Kinetic Theory of Turbulence Modeling: Smallness Parameter, Scaling and Microscopic Derivation of Smagorinsky Model

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Abstract

A mean-field approach (filtering out subgrid scales) is applied to the Boltzmann equation in order to derive a subgrid turbulence model based on kinetic theory. It is demonstrated that the only Smagorinsky type model which survives in the hydrodynamic limit on the viscosity time scale is the so-called tensor-diffusivity model. Scaling of the filter-width with Reynolds number and Knudsen number is established. This sets the first rigorous step in deriving turbulence models from kinetic theory.

1 Introduction

The application of a filtering procedure to equations of hydrodynamics (Navier-Stokes equations) in order to construct a subgrid model is often used for the turbulence modeling [1]. The aim of such models is to take into account the effects of subgrid scales as an extra stress term in the hydrodynamic equations for the resolved scale fields. Further, the subgrid scale terms should be representable in terms of the resolved fields. This procedure, like any other attempt to coarse-grain the Navier-Stokes equations, runs into the closure problem due to the nonlinearity of the equation and due to the absence of scale separation.
On the other hand, in statistical physics, good schemes to obtain closure approximations are known for nonlinear evolution equations (with a well-defined separation of scales). Unfortunately, attempts to borrow such schemes fail for the Navier-Stokes equations. The fundamental reason for this failure of the coarse-graining procedures on the Navier-Stokes equations is the absence of scale separation. Further, the length over which the equation is coarse-grained (the filter width in the present case) is completely arbitrary (and in practice dictated by the available computational resources), and cannot be justified a priori on physical grounds.

In this paper, we show that a coarse-grained description of hydrodynamics using the microscopic theories is possible. Specifically, we apply the standard filtering procedure (isotropic Gaussian filter) not on the Navier-Stokes equations but on the Boltzmann kinetic equation. We recall that the Navier-Stokes equations are a well defined limit of the Boltzmann equation (the hydrodynamic limit), whereas the filtering operation and going to the hydrodynamic limit are two distinct operations which do not commute, because kinetic fluctuations generally do not annihilate upon filtering. By doing so, we obtain the following results:

- **Smallness parameter**: The smallness parameter of the present theory is the usual kinetic-theory Knudsen number $\text{Kn}$,

$$
\text{Kn} = \frac{\nu}{Lc_s} \sim \frac{\text{Ma}}{\text{Re}},
$$

where $\text{Ma}$ is the Mach number and $\text{Re}$ is the Reynolds number, $\nu$ is the kinematic viscosity, $c_s$ is the sound speed and $L$ is the characteristic macroscopic length. Smallness of $\text{Kn}$ rules emergence of both, the usual viscosity terms, and the subgrid contributions, on the viscosity time scale of the filtered Boltzmann equation (that is, in the first-order Chapman-Enskog solution to the filtered Boltzmann equation).

- **Scaling**: In the coarse-grained representation obtained by filtering, the filter-width $\Delta$ (for the Gaussian filter, $\Delta^2$ is proportional to the covariance) is the smallest length-scale to be resolved. The requirement that contributions from the subgrid scales appear in the kinetic picture at the time scale of molecular relaxation time (viscosity time scale) sets the scaling of $\Delta$ with the Knudsen number as follows:

$$
\Delta = kL\sqrt{\text{Kn}},
$$

where $k$ is a nonuniversal constant which scales neither with $L$, nor with $\text{Kn}$. For the sake of simplicity, we set $k = 1$ in all the further computations. Equations (1) and (2) imply that the filter-width scales with the Reynolds number as follows:

$$
\Delta \sim \text{Re}^{-1/2}.
$$
While the Kolmogorov length, $l_K$, scales as $l_K \sim \text{Re}^{-3/4}$, we have

$$\frac{\Delta}{l_K} \sim \text{Re}^{1/4}.$$  \hfill (4)

Thus, the filtering scale is larger than the Kolmogorov scale when Re is large enough.

- **Subgrid model:** With the above smallness parameter (1), and the scaling (2), we rigorously derive the following subgrid pressure tensor $P^{SG}_{\alpha\beta}$, in addition to the usual (advection and viscosity) terms in the momentum equation:

$$P^{SG}_{\alpha\beta} = \frac{KnL^2 \overline{\rho}}{12} \left[ \overline{S}_{\alpha\gamma} - \overline{\Omega}_{\alpha\gamma} \right] \left[ \overline{S}_{\gamma\beta} + \overline{\Omega}_{\gamma\beta} \right]$$

$$= \frac{\nu \overline{\rho} c_s L}{12} \left[ \overline{S}_{\alpha\gamma} - \overline{\Omega}_{\alpha\gamma} \right] \left[ \overline{S}_{\gamma\beta} + \overline{\Omega}_{\gamma\beta} \right].$$ \hfill (5)

Here $\overline{\rho}$ is the filtered density, and summation convention in spatial components is adopted. For any function $X$, $\overline{X}$ denotes the filtered value of $X$. Furthermore, the filtered rate of the strain tensor $\overline{S}_{\alpha\beta}$ and the filtered rate of the rotation tensor $\overline{\Omega}_{\alpha\beta}$ depends only on the large scale velocity, $\overline{u}_\alpha$:

$$\overline{\Omega}_{\alpha\beta} = \frac{1}{2} \left\{ \partial_\alpha \overline{u}_\beta - \partial_\beta \overline{u}_\alpha \right\},$$

$$\overline{S}_{\alpha\beta} = \frac{1}{2} \left\{ \partial_\alpha \overline{u}_\beta + \partial_\beta \overline{u}_\alpha \right\}.$$ \hfill (6)

The derived subgrid model belongs to the class of Smagorinsky models [4], and the tensorial structure of the subgrid pressure tensor (5) corresponds to the so-called tensor-diffusivity subgrid model (TDSG) introduced by Leonard [5], and which became popular after the work of Clark et al [6]. Here, it is interesting to recall that in the class of existing Smagorinsky models the TDSG is one of only a few models in which the sub-grid scale stress tensor remains frame-invariant under arbitrary time-dependent rotations of reference frame [7]. Furthermore, the TDSG model belongs to a subclass of Smagorinsky models which take into account the backscattering of energy from the small scale to the large scales [1]. Beginning with the seminal work of Kraichnan [8], importance of the backscattering of energy in turbulence modeling is commonly recognized.

- **Uniqueness:** The result (5) requires only isotropy of the filter but otherwise is independent of the particular functional form of the filter. There are no other subgrid models different from (5) which can be derived from kinetic theory by the one-step filtering procedure. In other words, higher-order spatial derivatives are not neglected in an uncontrolled fashion, rather, they are of the order $Kn^2$, and thus do not show up on the viscosity time scale.

- **Nonarbitrary filter-width:** Unlike the phenomenological TDSGM where the prefactor in Eq. (5) remains an unspecified $\Delta^{2n}$, kinetic theory suggests that the filter-width cannot be set at will, rather, it must respect the phys-
tical parameterization (specific values of Re, Kn etc) of a given setup when
the subgrid model is used for numerical simulation. Recent findings that
simulations of the TDSG model become unstable for large $\Delta$ [9] is in qual-
itative agreement with the present result that the filter-width $\Delta$ cannot be
made arbitrary large.

The structure of the paper is as follows: In section 2 we set up the kinetic
theory for the subsequent coarse-graining and derivation of the subgrid model.
It is important to stress that the only requirement on the choice of the kinetic
equation in the present context is that it gives the Navier-Stokes hydrodynamic
equations in the appropriate fully resolved limit. For that reason we choose to
work with a recently introduced minimal kinetic model [2,3] which is sufficient
for our present purpose. Filtered kinetic equation is obtained in section 3. In
section 4 we derive the subgrid model (5) using the Chapman-Enskog method
[10] for the filtered kinetic model. This derivation uniquely defines the scaling
(3) from the requirement that the subgrid terms appear on the viscous time
scale. Finally, results are summarized, and some directions of future research
are discussed in section 6.

2 Kinetic theory

For the present discussion, the particular choice of the kinetic model is unim-
portant as long as the hydrodynamic limit of the kinetic theory is the usual
Navier-Stokes equations at least up to the order $O(Ma^3)$. We demonstrate the
whole procedure in detail for a recently introduced minimal discrete-velocity
kinetic model [2,3]. As the final result is just the same in two and three di-

The local equilibrium $f_i^{eq}$ is the conditional minimizer of the the entropy func-
tion $H$:

$$H = \sum_{i=1}^{9} f_i \ln \left( \frac{f_i}{W_i} \right),$$  (10)
under the constraint of local conservation laws:

\[
\sum_{i=1}^{9} f_{i}^{eq}\{1, C_{i}\} = \{\rho, \rho u\}.
\]  

(11)

The weights \( W_{i} \) in the equation (10) are:

\[
W_{i} = \frac{1}{36} \{16, 4, 4, 4, 1, 1, 1\}.
\]  

(12)

The explicit expression for \( f_{i}^{eq} \) reads:

\[
f_{i}^{eq} = \rho W_{i} \prod_{\alpha=1}^{9} \left( 2 - \sqrt{1 + 3u_{\alpha}^2} \right) \left( \frac{2u_{\alpha} + \sqrt{1 + 3u_{\alpha}^2}}{1 - u_{\alpha}} \right) C_{i\alpha}.
\]  

(13)

Below, it will prove convenient to work in the moment representation rather than in the population representation. Let us choose the following orthogonal set of basis vectors in the 9-dimensional phase space of the kinetic equation (7):

\[
\psi_{1} = \{1, 1, 1, 1, 1, 1, 1, 1\},
\]

\[
\psi_{2} = \{0, 1, 0, -1, 0, 1, -1, -1, 1\},
\]

\[
\psi_{3} = \{0, 0, 1, 0, -1, 1, 1, -1, 1\},
\]

\[
\psi_{4} = \{0, 0, 0, 0, 0, 1, -1, 1, -1\},
\]

\[
\psi_{5} = \{0, 0, 0, 1, -1, 1, 1, -1, 1\},
\]

(14)

\[
\psi_{6} = \{0, 1, -1, 1, -1, 0, 0, 0, 0\},
\]

\[
\psi_{7} = \{0, -2, 0, 2, 0, 1, -1, -1, 1\},
\]

\[
\psi_{8} = \{4, -5, -5, -5, -5, 4, 4, 4, 4\},
\]

\[
\psi_{9} = \{4, 0, 0, 0, 0, -1, -1, -1, -1\}.
\]

The orthogonality of the chosen basis is in the sense of the usual Euclidean scalar product, i.e.,

\[
\sum_{k=1}^{9} \psi_{ik} \psi_{kj} = d_{i}\delta_{ij},
\]  

(15)

where \( d_{i} \) are some constants needed for the normalization (the basis vectors are orthogonal but not orthonormal). We define new variables \( M_{i}, i = 1, \ldots, 9 \) as:

\[
M_{i} = \sum_{j=1}^{9} \psi_{ij} f_{j},
\]  

(16)

where \( \psi_{ij} \) denotes \( j \)th component of the 9-dimensional vector \( \psi_{i} \). Basic hydrodynamic fields are \( M_{1} = \rho, M_{2} = \rho u_{x}, \) and \( M_{3} = \rho u_{y} \). The remaining six moments are related to higher order moments of the distribution (the pressure tensor \( P_{\alpha\beta} = \sum f_{i} C_{i\alpha} C_{i\beta} \) and the third order moment \( Q_{\alpha\beta\gamma} = \sum f_{i} C_{i\alpha} C_{i\beta} C_{i\gamma} \) and so on), as: \( M_{4} = P_{xy}, \)

5
\[ M_5 = P_{xx} - P_{yy}, \]
\[ M_6 = 3 \sum f_i C_{iy} C_{ix} - 2M_2, \]
\[ M_7 = 3 \sum f_i C_{ix} C_{iy} - 2M_3 \]

The explicit form of the stress tensor in term of the new set of variables is:

\[ \begin{align*}
P_{xy} &= M_4, \\
P_{xx} &= \frac{2}{3} M_1 + \frac{1}{2} M_5 + \frac{1}{30} M_8 - \frac{1}{5} M_9, \\
P_{yy} &= \frac{2}{3} M_1 - \frac{1}{2} M_5 + \frac{1}{30} M_8 - \frac{1}{5} M_9. 
\end{align*} \tag{18} \]

The time evolution equations for the set of moments are:

\[ \begin{align*}
\partial_t M_1 + \partial_x M_2 + \partial_y M_3 &= 0, \\
\partial_t M_2 + \partial_x \left( \frac{2}{3} M_1 + \frac{1}{2} M_5 + \frac{1}{30} M_8 - \frac{1}{5} M_9 \right) + \partial_y M_4 &= 0, \\
\partial_t M_3 + \partial_x M_4 + \partial_y \left( \frac{2}{3} M_1 - \frac{1}{2} M_5 + \frac{1}{30} M_8 - \frac{1}{5} M_9 \right) &= 0, \\
\partial_t M_4 + \frac{1}{3} \partial_x (2M_5 + M_7) + \frac{1}{3} \partial_y (2M_2 + M_6) &= \frac{1}{\tau} (M_4^{eq}(M_1, M_2, M_3) - M_4), \\
\partial_t M_5 + \frac{1}{3} \partial_x (M_2 - M_6) + \frac{1}{3} \partial_y (M_7 - M_3) &= \frac{1}{\tau} (M_5^{eq}(M_1, M_2, M_3) - M_5), \\
\partial_t M_6 - \frac{1}{5} \partial_x (5M_5 - M_8 + M_9) + \partial_y M_4 &= \frac{1}{\tau} (M_6^{eq}(M_1, M_2, M_3) - M_6), \\
\partial_t M_7 + \partial_x M_4 + \frac{1}{3} \partial_y (5M_5 + M_8 - M_9) &= \frac{1}{\tau} (M_7^{eq}(M_1, M_2, M_3) - M_7), \\
\partial_t M_8 + \partial_x (M_2 + 3M_6) + \partial_y (M_3 + 3M_7) &= \frac{1}{\tau} (M_8^{eq}(M_1, M_2, M_3) - M_8), \\
\partial_t M_9 - \frac{1}{3} \partial_x (2M_2 + M_6) - \frac{1}{3} \partial_y (2M_3 + M_7) &= \frac{1}{\tau} (M_9^{eq}(M_1, M_2, M_3) - M_9). 
\end{align*} \tag{19} \]

The expression for the local equilibrium moments \( M_i^{eq}, i = 4, \ldots, 9 \) in terms of the basic variables \( M_1, M_2, \) and \( M_3 \) to the order \( u^2 \) is:
\[ M_{eq}^4(M_1, M_2, M_3) = \frac{M_2 M_3}{M_1}, \]
\[ M_{eq}^5(M_1, M_2, M_3) = \frac{M_2^2 - M_3^2}{M_1}, \]
\[ M_{eq}^6(M_1, M_2, M_3) = -M_2, \]
\[ M_{eq}^7(M_1, M_2, M_3) = -M_3, \]
\[ M_{eq}^8(M_1, M_2, M_3) = -3 \frac{M_2^2 + M_3^2}{M_1}, \]
\[ M_{eq}^9(M_1, M_2, M_3) = 5 \frac{3 M_1 - 3(M_2^2 + M_3^2)}{M_1}. \]  

(20)

The incompressible Navier-Stokes equations are the hydrodynamic limit of the system (19) and (20).

In the next section, we shall remove small scales through a filtering procedure on the moment system (19), (20). A precise definition of the small scales is postponed until later sections. For the time being, let us assume that there exist a length-scale \( \Delta \), and we wish to look at the hydrodynamics at length-scale larger than \( \Delta \) only.

3 Filtered kinetic theory

Coarse-grained versions of the Boltzmann equations have been discussed in the recent literature [11,12,13]. However, a systematic treatment is still lacking. In this section, we shall fill this gap.

3.1 Gaussian filter

For any function \( X \), the filtered function \( \overline{X} \) is defined as:

\[ \overline{X}(x) = \int_{R^3} G(r)X(x - r)dr. \]  

(21)

Function \( G \) is called the filter. In the sequel, we apply the filtering operation (21) on the moment system (19). We will need two relations. First, for any function \( X \),

\[ \overline{\partial_\alpha X} = \partial_\alpha \overline{X}. \]  

(22)

This relation is sufficient to filter the propagation terms in the equation (19) due to linearity of propagation in the kinetic picture. The latter is a useful
property which is not shared by the hydrodynamic Navier-Stokes equations, where the nonlinearity and nonlocality both come into the same \(u \nabla u\) term. Any isotropic filter, which satisfies the condition of commuting of the derivatives under the application of the filter (Eq. 22), will suffice for the present purpose. We choose a standard Gaussian filter \([1]\) which has the property (22):

\[
G(r, \Delta) = \left(\frac{6}{\pi \Delta^2}\right)^D \exp\left(-\frac{6r^2}{\Delta^2}\right). \tag{23}
\]

Let us recall the isotropy properties of a Gaussian filter:

\[
\int_{R^D} G(r, \Delta) \, dr = 1,
\]
\[
\int_{R^D} G(r, \Delta) \, r \, dr = 0,
\]
\[
\int_{R^D} G(r, \Delta) r_\alpha r_\beta \, dr = \frac{\Delta^2}{12} \delta_{\alpha\beta}. \tag{24}
\]

Second, in order to filter the nonlinear terms (20) in the right hand side of moment equations (19), we will also need the following relation for three arbitrary functions \(X, Y, Z\) which follow immediately from the isotropy property by second-order Taylor expansion:

\[
\overline{(XYZ)} = \overline{XY}Z + \frac{\Delta^2}{12} Z \left\{ (\partial_\alpha X)(\partial_\alpha Y) - \frac{2}{Z} (\partial_\alpha Z) \left( X \partial_\alpha Y + Y \partial_\alpha X + \frac{2XY}{Z} \partial_\alpha Z \right) \right\} + O(\Delta^4). \tag{25}
\]

The effect of a Gaussian filter need not be truncated to any order at the present step. The higher-order terms lumped under \(O(\Delta^4)\) in equation (25) can be computed from elementary Gaussian integrals. As we shall see it soon, higher than second order terms disappear in the hydrodynamic limit once the scaling of the filter-width versus Knudsen number is appropriately chosen.

In the next section, we shall filter the moment equations (19).

3.2 Filtering the moment system

Applying the filter (21) to the moment system (19), (20), using (22) and (25), and keeping terms up to the order \(u^2\), we obtain the following filtered moment system:
\[ \partial_t \overline{M}_1 + \partial_x \overline{M}_2 + \partial_y \overline{M}_3 = 0, \]
\[ \partial_t \overline{M}_2 + \partial_x \left( \frac{2}{3} \overline{M}_1 + \frac{1}{2} \overline{M}_5 + \frac{1}{30} \overline{M}_8 - \frac{1}{5} \overline{M}_9 \right) + \partial_y \overline{M}_4 = 0, \]
\[ \partial_t \overline{M}_3 + \partial_x \overline{M}_4 + \partial_y \left( \frac{2}{3} \overline{M}_1 - \frac{1}{2} \overline{M}_5 + \frac{1}{30} \overline{M}_8 - \frac{1}{5} \overline{M}_9 \right) = 0, \]
\[ \partial_t \overline{M}_4 + \frac{1}{3} \partial_x \left( 2 \overline{M}_3 + \overline{M}_7 \right) + \frac{1}{3} \partial_y \left( 2 \overline{M}_2 + \overline{M}_6 \right) = \frac{1}{\tau} \left( M_{1}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_4 \right) \]
\[ + \frac{\Delta^2}{12 \tau M_1} (\partial_x \overline{M}_2)(\partial_x \overline{M}_2) + O \left( \frac{\Delta^4}{\tau} \right), \]
\[ \partial_t \overline{M}_5 + \frac{1}{3} \partial_x \left( \overline{M}_2 - \overline{M}_6 \right) + \frac{1}{3} \partial_y \left( \overline{M}_7 - \overline{M}_3 \right) = \frac{1}{\tau} \left( M_{2}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_5 \right) \]
\[ + \frac{\Delta^2}{12 \tau M_1} \left\{ (\partial_x \overline{M}_2)(\partial_x \overline{M}_2) - (\partial_x \overline{M}_3)(\partial_x \overline{M}_3) \right\} + O \left( \frac{\Delta^4}{\tau} \right), \] (26)
\[ \partial_t \overline{M}_6 - \frac{1}{5} \partial_x \left( 5 \overline{M}_5 - \overline{M}_8 + \overline{M}_9 \right) + \partial_y \overline{M}_4 = \frac{1}{\tau} \left( M_{6}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_6 \right) \]
\[ \partial_t \overline{M}_7 + \partial_x \overline{M}_4 + \frac{1}{5} \partial_y \left( 5 \overline{M}_5 + \overline{M}_8 - \overline{M}_9 \right) = \frac{1}{\tau} \left( M_{7}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_7 \right), \]
\[ \partial_t \overline{M}_8 + \partial_x \left( \overline{M}_2 + 3 \overline{M}_6 \right) + \partial_y \left( \overline{M}_3 + 3 \overline{M}_7 \right) = \frac{1}{\tau} \left( M_{8}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_8 \right) \]
\[ - \frac{3\Delta^2}{12 \tau M_1} \left\{ (\partial_x \overline{M}_2)(\partial_x \overline{M}_2) + (\partial_x \overline{M}_3)(\partial_x \overline{M}_3) \right\} + O \left( \frac{\Delta^4}{\tau} \right), \]
\[ \partial_t \overline{M}_9 - \frac{1}{3} \partial_x \left( 2 \overline{M}_2 + \overline{M}_6 \right) - \frac{1}{3} \partial_y \left( 2 \overline{M}_3 + \overline{M}_7 \right) = \frac{1}{\tau} \left( M_{9}^{eq}(\overline{M}_1, \overline{M}_2, \overline{M}_3) - \overline{M}_9 \right) \]
\[ - \frac{3\Delta^2}{12 \tau M_1} \left\{ (\partial_x \overline{M}_2)(\partial_x \overline{M}_2) + (\partial_x \overline{M}_3)(\partial_x \overline{M}_3) \right\} + O \left( \frac{\Delta^4}{\tau} \right). \]

Thus, we are set up to derive the hydrodynamic equations as the appropriate limit of the filtered kinetic system (26). In passing, we note that different moments relax with different effective relaxation time scales, because the subgrid terms are not the same for all kinetic moments.

4 Hydrodynamic limit of the filtered kinetic theory

In the kinetic equation we have a natural length scale set by Knudsen number \( \text{Kn} \) (1). The Navier-Stokes dynamics is obtained in the limit \( \text{Kn} \ll 1 \). By filtering the kinetic equation we have introduced a new length scale as the size of the filter \( \Delta \). The hydrodynamic equations produced by the filtered kinetic equation will depend on how \( \Delta \) scales with the Knudsen number. In order to understand this issue, let us look at the filtered equation for one of the moments (26) in the non-dimensional form. In order to do this, let us
introduce scaled time and space variables,
\[
x' = \frac{x}{L}, \\
t' = \frac{t c_s}{L},
\]
where \(c_s = 1/\sqrt{3}\) for the present model. Let us also specify Knudsen number in terms of the relaxation time \(\tau\):
\[
Kn = \frac{\nu}{L c_s} = \frac{\tau c_s}{L},
\]
where, \(\nu\) is the kinematic viscosity, \(\nu = \tau c_s^2\) in the present model. Then, for example, the filtered equation for the moment \(M_4\) reads:
\[
\partial_t' M_4 + \frac{1}{3 c_s} \partial_{x'} \left( 2 M_3 + M_7 \right) + \frac{1}{3 c_s} \partial_{y'} \left( 2 M_2 + M_6 \right) = \frac{1}{Kn} \left( M_4^{eq}(M_1, M_2, M_3) - M_4 \right)
\]
\[
+ \frac{\Delta^2}{12 Kn L^2 M_1} \left\{ (\partial_{x'} M_2)(\partial_{x'} M_3) + (\partial_{y'} M_2)(\partial_{y'} M_3) \right\} + O \left( \frac{\Delta^4}{L^4 Kn} \right).
\]
We see that in absence of the filter (\(\Delta = 0\)), the usual situation of a singularly perturbed kinetic equation is recovered (and this results in the Navier-Stokes equations in the first-order Chapman-Enskog expansion). Let us consider the following three possibilities of dependence of \(\Delta\) on \(Kn\):
\begin{itemize}
  \item If \(\Delta/L \sim Kn^0\), then we do not have a singularly perturbed equation in (29) anymore. That is, the filter is too wide, and it affects the advection terms in the hydrodynamic equations.
  \item If \(\Delta/L \sim Kn\), then we do have a singularly perturbed system. However, the subgrid terms are of order \(Kn^2\), and they do not show up in the order \(Kn\) hydrodynamic equation. In other words, the filter is too narrow so that it does not affect hydrodynamic equations at the viscous time scale.
  \item Finally, there is only one possibility to set the scaling of filter-width with \(Kn\) so that the system is singularly perturbed, and the subgrid terms of the order \(\Delta^2\) contribute just at the viscous time scale. This situation happens if
\[
\frac{\Delta}{L} \sim \sqrt{Kn}.
\]
Note that, with the scaling (30), all the higher-order terms (of the order \(\Delta^4\) and higher) become of the order \(Kn\) and higher, so that they do not contribute at the viscous time scale.
\end{itemize}
Once the scaling of the filter-width (30) is introduced into the filtered moment equations (26), the application of the Chapman-Enskog method [10] becomes
a routine. We write:

$$\partial_t = \partial_t^{(0)} + Kn \partial_t^{(1)} + O(Kn^2),$$  \hspace{1cm} (31)

and for $i = 4, \ldots, 9$:

$$\mathcal{M}_i = M_i^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) + Kn \mathcal{M}_i^{(1)} + O(Kn^2).$$  \hspace{1cm} (32)

The hydrodynamics equations at the the order $O(1)$ are the Euler equations:

$$\begin{align*}
\partial_t^{(0)} \mathcal{M}_1 &= -\partial_x \mathcal{M}_2 - \partial_y \mathcal{M}_3, \\
\partial_t^{(0)} \mathcal{M}_2 &= -\partial_x \left( \frac{M_1 c_s^2 + \mathcal{M}_2 \mathcal{M}_2}{\mathcal{M}_1} \right) - \partial_y \left( \frac{\mathcal{M}_2 \mathcal{M}_3}{\mathcal{M}_1} \right), \\
\partial_t^{(0)} \mathcal{M}_3 &= -\partial_x \left( \frac{\mathcal{M}_2 \mathcal{M}_3}{\mathcal{M}_1} \right) - \partial_y \left( \frac{M_1 c_s^2 + \mathcal{M}_3 \mathcal{M}_3}{\mathcal{M}_1} \right).
\end{align*}$$  \hspace{1cm} (33)

Note that no subgrid terms appear at this time scale in the hydrodynamic equations (33). This means that large scale motion, even after filtering, is dictated just by the conservation laws. Zero-order time derivatives of the non-conserved moments are evaluated using the chain rule:

$$\partial_t^{(0)} M_i^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) = \frac{\partial M_i^{\text{eq}}}{\partial \mathcal{M}_1} \partial_t^{(0)} \mathcal{M}_1 + \frac{\partial M_i^{\text{eq}}}{\partial \mathcal{M}_2} \partial_t^{(0)} \mathcal{M}_2 + \frac{\partial M_i^{\text{eq}}}{\partial \mathcal{M}_3} \partial_t^{(0)} \mathcal{M}_3. \hspace{1cm} (34)$$

In particular, to the order $u^2$:

$$\begin{align*}
\partial_t^{(0)} M_4^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= 0, \\
\partial_t^{(0)} M_5^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= 0, \\
\partial_t^{(0)} M_6^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= \partial_x \left( M_1 c_s^2 + \frac{\mathcal{M}_2 \mathcal{M}_2}{\mathcal{M}_1} \right) + \partial_y \left( \frac{\mathcal{M}_2 \mathcal{M}_3}{\mathcal{M}_1} \right), \\
\partial_t^{(0)} M_7^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= \partial_x \left( \frac{\mathcal{M}_2 \mathcal{M}_3}{\mathcal{M}_1} \right) + \partial_y \left( M_1 c_s^2 + \frac{\mathcal{M}_3 \mathcal{M}_3}{\mathcal{M}_1} \right), \\
\partial_t^{(0)} M_8^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= 0, \\
\partial_t^{(0)} M_9^{\text{eq}}(\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3) &= -\frac{5}{3} \left[ \partial_x \mathcal{M}_2 + \partial_y \mathcal{M}_3 \right].
\end{align*}$$  \hspace{1cm} (35)

At the next order $O(Kn)$, correction to locally conserved moments is equal to zero,

$$\mathcal{M}_1^{(1)} = \mathcal{M}_2^{(1)} = \mathcal{M}_3^{(1)} = 0,$$
whereas corrections to the non-conserved moments, $M_i^{(1)}$, $i = 4, \ldots, 9$, are obtained by substituting Eq. (31), and Eq. (32) in Eq. (26) and eliminating the zeroth order time derivatives using Eq. (35):

$$M_4^{(1)} = -Lc_s \left[ \partial_x M_3 + \partial_y M_2 \right] + \frac{L^2}{12 M_1} \left\{ (\partial_x M_2) (\partial_x M_3) + (\partial_y M_2)(\partial_y M_3) \right\},$$

$$M_5^{(1)} = -2Lc_s \left[ \partial_x M_2 - \partial_y M_3 \right] + \frac{L^2}{12 M_1} \left\{ (\partial_x M_2)^2 - (\partial_x M_3)^2 + (\partial_y M_2)^2 - (\partial_y M_3)^2 \right\},$$

$$M_6^{(1)} = -Lc_s \left[ \partial_x \left( \frac{3(M_3^2)}{M_1} \right) \right] + \partial_y \left( \frac{6 M_2 M_3}{M_1} \right),$$

$$M_7^{(1)} = -Lc_s \left[ \partial_x \left( \frac{6 M_2 M_3}{M_1} \right) + \partial_y \left( \frac{3(M_2^2)}{M_1} \right) \right],$$

$$M_8^{(1)} = 6Lc_s \left[ \partial_x M_2 + \partial_y M_3 \right] - \frac{3L^2}{12 M_1} \left\{ (\partial_x M_2)^2 + (\partial_y M_2)^2 + (\partial_x M_3)^2 + (\partial_y M_3)^2 \right\},$$

$$M_9^{(1)} = 6Lc_s \left[ \partial_x M_2 + \partial_y M_3 \right] - \frac{3L^2}{12 M_1} \left\{ (\partial_x M_2)^2 + (\partial_y M_2)^2 + (\partial_x M_3)^2 + (\partial_y M_3)^2 \right\},$$

and the first-order time derivative of the conserved moments are:

$$\partial_t M_1 = 0,$$

$$\partial_t M_2 = -\partial_x \left( \frac{1}{2} M_5^{(1)} + \frac{1}{30} M_8^{(1)} - \frac{1}{5} M_9^{(1)} \right) - \partial_y M_4^{(1)},$$

$$\partial_t M_3 = -\partial_x M_4^{(1)} - \partial_y \left( \frac{1}{2} M_5^{(1)} + \frac{1}{30} M_8^{(1)} - \frac{1}{5} M_9^{(1)} \right).$$

These equations shows that the viscous term and the subgrid term both appear as the $O(Kn)$ contribution. We remind that no assumption was made about relative magnitude of the subgrid term as compared with the viscous terms. The only requirement that is set on the subgrid scale term is that they appear at the viscous time scale rather than the time scale of the advection. We can write the complete hydrodynamics equation by using Eq. (31), Eq. (32), Eq. (33), Eq. (36), and Eq. (37) to obtain the hydrodynamics equations correct up to the order $O(Kn^2)$ (at this stage one recovers the Navier-Stokes equations using the unfiltered kinetic equation). In the next section, we shall see how the subgrid scale terms affect the Navier-Stokes description.
5 Hydrodynamic equations

The final set of hydrodynamics equation, valid up to the order $O(Kn^2)$ is:

$$
\begin{align*}
\partial_t \rho + \partial_x \rho u_x + \partial_y \rho u_y &= 0 \\
\partial_t \rho u_x + \partial_x \rho u_x + \partial_y \rho u_y &= 0 \\
\partial_t \rho u_y + \partial_x \rho u_y + \partial_y\rho u_y &= 0,
\end{align*}
$$

where

$$
\begin{align*}
\mathbf{P}_{xx} &= \left[ \mathbf{P} + \frac{\rho u_x^2}{p} - 2\nu \rho S_{xx} \right] + P^{SG}_{xx}, \\
\mathbf{P}_{xy} &= \left[ \frac{\rho u_x \rho u_y}{p} - 2\nu \rho S_{xy} \right] + P^{SG}_{xy}, \\
\mathbf{P}_{yy} &= \left[ \mathbf{P} + \frac{\rho u_y^2}{p} - 2\nu \rho S_{yy} \right] + P^{SG}_{yy},
\end{align*}
$$

with $\mathbf{P} = \rho c_s^2$, as the thermodynamic pressure and

$$
P^{SG}_{\alpha\beta} = \frac{KnL^2 p}{12} \left[ S_{\alpha\gamma} - \Omega_{\alpha\gamma} \right] \left[ S_{\gamma\beta} + \Omega_{\gamma\beta} \right] = \frac{\nu p L}{12 c_s} \left[ S_{\alpha\gamma} - \Omega_{\alpha\gamma} \right] \left[ S_{\gamma\beta} + \Omega_{\gamma\beta} \right].
$$

Thus, we have obtained a closed set of hydrodynamics equations, for appropriate choice of filtering width. This set of equations, written in the nondimensional form up to the order, $u^2$ is:

$$
\partial_t \bar{u}_\alpha = 0,
$$

$$
\begin{align*}
\partial_t (\bar{u}_\alpha) + \partial_\beta (\bar{u}_\alpha \bar{u}_\beta) &= -\partial_\alpha P + 2 K n \partial_\beta \left( S_{\alpha\beta} \right) \\
&- \frac{Kn}{12} \partial_\beta \left\{ (S_{\alpha\gamma} - \Omega_{\alpha\gamma}) (S_{\gamma\beta} + \Omega_{\gamma\beta}) \right\}.
\end{align*}
$$

Note that the pressure appearing in the momentum equation is not the thermodynamic pressure anymore, but needs to be computed from the incompressibility condition (Eq. (40) [15]). Significance of the Knudsen number appearing in the equation (41) is explained below in section 6.

Similar to the case of the Navier-Stokes equation, the subgrid model (5) enjoys the consistent derivation from the kinetic theory. We should remind here again
that the result is independent of the particular kinetic model used for the derivation. Any kinetic model which recovers the Navier-Stokes equations in the hydrodynamic limit will lead to the same result.

6 Discussion and conclusion

Now we shall summarise the results obtained in the present work and their limitations:

- It is possible to derive rigorously a coarse-grained closed set of equation for hydrodynamics, a long cherished goal in turbulence modeling.
- The scale-separation present in the kinetic theory provides a natural way to obtain coarse models.
- Arbitrary choice of filter-width is not allowed.
- In this work, we have shown that the operation of solving the Boltzmann equation (Chapman-Enskog expansion) and coarse-graining (filtering) do not commute. In the usual procedure of producing filtered hydrodynamic equation, the filtering is done on the solution of the Boltzmann equation (Navier-Stokes equations), which leads to closure problems. On the other hand, reversing the order of these two operations, provides a physical meaning to the filtering width and produces a closed set of equations in the hydrodynamic limit.
- As the smallest length scale needed to be resolved in the new set of equations is \( \Delta \sim Kn^{1/2} \sim Re^{-1/2} \), the cost of numerical computation reduces drastically as compared to the fully resolved simulation of the Navier-Stokes equations. We can get an estimate of this gain as follows: The smallest scale needed to be resolved in the numerical simulation is proportional to the \( Re^{-1/2} \) rather than \( Re^{-3/4} \) (Kolmogorov scale). This changes the scaling of number of degrees of freedom in a three-dimensional simulation with \( Re \) from \( Re^{9/4} \) to \( Re^{3/2} \) (number of grid point is \( \propto \delta x^{-3} \), where \( \delta x \) is the grid spacing). Further, a rough estimate of the scaling of the cost of time integration with \( Re \) is \( Re^{3/4} \) (number of time steps is \( \propto \delta x^{-1} \)) in the case of fully resolved simulation of the Navier-Stokes equations [1]. However, in the present case this scaling will be \( Ma^{-1} \). This happens because any numerical scheme has to take a time-step dictated by the sound speed (or an analog of it pertinent to the discretization in time chosen). Thus the scaling of the total cost of computation with the \( Re \) changes from \( Re^{3} \) for the Navier-Stokes equations to \( Re^{3/2} \) for the present equation.
- In the above estimation, the Mach number \( Ma \) appearing in the equation for the filter-width \( \Delta \) (\( \Delta^2 \propto Re^{-1} \)) was not taken into the account. This is justified as long as \( Re \) is sufficiently large and the Mach number \( Ma \) is not zero. An acceptable limit for the incompressible limit of the Navier-Stokes equation is \( Ma \sim 0.1 \) (for example, most of the lattice-Boltzmann
simulations of the incompressible Navier-Stokes uses $Ma \sim 0.05 - 0.1$.
Let us consider the case when the number of grid points in each direction
is 1024, then a fully resolved simulation of the Navier-Stokes equations is
possible by taking the Reynolds number as $Re \sim O(10^4)$, while a fully
resolved simulation using the present subgrid model is possible by taking
the Reynolds number as $Re \sim O(10^5)$, for $Ma \sim 0.07$.

- One interpretation of the subgrid scale terms is that the removal of the
small-scales in the kinetic picture appears naturally as the force term. As the
extra terms appearing in the evolution equations for non-conserved variables
can also be generated in the unfiltered kinetic equation by an appropriate
choice of the external force field (dependent on the position as well as molec-
ular velocity). Thus at least formally, we can find a force-field which will
act like a filter and remove the small scales of motion present in the kinetic
equation. Thus the physical meaning of the filtering (a purely mathemati-
cal operation) at the kinetic level is the application of some self-consistent
mean-field force which removes the small scale of the motions from the ki-
netic equation. The technical advantage of the search for a mean-field force
(appearing in the filtered kinetic equation), rather than an effective viscos-
ity term (attempts to absorb subgrid scale contributions in the viscous term
of the Navier-Stokes equations) is that the one does not have to deal with
the difficult question of what to do with the nonlinearity and nonlocality
present in the convective term of the Navier-Stokes equations.

Finally, let us mention some further possible directions of study:

- From a practical standpoint, a major goal of going beyond a Navier-Stokes-
based coarse graining, is to make a (filtered) kinetic theory work at possibly
large ratios $\Delta/L$. Indeed, successful kinetic subgrid models have been
known empirically for some time [14]. However, it is unclear why kinetic
subgrid scale models work better than models of the Navier-Stokes equa-
tions (for example, a recent comment on the kinetic models of turbu-
ence was: “Whether the approach can be supported by rigorous theory remains
to be shown” [16]). Our analysis shows that everything is eventually ruled
by the smallness of the Knudsen number, a well defined smallness param-
eter present in the kinetic theory. This is the first rigorous step in the ki-
netic modeling of the turbulence. For example, the choice of the filter-width
(2), based on the integer-power (standard) Chapman-Enskog analysis is a con-
servative estimate only. In order to achieve a subgrid model between
the advection time scale ($Kn^0$) and the viscosity time scale ($Kn^1$), that is,$$
\Delta/L \sim Kn^\gamma$$
with $0 < \gamma < 1/2$ requires a generalization of the Chapman-
Enskog method to noninteger series expansion in Knudsen number. This
interesting possibility needs to be studied separately. The application of
the method of the invariant manifold [17], which does not require Knudsen
number $Kn$ to be small, on the filtered kinetic equation for $0 < \gamma < 1/2$
is a possible extensions of the present work. The possibility of doing exact
Chapman-Enskog expansion [18,19], also need to be investigated further. Another possible extensions is the use of “renormalization-group” ideas by applying several filters of increasing filter-widths.

- When the discrete-velocity kinetic theory of section (2) is appropriately discretized in time and space, one arrives at the so-called entropic lattice Boltzmann method [2,3] (ELBM). In the ELBM, the thermodynamic stability (Boltzmann’s $H$-theorem) is maintained by the discrete-time $H$-theorem [20,21,22,23] which results in unconditionally stable simulation algorithm for hydrodynamics. It was argued [21] that ELBM is a built-in subgrid model. It would be interesting therefore to establish a closer relation between ELBM and the present theory.

- Filtering the kinetic equations as above can be applied to a wide class of kinetic theories with a well-defined separation of time scales enrich existing resolved macroscopic models with physically sound subgrid contribution (for example, the kinetic equations for the granular flows [24]).

To conclude, the presented coarse-grained equations are the first rigorously derived subgrid model. Effectiveness of the model in practice needs to be investigated further numerically. Work in this direction is currently in progress.

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