical situations. In fact, it is somewhat of a turbulent analog of the Maxwellian equilibrium condition in (2.12) for the fluid particle velocities, assumed without rigorous justification.

Under the isotropic assumption in (4.17), the equation for the turbulent energy transport in (4.16) becomes

\[(4.18) \quad \frac{\partial E_t}{\partial t} + \text{div}(E_t u^*) + \frac{2}{3} \left( \text{div} u^* + \frac{\mu}{\rho} \Delta + \frac{\mu}{\rho^2} \frac{\|\nabla \rho\|^2}{\rho} - \frac{5}{3} \frac{\mu}{\rho^3} \right) E_t + \rho \varepsilon_t = 0.\]

There are two problems with this equation. First, the diffusion term above is clearly ill-posed, which means that the turbulent energy will be amplified by this term at small scales, rather than damped. The second problem with the equation above is that it has no means of producing turbulent energy from zero initial condition. At the same time, it is very well known that the turbulence appears even if there was none to begin with, from the interactions of the large-scale motions with the small-scale viscous dissipation. Thus, the only way to create such interaction is to couple the higher-order Reynolds averages in (4.16) to the coarse-grained variables, rather than assuming isotropy. In a broad sense, the turbulence is produced by the anisotropy of the large-scale flow.

4.2. Coupling the turbulent Reynolds averages to the coarse-grained variables. Here we assume that on the fine-grained scale the fluid satisfies the Navier-Stokes approximations in (2.27). We also assume that replacing the viscosity \(\mu\) and heat conductivity \(\kappa\) in (2.27) with their corresponding Reynolds averages is an acceptable approximation. Then, the Reynolds averages of the turbulent fluctuations \(\overline{S'}\) and \(\overline{q'}\) can be expressed via the coarse-grained stress \(\overline{S^*}\) and heat flux \(\overline{q^*}\), and the Reynolds-averaged Navier-Stokes approximations for the fine-grained stress and heat flux as follows:

\[(4.19a) \quad \overline{S'} = \overline{S} - \overline{S^*} = -\overline{S^*} - 2\mu [\nabla \otimes u^*]_{TS'},\]

\[(4.19b) \quad \overline{q'} = \overline{q} - \overline{q^*} = -\overline{q^*} - \kappa \nabla \left( \frac{\overline{p'}}{\rho} \right) = -\overline{q^*} - \kappa \nabla \left( \frac{\overline{p^*}}{\rho} \right) + \frac{2}{3} \kappa \nabla \left( \frac{E_t}{\rho} \right).\]
Substituting the above expressions into the transport equation for the turbulent energy yields

\[\frac{\partial E_t}{\partial t} + \text{div}(E_t u^*) + \frac{2}{3} \left( \text{div}u^* + \frac{\mu}{\rho} \Delta + \mu \frac{\Delta \rho}{\rho^2} - \frac{5}{3} \mu \frac{\| \nabla \rho \|^2}{\rho^3} \right) E_t = \frac{2}{3} \text{div} \left( \kappa \nabla \left( \frac{E_t}{\rho} \right) \right) + \left( \nabla \otimes u^* + \frac{\mu}{\rho^2} (\nabla \otimes \nabla) + \frac{2 \mu}{\rho^2} (\nabla \otimes \nabla) \rho - \frac{5 \mu}{3 \rho^3} (\nabla \rho \otimes \nabla \rho) \right) : (S^* + 2 \mu [\nabla \otimes u^*]_{TS}) + \text{div} q^* + \text{div} \left( \kappa \nabla \left( \frac{p^*}{\rho} \right) \right) - \frac{3}{2} \text{div}(p^* u^*) + \frac{\rho}{\rho} \cdot p^* u^* + \rho_\varepsilon = 0.\]

The unknown term $p^* u^*$ is still present, and needs either its own separate transport equation (which will, of course, involve yet higher-order moment combinations of turbulent quantities), or a suitable closure. For simplicity, here we propose a closure under the assumption of Bernoulli’s principle. For that, first observe the following relation:

\[\frac{\partial}{\partial t} \overline{S' u'} = \overline{S u'} - 2 \mu \left[ \nabla \otimes u \right]_{TS} u' = -2 \mu \left[ \nabla \otimes u \right]_{TS} u' = -2 \mu \left[ \nabla \otimes u \right]_{TS} u' = -\mu \left( \nabla \otimes u' + (\nabla \otimes u')^T - \frac{2}{3} (\text{div} u') I \right) u',\]

where, as before, the Navier-Stokes approximation is used for the Reynolds average of the fine-grained stress $\overline{S}$. For the separate terms above we have, with the help of (4.1),

\[(4.22a) \quad \left( \nabla \otimes u' \right) u' = -\frac{3}{2} \nabla \left( \frac{\overline{p'}^*}{\rho} \right) = \nabla \left( \frac{E_t}{\rho} \right),\]

\[(4.22b) \quad (\nabla \otimes u')^T u' = \frac{1}{\rho} \text{div}(\rho u' \otimes u') = -\frac{1}{\rho} \text{div} S' + \frac{2}{3} \nabla \left( \frac{E_t}{\rho} \right) - \frac{2}{3} E_t \frac{\nabla \rho}{\rho^2},\]

\[(4.22c) \quad \text{div}(u' u') = -\left( u' \otimes u' \right) \frac{\nabla \rho}{\rho} = S' \frac{\nabla \rho}{\rho^2} - \frac{2}{3} E_t \frac{\nabla \rho}{\rho^2},\]

which, when assembled together, lead to the expression of $\overline{S' u'}$ in terms of the Reynolds average of the turbulent stress fluctuation $\overline{S'}$ and the turbulent kinetic energy $E_t$:

\[\frac{\partial}{\partial t} \overline{S' u'} = \left( \frac{\mu}{\rho} \text{div} + \frac{2 \mu}{3 \rho^2} \nabla \rho \right) \overline{S'} - \frac{5}{3} \mu \nabla \left( \frac{E_t}{\rho} \right) - \frac{10}{9} \frac{\mu E_t}{\rho^2} \frac{\nabla \rho}{\rho^2}.\]

Combining (4.23) with (4.4d) and (4.19), we obtain

\[(4.24) \quad q^* + \kappa \nabla \left( \frac{p^*}{\rho} \right) - \frac{2}{3} \kappa \nabla \left( \frac{E_t}{\rho} \right) = -\overline{q'} = -\left( \frac{\mu}{\rho} \text{div} + \frac{2 \mu}{3 \rho^2} \nabla \rho \right) \left( S^* + 2 \mu [\nabla \otimes u^*]_{TS} \right) - \frac{5}{3} \mu \nabla \left( \frac{E_t}{\rho} \right) - \frac{10 \mu}{9 \rho^2} E_t \nabla \rho + \frac{5}{2} \overline{p^* u'} + \frac{1}{2} \frac{\rho}{\rho} \|u'\|^2 u'.\]
or, after rearranging the terms,

\[
\frac{5}{2} p' u' + \frac{1}{2} \rho \| u' \|^2 u' = q^* + \kappa \nabla \left( \frac{p^*}{\rho} \right) + \frac{5\mu - 2\kappa}{3} \nabla \left( \frac{E_t}{\rho} \right) + \frac{10\mu}{9\rho^2} E_t \nabla \rho + \\
+ \left( \frac{\mu}{\rho} \text{div} + \frac{2\mu}{3\rho^2} \nabla \rho \right) \left( S^* + 2\mu [\nabla \otimes u^*]_{TS} \right).
\]

Observe that the Reynolds averages of turbulent fluctuations in the left-hand side above are expressed entirely in terms of the coarse-grained variables and the turbulent energy \(E_t\) in the the right-hand side. However, in order to close the turbulent energy transport equation in terms of the coarse-grained variables and the turbulent energy itself, one has to surmise a plausible relation between the Reynolds averages \(p' u'\) and \(\| u' \|^2 u'\). There is certainly more than one way to do that (as an example, one could postulate \(\| u' \|^2 u' = 0\), for a simplest closure), and we here choose what we perceive as the most physically realistic. Namely, we recall Bernoulli’s principle, which states that the change in the local flow velocity tends to affect the pressure in the flow in a manner as to preserve the total energy. If we treat the turbulent velocity fluctuation \(u'\) as the primary cause for the turbulent pressure fluctuation \(p'\) at the same location, Bernoulli’s principle then leads to the relation

\[
(4.26) \quad p' = -\frac{1}{3} \rho \| u' \|^2.
\]

Of course, we understand that in reality the relation in (4.26) cannot hold at each spatial point exactly, as Bernoulli’s principle is merely an approximation. However, we note that the exact relation (4.4b) is precisely the Reynolds-averaged relation (4.26). So, we surmise that it is plausible to incorporate an approximate relation in (4.26) into the relation between \(p' u'\) and \(\| u' \|^2 u'\) as follows:

\[
(4.27) \quad \bar{p}' u' = -\frac{1}{3} \rho \| u' \|^2 u', \quad \text{or} \quad \frac{5}{2} \bar{p}' u' + \frac{1}{2} \rho \| u' \|^2 u' = \bar{p}' u'.
\]

In particular, as a result of Bernoulli’s assumption, the Reynolds average of the turbulent heat flux becomes the Reynolds average of the product of the turbulent velocity with the turbulent pressure matrix, taken with the opposite sign:

\[
(4.28) \quad \bar{q}' = -\bar{P}' u', \quad \bar{P}' = p' I + S'.
\]

This results in the following expression for \(\bar{p}' u'\) in terms of the coarse-grained variables and the turbulent energy \(E_t\):

\[
(4.29) \quad \bar{p}' u' = q^* + \kappa \nabla \left( \frac{p^*}{\rho} \right) + \frac{5\mu - 2\kappa}{3} \nabla \left( \frac{E_t}{\rho} \right) + \frac{10\mu}{9\rho^2} E_t \nabla \rho + \\
+ \left( \frac{\mu}{\rho} \text{div} + \frac{2\mu}{3\rho^2} \nabla \rho \right) \left( S^* + 2\mu [\nabla \otimes u^*]_{TS} \right).
\]
Rearranging the terms, we further obtain

\begin{equation}
\frac{\partial E_t}{\partial t} + \text{div}(E_t \mathbf{u}^*) + \frac{2}{3} \left( \text{div}\mathbf{u}^* + \frac{\mu}{\rho} \Delta + \mu \frac{\Delta \rho}{\rho^2} - \frac{5}{3} \mu \frac{\|\nabla \rho\|^2}{\rho^3} \right) E_t - \frac{2}{3} \text{div} \left( \kappa \nabla \left( \frac{E_t}{\rho} \right) \right) + \\
+ \left( \nabla \frac{\rho}{\rho^2} - \frac{3}{2} \nabla \right) \cdot \left( \frac{5 \mu - 2 \kappa}{3} \nabla \left( \frac{E_t}{\rho} \right) + \frac{10 \mu}{9 \rho^2} E_t \nabla \rho \right) + \left( \nabla \frac{\rho}{\rho^2} - \frac{1}{2} \nabla \right) \cdot \left( q^* + \kappa \nabla \left( \frac{p^*}{\rho} \right) \right) + \\
+ \left( \nabla \otimes \mathbf{u}^* + \frac{\mu}{\rho} \nabla \otimes \nabla \mathbf{u} + \frac{\mu}{\rho^2} \left( (\nabla \otimes \nabla) \rho - \frac{5 \mu}{3 \rho^3} (\nabla \rho \otimes \nabla \rho) \right) \right) : \left( \mathbf{S}^* + 2 \mu [\nabla \otimes \mathbf{u}^*]_{TS} \right) + \\
+ \left( \frac{3}{2} \nabla - \frac{3}{2} \nabla \right) \cdot \left( \left( \frac{\mu}{\rho} \text{div} + \frac{2 \mu}{3 \rho^2} \nabla \rho \right) \left( \mathbf{S}^* + 2 \mu [\nabla \otimes \mathbf{u}^*]_{TS} \right) \right) + \rho \varepsilon_t = 0.
\end{equation}

Rearranging the terms, we further obtain

\begin{equation}
\frac{\partial E_t}{\partial t} + \text{div} \left( E_t \left( \mathbf{u}^* + \frac{15 \mu - 4 \kappa}{3 \rho^2} \nabla \rho + \frac{\nabla (2 \kappa - 15 \mu)}{6 \rho} \right) \right) + \frac{2}{3} E_t \left( \text{div}\mathbf{u}^* + \frac{15 \mu - 2 \kappa}{2} \frac{\|\nabla \rho\|^2}{\rho^3} + \\
+ \frac{1}{\rho^2} \nabla (\kappa - 5 \mu) \cdot \nabla \rho + \text{div} \left( \frac{\nabla (2 \kappa - 15 \mu)}{4 \rho} \right) + \frac{2 \kappa - 11 \mu}{6 \rho} \Delta E_t = F_t^* - \rho \varepsilon_t,
\end{equation}

where $F_t^*$ is the coarse-grained forcing:

\begin{equation}
F_t^* = \left( \frac{1}{2} \nabla - \frac{3 \nabla}{2} \right) \cdot \left( q^* + \kappa \nabla \left( \frac{p^*}{\rho} \right) \right) - \\
\left( \nabla \otimes \mathbf{u}^* + \frac{\mu}{\rho} \nabla \otimes \nabla \mathbf{u} + \frac{\mu}{\rho^2} \left( (\nabla \otimes \nabla) \rho - \frac{5 \mu}{3 \rho^3} (\nabla \rho \otimes \nabla \rho) \right) \right) : \left( \mathbf{S}^* + 2 \mu [\nabla \otimes \mathbf{u}^*]_{TS} \right) + \\
+ \left( \frac{3}{2} \nabla - \frac{3}{2} \nabla \right) \cdot \left( \left( \frac{\mu}{\rho} \text{div} + \frac{2 \mu}{3 \rho^2} \nabla \rho \right) \left( \mathbf{S}^* + 2 \mu [\nabla \otimes \mathbf{u}^*]_{TS} \right) \right).
\end{equation}

Here observe the following properties:

- For the Prandtl number of the ideal gas, $Pr = 2/3$, and the assumption that the spatial derivatives of $\mu$ and $\kappa$ can be neglected, the advection term in (4.31) is exactly the same as it is for the usual pressure variable.
- The Laplace diffusion term in (4.31) is well posed as long as $Pr > 5/11$, which includes the ideal gas.
- The term with $\|\nabla \rho\|^2$ in (4.31) is linear damping as long as $Pr > 1/3$, which again includes ideal gas.

For a strong turbulence (that is, large coarse-grained stress $S^*$ and heat flux $q^*$) and small microscale viscosity $\mu$ and heat conductivity $\kappa$, one likely can drop the terms scaled by $\rho \varepsilon_t$, the latter in (4.31) and (4.32), except the one for the diffusion, as it could potentially be the highest-order differential operator, given the lack of information on $\rho \varepsilon_t$.
simplified equation is given by
\[
\frac{\partial E_t}{\partial t} + \text{div}(E_t u^*) + \frac{2}{3} E_t \text{div} u^* + \frac{2\kappa - 11\mu}{6\rho} \Delta E_t = \left( \frac{1}{2} \nabla - \frac{\nabla \rho}{\rho} \right) \cdot q^* - S^* : (\nabla \otimes u^*) - \rho\varepsilon_t. \]

Observe that this simplified transport equation for the turbulent energy is the same as the one for the Euler approximation of the pressure equation, but with the additional forcing via the coarse-grained variables \( S^* \) and \( q^* \), small scale dissipation \( \rho\varepsilon_t \), and a weak diffusion.

At this point, it becomes clear how the turbulence is produced from an initial condition which belongs to the fully resolved coarse-grained scale, with zero stress and heat flux. Schematically, this process can be illustrated as

\[
\begin{align*}
2p^* \left[ \nabla \otimes u^* \right]_{TS} & \rightarrow S^* \\
\frac{5}{2} p^* \nabla \left( \frac{p^*}{\rho} \right) & \rightarrow q^* \\
\rightarrow E_t,
\end{align*}
\]

where there are two stages:

1. As the stress and heat flux are zero initially, the coarse-grained strain rate term \( 2p^* \left[ \nabla \otimes u^* \right]_{TS} \) and the coarse-grained temperature gradient term \( \frac{5}{2} p^* \nabla \left( \frac{p^*}{\rho} \right) \) act as external forcing in the equations for the coarse-grained stress (3.6d) and heat flux (3.6e), respectively, causing deviation from the Maxwellian equilibrium on the coarse-grained scale.

2. In turn, the nonzero coarse-grained stress \( S^* \) and heat flux act \( q^* \) act as external forcing in the turbulent energy equation (4.31), causing the nonzero turbulent energy to appear.

In particular, this means that the coarse-grained collision terms \( C^*_S \) and \( c^*_q \) provide weaker damping rate than their fine-grained counterparts even when there is no turbulence developed yet.

5. Collision terms and moment closures for the coarse-grained transport equations

Thus far, we developed the following ingredients of the coarse-grained transport framework for a turbulent flow:

- A hierarchy of the new coarse-grained variables in (3.5) and the corresponding hierarchy of the transport equations in (3.6). Although the expressions for the coarse-grained variables in (3.5) and the corresponding equations (3.6) only include the moments up to the heat flux, clearly the full set of moments is infinite, and requires either infinitely many transport equations, or an approximate closure. The derivation was done under the general assumption that, microscopically, the flow is described by the Boltzmann equation for a monatomic ideal gas (2.1).

- The relations for the corresponding Reynolds-averaged turbulent fluctuations. Those are given in the form of the turbulent energy (or, equivalently, turbulent...
pressure) transport equation in (4.31), and the relations for the turbulent stress and heat flux in (4.19). This was done under the following assumptions:

1. Validity of the Navier-Stokes approximations for the fine-grained stress and heat flux (2.27);
2. Invariance of the density $\rho$ under the Reynolds averaging and the resulting anelastic turbulence approximation (4.1);
3. Approximation of the microscale viscosity $\mu$ and heat conductivity $\kappa$ by their own Reynolds averages;
4. Bernoulli’s principle for the turbulent velocity fluctuations in (4.27).

In order to make the resulting system of equations suitable for practical computations and modeling, two further parameterizations need to be developed:

1. A closure of the hierarchy of the coarse-grained equations in (3.6). Namely, we need to relate the coarse-grained skewness moment $Q^*$ and the contracted fourth-order moment $R^*$ to the coarse-grained density, pressure, stress and heat flux.
2. Suitable parameterizations of the coarse-grained collision operators $C^*_S$ and $c^*_q$, and the turbulent energy dissipation rate $\rho \varepsilon_t$.

Below we elaborate on the first subject to the extent it allows to avoid the second subject. The reason for this is that the collision operators and the turbulent energy dissipation rate are the Reynolds averages of nonlinear (with respect to the transported variables) quantities, and thus should likely be modeled depending on a particular application, with more detailed assumptions on the flow properties put into place. Nonetheless, in Section 6 we suggest some crude parameterizations for $C^*_S$, $c^*_q$ and $\rho \varepsilon_t$.

5.1. Grad closure for the coarse-grained transport equations. Generally, there is little that can be concluded about the local entropy state $S_l[f]$ of $f$. As Girimaji pointed out in [12], the problem here is that $f$ is the statistical ensemble average of many realizations of $f$, where each realization of $f$ generally has its own density $\rho$, velocity $u$, and pressure $p$ at a given spatial point $x$. Therefore, even if we assume that each $f$ in the statistical ensemble is the corresponding Maxwellian state (2.12) with its own $\rho$, $u$ and $p$, the averaged sum of these states does not have to be near a Maxwellian state. However, if $f$ is far from a Maxwellian, then both the Euler and the Navier-Stokes approximations for the moments of such distribution become rather questionable.

In contrast to the local entropy state, it turns out that the global entropy state of the Reynolds-averaged Boltzmann equation behaves similarly to the Reynolds average of the global entropy. In order to better argue our point here, we first note that the Reynolds operator satisfies Jensen’s inequality.

**Proposition 3** (Jensen’s inequality). The Reynolds operator satisfies Jensen’s inequality: for a convex function $\phi$ and a function of the statistical ensemble $h$,

\[
\phi(h) \geq \phi(\bar{h}).
\]

**Proof.** Follows from the fact that the Reynolds operator is a statistical average. \qed

This results in the following estimate for the entropy of the Reynolds-averaged solution of the Boltzmann equation (2.1):

\[
S_l[\bar{f}] \leq S_l[f].
\]
**Proposition 4** (Entropy of the Reynolds-averaged Boltzmann equation). Let \( \bar{f} \) be the
Reynolds-averaged distribution \( f \) of the Boltzmann equation in (2.1), which apparently satisfies
\[
\frac{\partial \bar{f}}{\partial t} + v \cdot \nabla_x \bar{f} = C(f).
\]
Then, both the local and global entropies of \( \bar{f} \) are bounded from below by the Reynolds averages of
the local and global entropies of \( f \), respectively:
\[
S_l[\bar{f}] \geq S_l[f], \quad S_g[\bar{f}] \geq S_g[f].
\]
Proof. Observe that \( \phi(f) = f \ln f \) is convex. Therefore, Jensen’s inequality yields
\[
S_l[\bar{f}](t,x) = -\int f \ln f \, dv \geq -\int \bar{f} \ln \bar{f} \, dv = S_l[f](t,x).
\]
The corresponding inequality for the global entropy is obtained by integrating in \( x \). \( \square \)

The above result is not of much use for estimating the local behavior of \( \bar{f} \) at a spatial
point \( x \); indeed, while the lower bound estimate is valid, the upper bound for \( S_l[\bar{f}] \) can
be different from the upper bound for \( S_l[f] \), due to the fact that the local density, mo-
mentum and pressure are not preserved between the members of the statistical ensemble
(if they were, there would likely be little need for the Reynolds averaging to begin with).
However, it is quite reasonable to assume that the members of the statistical ensemble
share the total mass, momentum and energy constraints, because they have to be dif-
ferent realizations of the same large-scale flow scenario, rather than being completely
unrelated. Therefore, the statistical ensemble members also share the maximum global
entropy state \( \rho^g_M \) under these constraints, which means that the maximum global entropy
state is invariant under the Reynolds averaging. As a result, one can show the following
inequality for the global relative entropy,
\[
H_g[\bar{f}] = -S_g[\bar{f}] - \int \bar{f} \ln \rho^g_M \, dv \, dx \leq -S_g[f] - \int \bar{f} \ln \rho^g_M \, dv \, dx = H_g[f].
\]
The latter means that the global relative entropy of the Reynolds-averaged distribution
\( \bar{f} \) decays at the same rate as the Reynolds average of the ensemble global entropy states
(that is, \( O(t^{-\infty}) \), as shown by Desvillettes and Villani [10]).

This situation is similar to what usually happens in the dynamics of rarefied gases
[8,14,15,21,22] where there is little time scale separation between the growth rates of the
local and global entropies, and thus the higher-order moments do not rapidly converge
to their local equilibrium values, while still maintaining global convergence on a slower
time scale. Thus, the Grad closure [14,15] appears to be a suitable option for closing
the transport equations in (3.6) for the coarse-grained variables in (3.5). Applying the
Grad closure to the coarse-grained moment transport equations in (3.6) is identical to
that of the usual moment transport equations in (2.7), as the Grad closure imposes no
restrictions on the structure of the collision terms, whether Reynolds-averaged or not.
The resulting system of equations for the coarse-grained variables is the same as the one
in (2.32), except that the collision terms are different:

\[
(5.6a) \quad \frac{\partial \rho^*}{\partial t} + \text{div}(\rho^* u^*) = 0,
\]

\[
(5.6b) \quad \frac{\partial (\rho^* u^*)}{\partial t} + \text{div}(\rho^* u^* \otimes u^* + p^* I + S^*) = 0,
\]

\[
(5.6c) \quad \frac{\partial p^*}{\partial t} + \text{div}(p^* u^*) + \frac{2}{3} [p^* \text{div} u^* + S^* : (\nabla \otimes u^*) + \text{div} q^*] = 0,
\]

\[
(5.6d) \quad \frac{\partial S^*}{\partial t} + (u^* \cdot \nabla) S^* + \text{div}(u^*) S^* + 2 [S^* (\nabla \otimes u^*)]_{TS} + \frac{4}{5} [\nabla \otimes q^*]_{TS} + 2 p^* [\nabla \otimes u^*]_{TS} = C^*_S,
\]

\[
(5.6e) \quad \frac{\partial q^*}{\partial t} + \frac{7}{5} (\text{div}(q^* \otimes u^*) + (q^* \cdot \nabla u^*) + \frac{2}{5} ((\nabla \otimes u^*) q^* - (u^* \cdot \nabla) q^*) - \frac{1}{\rho^*} \left(\frac{5}{2} p^* I + S^*\right) \text{div}(p^* I + S^*) + \text{div} \left(\frac{5 p^*}{2 \rho^*} I + \frac{7 p^*}{2 \rho^*} S^*\right) = c^*_q.
\]

The following arguments can be made in favor of the Grad closure in (5.6):

- The ability to set the prescribed stress and heat flux. It cannot be assumed that the coarse-grained stress $S^*$ and heat flux $q^*$ are zero (or nearly zero), as there is not enough information about rapid Reynolds-averaged local entropy growth (or, equivalently, decay of $H_l[f]$) to substantiate that. Thus, a suitable moment closure must account for that. At the same time, the moments of such closure must be explicitly computable in terms of elementary functions, for the transport equations to have an explicit form. Also, one must remember that, due to Proposition 4, the Reynolds average $\bar{f}$ has a global tendency to dissipate towards a normal distribution on a long time scale, and thus the closure should not be “too far away” from this state. The Grad closure meets all of these conditions: it is built around (2.12), its moments are explicitly computable, and it also possesses the prescribed stress and heat flux, in addition to prescribed density, velocity and pressure.

- Few restrictions for the parameterization of the coarse-grained collision terms. As the coarse-grained collision terms $C^*_S$ and $c^*_q$ are nonlinear and require separate (quite possibly empirical or semi-empirical) treatment, any need in prior assumptions on the structure of the collision terms (as in the Navier-Stokes approximation, for example) is undesirable. In the Grad closure, there are no \textit{a priori} assumptions on the form of collision terms, as they enter the equations as unspecified parameters.

- Backward consistency with a weak/vanishing turbulence scenario. If the turbulence is weak or vanishing, then the coarse-grained variables in (3.5) become the corresponding fine-grained variables in (2.5). Then, the Grad equations for the coarse-grained variables naturally transition into the ordinary Grad equations in (2.32), with appropriate collision terms.
Generalization of Millionschikov’s hypothesis. In 1941, Millionschikov \[23,24\] asserted that the relations between the second and fourth turbulent statistical moments are related in approximately the same way as the corresponding moments of the normal distribution. Later in 1948, Heisenberg \[16\] independently proposed the same hypothesis. Since then, some evidence was accumulated in favor of this hypothesis (see \[25,26\] and references therein). The Grad distribution generalizes Millionschikov’s hypothesis, providing the explicit dependence of higher-order turbulent moments on the stress and heat flux in addition to the density, velocity and pressure.

However, there are also the following drawbacks:

- Increased computational complexity. Observe that the usual Navier-Stokes equations incorporate only five prognostic variables: the density, three velocity components, and pressure. For the Grad closure, the number of prognostic variables increases to 13 (plus one more for the turbulent energy \(E_t\)).
- Somewhat questionable numerical stability. There are at least two types of possible numerical instabilities which can manifest in the Grad equations. The first one arises when the contribution of the collision terms for the stress and heat flux is very large, so that these variables are strongly damped, and thus the numerical stiffness (that is, oscillation of the numerical time-discretization polynomial) arises for high-accuracy integration schemes unless the time step is very small, or a specially tailored scheme, such as an implicit BDF, is used. The second numerical instability will arise if the collision terms \(C^*_S\) and \(c^*_q\) do not include diffusion, in which case the numerical solution will develop shock waves \[14\] which will transfer the energy to high Fourier wavenumbers and cause the Gibbs oscillations. Below in Section \(6\) we suggest an option to mitigate this problem.

5.2. Coarse-grained viscosity and heat conductivity approximations. Observe that as the turbulence vanishes, the coarse-grained variables in \(3.5\) naturally become the fine-grained variables in \(2.5\), while the coarse-grained transport equations in \(3.6\) become the fine-grained transport equations in \(2.7\). The latter suggests that, under the conditions of sufficiently weak turbulence, the coarse-grained collision terms \(C^*_S\) and \(c^*_q\) can be represented as linear damping via the coarse-grained viscosity \(\mu^*\) and heat conductivity \(\kappa^*\) as follows:

\[
(5.7a) \quad C^*_S \approx -\frac{p^*}{\mu^*} S^*,
\]

\[
(5.7b) \quad c^*_q \approx -\frac{5}{2} \frac{p^*}{\kappa^*} q^*,
\]

where \(\mu^*\) and \(\kappa^*\), of course, remain unspecified quantities and must be somehow parameterized, possibly semi-empirically. However, this situation is much simpler than what it was before from the modeling perspective, as now two scalar quantities need to be estimated, rather than two general collision operators. Below in Section \(6\) we suggest a crude approximation for both \(\mu^*\) and \(\kappa^*\), which could serve as a starting point in practical modeling, at least until the properties of \(C^*_S\) and \(c^*_q\) become better studied.
The main drawback of the linear damping parameterization is the following. In practice, the microscale viscosity and heat conductivity are very small, while the turbulent fluctuations are large. In a typical turbulent flow situation, $S' \gg S$ and $q' \gg q$, such that the coarse-grained stress $S^*$ and heat flux $q^*$ consist largely of the Reynolds-averaged turbulent fluctuations,

$$S^* \approx -S', \quad q^* \approx -q'.$$

In this setting, there is simply not enough information to determine whether $p*S$ and $p*q$ (which are very small quantities) are collinear, respectively, to $p^*S^*$ and $p^*q^*$ (which are large quantities), as the latter are determined largely by the statistical physics of the turbulent flow, rather than microscale collisions. However, this collinearity is a necessary condition to justify scalar quantities $\mu^*$ and $\kappa^*$.

5.3. Coarse-grained Navier-Stokes equations. If, in addition to (5.7), the coarse-grained viscosity $\mu^*$ and heat conductivity $\kappa^*$ are sufficiently small, it enables the Navier-Stokes approximation of the form (2.25)–(2.27), that is,

$$S^* = -2\mu^* \left[ \nabla \otimes u^* \right]_{TS},$$

$$q^* = -\kappa^* \nabla \left( \frac{p^*}{\rho} \right),$$

so that the coarse-grained Grad equations in (5.6) simplify to the coarse-grained Navier-Stokes equations:

$$\frac{\partial \rho^*}{\partial t} + \text{div} (\rho^* u^*) = 0,$$

$$\frac{\partial (\rho^* u^*)}{\partial t} + \text{div} (\rho^* u^* \otimes u^*) + \nabla p^* = 2 \text{div} \left( \mu^* \left[ \nabla \otimes u^* \right]_{TS} \right),$$

$$\frac{\partial p^*}{\partial t} + \text{div} (p^* u^*) + \frac{2}{3} p^* \text{div} u^* = \frac{4}{3} \mu^* \left\| \left[ \nabla \otimes u^* \right]_{TS} \right\|^2 + \frac{2}{3} \text{div} (\kappa^* \nabla (p^*/\rho^*)), $$

where, as in (2.28), one could consider dropping the term with $\mu^*$ in the coarse-grained pressure equation, since it acts as unbalanced forcing which tends to increase $p^*$. In this situation, the coarse-grained forcing $F^*_t$ in the turbulent energy transport equation (4.31) becomes

$$F^*_t = \left( \frac{1}{2} \nabla - \frac{\nabla \rho}{\rho} \right) \cdot \left( (\kappa - \kappa^*) \nabla \left( \frac{p^*}{\rho} \right) \right) -$$

$$- 2(\mu - \mu^*) \left( \nabla \otimes u^* + \frac{\mu}{\rho^2} \left( \nabla \otimes \nabla \right) \rho + \frac{\mu}{\rho^2} (\nabla \otimes \nabla) \rho - \frac{5\mu}{3\rho^3} \left( \nabla \rho \otimes \nabla \rho \right) \right) : \left[ \nabla \otimes u^* \right]_{TS} +$$

$$+ \left( 3\nabla - 2\frac{\nabla \rho}{\rho} \right) \cdot \left( \frac{\mu}{\rho} \text{div} + \frac{2\mu}{3\rho^2} \nabla \rho \right) \left( (\mu - \mu^*) \left[ \nabla \otimes u^* \right]_{TS} \right) .$$

Assuming that the coarse-grained viscosity $\mu^*$ and heat conductivity $\kappa^*$ are large enough in comparison to the microscale viscosity $\mu$ and heat conductivity $\kappa$ (but at the same time
still small enough to enable the Navier-Stokes approximations in (5.9), one can simplify the above expression as

\[
F_t^* = -\left( \frac{1}{2} \nabla - \frac{\nabla \rho}{\rho} \right) \cdot \left( \kappa^* \nabla \left( \frac{p^*}{\rho} \right) \right) + 2\mu^* \left\| \nabla \otimes \mathbf{u}^* \right\|_{TS}^2.
\]

The main advantage of the coarse-grained Navier-Stokes equations in (5.10) is that they are technically not very different from the usual Navier-Stokes equations, for which many computational methods have already been developed. Here, we have the additional transport equation for the turbulent energy transport in (4.31), but, again, it is not much different from the usual pressure transport equation, except that it has the additional forcing, dissipation, and diffusion.

The main drawback of the coarse-grained Navier-Stokes approximation is, however, the following. Even if linear damping (5.7) applies for a given type of turbulence (which does not restrict the use of the coarse-grained Grad equations in (5.6)), the necessary condition for the coarse-grained Navier-Stokes approximation in (5.10) to be viable is that the evolution time scale of the coarse-grained stress and heat flux must be much faster than that for the density, velocity and pressure. This condition requires that both the coarse-grained viscosity and heat conductivity must be very small (which is usually the case for the conventional microscale \( \mu \) and \( \kappa \)). However, often in the models with the turbulent viscosity approximation these parameters can be several orders of magnitude larger than the microscale viscosity. In this situation, the time-scale separation is unlikely to exist, and thus the turbulent Navier-Stokes approximation may not apply.

5.4. Coarse-grained Burnett and super-Burnett equations. A key advantage of the new coarse-grained variables in (3.5) is that they obey the well-studied hierarchy of the moment equations in (3.6). Because of this, one has an opportunity to use existing closure methods for these equations. Above we showed how to derive the coarse-grained Grad (5.6) and Navier-Stokes (5.10) closures for this hierarchy, but one does not have to stop there. Using the ratio \( \mu^*/p^* \) (or, equivalently, \( \kappa^*/p^* \)) as a small parameter akin to the usual Knudsen number in the molecular kinetics, one can carry out the standard Chapman-Enskog perturbation expansion into the higher orders, obtaining the coarse-grained Burnett [9] and super-Burnett [32] equations in the same way they are derived for the conventional transport equations. While these equations are generally ill-posed, some relaxation-type regularizations were developed for them [17]. Here we do not elaborate on this further, as the derivation itself is straightforward, while a more detailed study of the resulting coarse-grained Burnett or super-Burnett equations is an entirely separate topic. With the higher-order Chapman-Enskog expansion, the expressions for \( S^* \) and \( q^* \) in (5.9) will contain additional terms, scaled by powers of \( \mu^*/p^* \) and \( \kappa^*/p^* \), which will accordingly affect the expression for \( F_t^* \) in (5.11). The transport and dissipation parts of the equation for \( E_t \) in (4.31) will remain the same.

6. Practical considerations for a computational implementation

In this section we discuss possible issues arising in the course of numerical implementation and modeling of the transport equations, developed above.
6.1. **Inclusion of the coarse-grained spatial scale information.** A key subject which was thus far left out of the picture is the spatial scale information about the coarse-grained and turbulent scales. While this scale information can be avoided in the formal coarse-grained transport formulation presented above (simply due to the fact that the Boltzmann equation is linear except for its collision operator), it naturally resurfaces when one has to discretize the transport equations for a numerical simulation. For example, if the discretization scale is so fine that it resolves the viscous molecular dissipation, then, clearly, the turbulent energy $E_t$ must be (nearly) zero, as should be the coarse-grained stress $S^*$ and heat flux $q^*$. On the other hand, if one chooses to coarsen the spatial discretization mesh, then $E_t$, $S^*$ and $q^*$ should naturally become larger, which means that their corresponding dissipation terms must be weakened appropriately. The only way to set these conditions in the transport equations is to adjust the turbulent energy dissipation rate $\rho_\varepsilon t$ and damping in the coarse-grained collision terms $C^*_S$ and $c^*_q$ (or, alternatively, coarse-grained viscosity $\mu^*$ and heat conductivity $\kappa^*$), solely because there is nothing else in the transport equations that can be changed.

At first, this situation appears to conflict with the way the Reynolds average is initially set up as a statistical average, since the ensemble averaging is formally unrelated to the spatial filtering (like the one in the LES). To clarify the situation, here we offer an informal explanation how the spatial scaling information can be incorporated into the Reynolds averaging. The Reynolds averaging process consists of two stages – first, “ensemble generation”, and, second, “ensemble averaging” (as purely a thought process, of course, since there is no explicit numerical ensemble generation or averaging involved). Here we claim that the spatial scale information is taken into account during the “ensemble generation” stage. Indeed, observe that all ensemble members must share the coarse-grained scale features (as it is the “resolved” scale), while, of course, differing on the turbulent scale. Therefore, if the coarse-grained scale is in fact so fine that it resolves even the molecular viscosity effects, the corresponding statistical ensemble must, essentially, consist of a single member (or many identical members), as any difference between the ensemble members on the unresolved scale is nearly instantaneously damped to zero by the molecular viscosity. Conversely, if the coarse-grained scale is not too fine, then it lifts the difference between the ensemble members into larger spatial scales, and hence weakens their dissipation.

This leads to the natural conclusion that the spatial scale information must be encoded into the dissipative terms parameterizing the turbulent energy decay rate $\rho_\varepsilon t$ and the coarse-grained collision terms $C^*_S$ and $c^*_q$. Particularly, in the limit as the coarse-grained scale becomes fine enough to resolve the molecular viscosity scale, the turbulent energy decay rate $\rho_\varepsilon t$ must be strong enough to ensure that the turbulent energy $E_t$ is (almost) zero, while the coarse-grained collision terms $C^*_S$ and $c^*_q$ must transform into their fine-grained analogs in (2.23).

6.2. **Numerical stability and possible shock formation.** From what is developed above, one can envision three general scenarios of a practical computational set-up:

1. The coarse-grained Grad transport equations (5.6) with the specific, problem-dependent parameterization of the collision terms;
(2) The coarse-grained Navier-Stokes transport equations (5.10) with the coarse-grained viscosity and heat conductivity;

(3) The coarse-grained Grad transport equations (5.6) with collision terms parameterized via linear damping as in (5.7), with coarse-grained viscosity and heat conductivity.

There is not much to comment on in the first two scenarios, because the latter is comprised by the well-studied Navier-Stokes equations, while the computational properties of the former heavily depend on the implementation of the coarse-grained collision terms. The third scenario is, however, of more interest, since it is typically used in rarefied gas dynamics [14,15,34,35,37]. In the turbulent flow simulations, the third scenario is likely to appear when the turbulence is still weak enough to parameterize the collisions by linear damping (5.7), but at the same time the coarse-grained viscosity $\mu^*$ and heat conductivity $\kappa^*$ are not small enough to enable the Navier-Stokes approximations of $S^*$ and $q^*$ via (5.9). In this situation, observe that the resulting transport equations for the coarse-grained variables do not have any diffusion terms, which leads to the creation of shocks at high Mach numbers [14].

In this scenario, one might consider the regularization strategy proposed by Struchtrup and Torrilhon [35,37], which is, roughly put, a type of the Chapman-Enskog expansion built around the Grad state in (2.29), and applied to the transport equations for $Q^*$ and $R^*$. The way this regularization works is the same as in the Navier-Stokes parameterizations in (2.25)–(2.27), yielding additional diffusion terms in the transport equations for the coarse-grained stress (5.6d) and heat flux (5.6e), and thus dissipating the shock formation. The diffusion from these extra terms manifests on the scale $\mu^*/p^*$ (or, alternatively, $\kappa^*/p^*$), and extends to the larger scales as the coarse-grained viscosity and heat conductivity increase, thus allowing for coarser computational discretization.

### 6.3. A crude approximation for the turbulent energy dissipation rate

The simplest way to model the turbulent energy dissipation rate $\rho \varepsilon_t$ is by using the dimensional analysis. Above, we concluded that a parameterization for $\rho \varepsilon_t$ should depend on a length scale parameter which characterizes the coarse-grained spatial scale (such as the spatial discretization size). Let us now assume that $\varepsilon_t$ may only depend on such a spatial scale parameter $L$, and the turbulent energy $E_t$ itself, scaled by the density $\rho$:

\[
\varepsilon_t \propto (E_t / \rho)^\alpha L^\beta,
\]

where the constants $\alpha$ and $\beta$ must be determined by considering physical dimensions. Now, observe that the dimension of $E_t / \rho$ is length$^2$/time, while the dimension of $\varepsilon_t$ is length$^2$/time$^3$. Thus, the only way to equalize dimensions in the expression above is to set $\alpha = 3/2, \beta = -1$, which yields

\[
\varepsilon_t \propto E_t^{3/2} / \rho^{3/2} L, \quad \rho \varepsilon_t \propto E_t^{3/2} / \rho^{1/2} L.
\]

This well-known simple parameterization was proposed by Taylor [36]. Observe that it is in agreement with what was concluded earlier; namely, it disappears when $E_t \to 0$ (and thus does not let $E_t$ become negative), and increases for fixed $E_t$ as $L \to 0$, thus
more strongly driving $E_t$ towards zero in the case the coarse-grained spatial resolution scale becomes more refined.

However, we can immediately see that the simple parameterization above has a serious drawback. Recall that we agreed in Section 3 that the new coarse-grained transport equations must have solutions which do not exhibit rapid oscillations at small scales, otherwise the very point of introducing the coarse-grained equations would become moot. Nonetheless, with the turbulent energy decay rate $\rho \varepsilon_t$ given as above in (6.2), the turbulent energy transport equation in (4.31) has no diffusive terms of sufficient strength (the existing diffusion term there manifests on the molecular scale), and in that respect the equation in (4.31) is no different from the conventional transport equations in (2.7) we started with.

Therefore, here we contend that the turbulent energy decay rate $\rho \varepsilon_t$ must incorporate a diffusion term which manifests on the coarse-grained scale. In particular, we propose a simple extension of (6.2) based, again, on a dimensional argument:

\[ (6.3) \quad \rho \varepsilon_t \propto \left( \frac{E_t}{\rho} \right)^{1/2} \left( \frac{E_t}{L} + \alpha L \Delta E_t \right), \]

where $\alpha$ is a scalar non-dimensional parameter. Observe that above the first term is exactly the Taylor parameterization from (6.2). The additional term, scaled by $\alpha$, is a diffusion term, which, contrary to the linear damping term, increases when $L$ becomes large, extending the diffusion scale proportionally to the coarse-grained scale parameter $L$. Conversely, the diffusion term disappears as the coarse-grained scale becomes more refined. This seems to be in consistence with what one would expect from the behavior of the turbulent energy.

Of course, the parameterization in (6.3) is the simplest model for $\rho \varepsilon_t$ one could possibly come up with, but at least it seems to be a reasonable starting point for use in computational modeling. There also exist more sophisticated models for $\varepsilon_t$ (such as, for example, the $k$-$\varepsilon$ and $k$-$\omega$ models [38]) but they require a separate transport equation for $\varepsilon_t$, which, in turn, introduces additional closure problems via unspecified parameters.

6.4. Crude approximations for the coarse-grained collision terms. Here we offer a very crude parameterization of the coarse-grained collision terms in the form of a linear damping, which, of course, will not stand any critique when the properties of the coarse-grained collision terms become better studied, but at present may at least serve as a starting point in the computational modeling. Here we assume that the coarse-grained collision terms $C_S^*$ and $c_q^*$ can be modeled by a linear damping of the form (5.7), where the coarse-grained viscosity $\mu^*$ and heat conductivity $\kappa^*$ are to be approximated somehow. From the prior considerations, we expect that $\mu^*$ and $\kappa^*$ must be proportional to the coarse-grained length scale (that is, they must become small when the length scale is short, and vice versa). At the same time, we know that, as the coarse-grained length scale becomes short, $\mu^*$ and $\kappa^*$ must become their microscale counterparts $\mu$ and $\kappa$, respectively. The form of the microscale $\mu$ and $\kappa$ is given in Grad [14] as

\[ (6.4) \quad \mu, \kappa \propto \frac{m}{\sigma^2} \left( \frac{p}{\rho} \right) = \mu_m \frac{\sigma}{\sigma^2} \left( \frac{p}{\rho} \right)^{1/2} = \rho_m \sigma \left( \frac{p}{\rho} \right)^{1/2}, \]
where \( m \) is the mass of the molecule, \( \sigma \) is its linear size (diameter or radius), and \( \rho_m \) is the “density” of a molecule. Now, with help of a vivid imagination, one could interpret the collision processes on a coarse-grained scale as ones with rather large and soft molecules. This means that for the coarse-grained viscosity or heat conductivity one likely has to keep the “density” \( \rho_m \) fixed, but increase the “size” of the molecule to be that of the characteristic length of the coarse-grained scale, while at the same time also parameterizing \( p \) via either its coarse-grained counterpart, or its Reynolds average:

\[
\mu^*, \kappa^* \propto \left( \frac{p}{\rho} \right)^{1/2} L \propto \begin{cases} 
\left( \frac{p^*}{\rho} \right)^{1/2} L, & \text{or} \\
\left( \frac{p}{\rho} \right)^{1/2} L = \left( \frac{3p^* - 2E_t}{3\rho} \right)^{1/2} L,
\end{cases}
\]

where the choice is between the lack of feedback from the small scales, or a feedback which damps the viscosity and heat conductivity if the turbulent energy becomes too large. The coefficients of proportionality should likely be chosen so that in the limit as the resolved scale becomes the molecular viscosity scale, both \( \mu^* \) and \( \kappa^* \) become their microscale counterparts. In fact, they do not necessarily have to be constants, as that would impose the same Prandtl number on the coarse-grained scale, which may not necessarily be the case in practice.

The relation above constitutes the simplest, crudest parameterization for the coarse-grained viscosity and heat conductivity. This parameterization is, however, consistent with what is expected of it, namely, it increases the coarse-grained viscosity and heat conductivity in proportion to the coarse-grained spatial scale, and, if the turbulent energy feedback option is chosen, it also tends to decrease them as \( E_t \) increases, thus providing an additional balancing mechanism. Note, however, that a regularization along the lines of Struchtrup and Torrilhon [35, 37] is needed for a linear damping parameterization in (6.5) to improve the numerical stability of the coarse-grained Grad equations in (5.6). Alternatively, if the resulting \( \mu^* \) and \( \kappa^* \) are found to be small enough to allow the steady-state parameterization of the kind in (5.9), then one can optionally use the coarse-grained Navier-Stokes equations (5.10) instead of the coarse-grained Grad equations (5.6) (or suitably regularized Burnett/super-Burnett expansions, for better accuracy with not-so-small \( \mu^* \) and \( \kappa^* \)).

### 7. Summary and future research

In this work, we propose a new framework for the coarse-grained transport of a turbulent flow, which is based on the Reynolds averaging of the Boltzmann equation in (2.1), rather than the conventional Reynolds averaging of the Navier-Stokes equations in (2.28). The proposed framework consists of the equations in (3.6) for the transport of the coarse-grained variables of the flow in (3.5), and the equation for the transport of the turbulent energy in (4.31) under the approximation of the anelastic turbulence. We also propose two different closures for the hierarchy of the transport equations for the coarse-grained variables: the more general Grad closure in (5.6), and the more simple Navier-Stokes closure formulation in (5.10), which can likely be expanded into the higher Burnett or super-Burnett orders to improve accuracy. The proposed transport
model includes three unknown parameters: the turbulent energy dissipation rate $\rho_\varepsilon t$ in the turbulent energy equation (4.31), the coarse-grained stress collision operator $C^*_S$ (or, equivalently, the corresponding coarse-grained viscosity $\mu^*$) in the coarse-grained stress equation (5.6d), and the coarse-grained heat flux collision operator $c^*_q$ (or, equivalently, the corresponding coarse-grained heat conductivity $\kappa^*$) in the coarse-grained heat flux equation (5.6e). These three parameters cannot be defined exactly within the scope of the new transport model, as they depend on the properties of the nonlinear fluid-fluid interactions, and require separate treatment. We also suggest crude parameterizations for $\rho_\varepsilon t$, $C^*_S$ and $c^*_q$ based on dimensional analysis, to be used as a starting point in the practical computational modeling.

**Future research.** The main deficiency of the developed coarse-grained transport framework is that it is derived under the assumption of a monatomic ideal gas model. While this assumption greatly simplifies calculations, at the same time it severely restricts the applicability of the framework, as most gases in the surrounding nature are at least diatomic (e.g., the air). At the same time, such a framework would likely be of use in the applications which involve the circulation of the large scale atmosphere, as it is well known that the atmosphere is a highly turbulent medium, and at the same time present computational limitations restrict the spatial resolution of the global circulation models to rather coarse meshes. Thus, the development of the analogous coarse-grained transport framework for the polyatomic (or at least diatomic) ideal gases is presently our main priority.

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