Consistent subgrid scale modelling for lattice Boltzmann methods

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The lattice Boltzmann method has become a widely used tool for the numerical simulation of fluid flows and in particular of turbulent flows. In this frame the inclusion of subgrid scale closures is of crucial importance and is not completely understood from the theoretical point of view. Here, we propose a consistent way of introducing subgrid closures in the BGK Boltzmann equation for large eddy simulations of turbulent flows. Based on the Hermite expansion of the velocity distribution function, we construct a hierarchy of subgrid scale terms, which are similar to those obtained for the Navier–Stokes equations, and discuss their inclusion in the lattice Boltzmann method scheme. A link between our approach, with the standard way on including eddy viscosity models in the lattice Boltzmann method is established. It is shown that the use of a single modified scalar relaxation time to account for subgrid viscosity effects is not consistent in the compressible case. Finally, we validate the approach in the weakly compressible case by simulating the time developing mixing layer and comparing with experimental results and direct numerical simulations.

Key words: Lattice Boltzmann method, Large-Eddy Simulation, Turbulence, Mixing layer, Kinetic theory

1. Introduction

Turbulent flows are present in many engineering applications, such as flows past cars or aircrafts, and their study is of primary importance for the design of such devices. The range of scales involved in the evolution of efficient systems is so wide that their direct numerical resolution becomes rapidly intractable for even the most powerful computers. A possible workaround for still being able to simulate such complex flows lies in the large eddy simulation (LES) class of techniques, where the larger scales are simulated while the smallest are modelled.

Many models have been proposed within the Navier–Stokes framework (see Sagaut (2005); Sagaut et al. (2006)), since closing the momentum equations is observed to be a very difficult task. Calibration of the model by tuning arbitrary parameters it contains necessitates to account for both filter and flow features, e.g. Meyers et al. (2006); Meyers & Sagaut (2006), and also numerical discretization Meyers et al. (2007). Multiphysics models have been developed during the past decades, e.g. to account for heat transfer Labbé et al. (2002) or noise generation Seror et al. (2001). Increasing efficiency of LES by combining it with multiresolution techniques, e.g. Quéméré et al. (2001, 2002), is

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It appears that subgrid closures within the lattice Boltzmann method (LBM) framework are almost exclusively limited to eddy viscosities models, only very few non-eddy-viscosity closures having been proposed Sagaut (2010); Malaspinas & Sagaut (2011). Furthermore, the vast majority of these LBM models are based on heuristic extrapolations of Navier–Stokes eddy viscosity models (see Hou et al. (1996); Eggels (1996); Filippova et al. (2001); Krafczyk et al. (2003); Kerimo & Girimaji (2007); Dong et al. (2008); Premnath et al. (2009); Chen (2009); Weickert et al. (2010) among others), by simply adding an efficient relaxation time in the collision operator. All these models are only valid in the weakly compressible limit while, the lattice Boltzmann method can in principle also be applied to fully compressible flows (see Nie et al. (2008); Scagliarini et al. (2010b,a); S. et al. (2010)).

Only a handful of papers propose alternative approaches. Among others, Chen et al. (1999) apply the renormalization group theory to the BGK Boltzmann equation and derive a subgrid scale viscosity model. Then Chen et al. (2003) propose an efficient way of modelling turbulence with an extended Boltzmann equation. In Chen et al. (2004) the authors carry the Chapman–Enskog expansion up to the second order and show a similarity between the subgrid stress tensor and non-linear $k − \varepsilon$ models. In Ansumali et al. (2004) a turbulence model based on kinetic theory is derived and a link with Smagorinsky like models is made. Finally, in Girimaji (2007) a subgrid scale closure for the filtered Boltzmann equation in the weakly compressible limit is presented and applied to the Smagorinsky model.

In the present paper we propose a consistent a priori approach for including subgrid scale closures to the lattice Boltzmann method (Chen & Doolen (1998); Wolf-Gladrow (2000); Succi (2001); Shau et al. (2006); Aidun & Clausen (2010) for complete references on the LBM), by applying the filtering procedure proposed by Leonard (1974). This approach allows to explicitly express the subgrid scale tensors to be modelled and provide a formula to include them into the model. We also show that the standard approach, which consists in modifying the relaxation time locally, holds as long as the Chapman–Enskog expansion commutes with the filtering operation. Furthermore, modifying the relaxation time locally can induce complications when computing the strain rate tensor directly from the distribution functions. We give an explicit formula for computing it in the case of a Smagorinsky model. Our approach is finally applied on the time developing mixing layer and it is shown to give results that are in good agreement with the DNS results of Rogers & Moser (1994).

We point out, that although our paper is focused on large eddy simulation in the lattice Boltzmann method framework, it does not deal with kinetic theory approaches to model turbulence. It rather shows how to include consistently existing Navier–Stokes models in the BGK Boltzmann equation.

The paper is organized as follows. In Section 2 we introduce the notations to be used in the paper by shortly reminding the basics of the filtering procedure for the incompressible Navier–Stokes equations. Then the macroscopic limits of the BGK equation are presented and then the standard way of including eddy viscosity models in the BGK is presented, in Section 3. In Section 4 the consistent inclusion of subgrid closures is described. The link between our approach and the classical existing “eddy relaxation time” is made in Section 5. Then an accurate way of computing the strain rate tensor from the distribution function for Smagorinsky-like models is shown in Section 6. In Section 7 the developments of Sections 4-6 are validated on the time developing mixing layer benchmark. Finally this work is concluded in Section 8.
2. Reminder: the filtered Navier–Stokes equations

It is recalled that LES consists essentially in solving governing equations for flow motion on a grid which is too coarse to capture small scales of the exact flow solution. In order to write governing equations for this truncated problem, one needs to mimic this removal of small scales. Physical intuition leads to the idea that the solution computed on the coarse grid is smoother than the exact solution. From classical signal processing theory, this smoothing of the solution can be modelled as a application of a regularizing filter to the exact solution.

We first remind the filtering techniques inspired by the work of Leonard (1974) for the Navier–Stokes equations, in order to introduce the notations and understand the procedure that will be applied to the the BGK equation afterwards.

With $G$ an homogeneous convolution filter kernel, and denoting the filtered counterpart of any quantity, $a$, as

$$\tilde{a} \equiv G * a = \int_{-\infty}^{\infty} G(x - y) a(y) \, dy,$$

one can write the filtered incompressible Navier–Stokes equations as

$$\nabla \cdot \tilde{u} = 0,$$

$$\rho \left( \partial_t \tilde{u} + (\tilde{u} \cdot \nabla) \tilde{u} \right) = -\nabla \tilde{p} + 2\nabla \cdot (\mu S) - \nabla \cdot T,$$

where $\mu = \rho \nu$ is the dynamic viscosity and where $\nu$ the kinematic viscosity, $\tilde{S} \equiv (\nabla \tilde{u} + (\nabla \tilde{u})^T)/2$ is the filtered strain rate tensor, $\tilde{u}$ and $\tilde{p}$, respectively, the filtered velocity and pressure, and $T$ is the subgrid stress tensor defined as

$$T \equiv \tilde{u} \tilde{u} - \tilde{u} \tilde{u}.$$

The appearance of the subgrid scale stress tensor is due to the fact that the filtering operation does not commute with the non-linear term of the Navier–Stokes equation. This term, which cannot be computed exactly, needs to be modelled. One very common class of models for the subgrid scale (SGS) stress tensor consists of assuming that $T = -2\mu_{\text{sgs}} \tilde{S}$ (Boussinesq approximation), where $\mu_{\text{sgs}}$ is the subgrid scale viscosity which for example in Smagorinsky (1963) is proportional to the norm of the filtered strain rate tensor,

$$||\tilde{S}|| \equiv \sqrt{2\pi (\tilde{S} \cdot \tilde{S})}$$

and is given by $\mu_{\text{sgs}} = \rho(C\Delta)^2 ||\tilde{S}||$ ($C$ being the Smagorinsky constant and $\Delta$ the filter width).

The momentum conservation equation (2.3) can thus be rewritten as

$$\rho \left( \partial_t \tilde{u} + (\tilde{u} \cdot \nabla) \tilde{u} \right) = -\nabla \tilde{p} + 2\nabla \cdot (\mu_{\text{eff}} \tilde{S}),$$

where $\mu_{\text{eff}}$ is the efficient viscosity defined as

$$\mu_{\text{eff}} \equiv \mu + \mu_{\text{sgs}}.$$

3. Subgrid scale closures of the Boltzmann BGK equation

In this section, we first introduce very shortly the Boltzmann-BGK equation (for Bhatnagar, Gross and Krook, see Bhatnagar et al. (1954)). Then we provide the basic steps used in the lattice Boltzmann framework in order to recover the Navier–Stokes-like macroscopic limits of the BGK equation. Finally we present the standard way of including eddy viscosity closure models in this framework (see Hou et al. (1996); Krafczyk et al. (2003) among others).
3.1. The BGK equation and its macroscopic limit

The Boltzmann equation describes the time evolution of the velocity density probability distribution \( f(x, \xi, t) \) of finding a particle with velocity \( \xi \) at position \( x \) and time \( t \) in terms of particle collisions only, and reads in absence of a force as

\[
\partial_t f(x, \xi, t) + (\xi \cdot \nabla)f(x, \xi, t) = \Omega(f),
\]

(3.1)

where \( \Omega \) is the collision operator. The macroscopic fields such as the density \( \rho \), the velocity \( u \), the stress tensor \( P \), the temperature \( \theta \) (actually the temperature times the Boltzmann constant), the internal energy \( \varepsilon \) and the internal energy flux \( q \) are given by the following moments of the distribution function

\[
\rho = \int f(x, \xi, t) \, d\xi,
\]

(3.2)

\[
\rho u = \int \xi f(x, \xi, t) \, d\xi,
\]

(3.3)

\[
P = \int c c f(x, \xi, t) \, dc,
\]

(3.4)

\[
\rho \theta = 2 \frac{D \rho \varepsilon}{D} = \frac{1}{D} \int c^2 f(x, \xi, t) \, dc,
\]

(3.5)

\[
q = \frac{1}{2} \int c^2 c f(x, \xi, t) \, dc,
\]

(3.6)

where \( c = \xi - u \) is the microscopic velocity in the co-moving frame and \( D \) is the dimension of the momentum space. The most widely used model for computational fluid dynamics for the collision operator is the BGK, single relaxation time approximation, in which the Boltzmann equation reads

\[
\partial_t f(x, \xi, t) + (\xi \cdot \nabla)f(x, \xi, t) = -\frac{1}{\tau} \left( f(x, \xi, t) - f^{(0)}(\rho, u, \theta) \right),
\]

(3.7)

where \( \tau \) the relaxation time, and \( f^{(0)} \) is the local Maxwell–Boltzmann equilibrium distribution function, in non-dimensional units,

\[
f^{(0)} = \frac{\rho(x, t)}{(2\pi \theta(x, t))^{D/2}} \exp \left( -\frac{(u(x, t) - \xi)^2}{2\theta(x, t)} \right).
\]

(3.8)

Here, our approach stops following kinetic theory textbooks. Since we are interested in numerically solving Eq. (3.7) in an efficient fashion that nevertheless represents accurately continuum fluid flows, certain simplifications will be made. In particular instead of considering the complete form of the Maxwell–Boltzmann distribution function, only a polynomial approximation will be used.

Following an idea by Grad (1949b) (or Shan et al. (2006) for the original use of this expansion in this framework), one can expand the distribution functions \( f \) and \( f^{(0)} \), in Hermite polynomials up to an arbitrary order \( N \) (see Grad (1949a) for a summary on Hermite polynomials)

\[
f^N = w(\xi) \sum_{n=0}^{N} \frac{1}{n!} \mathcal{H}(\xi)^{(n)} : a^{(n)},
\]

(3.9)

\[
f^{(0)}^N = w(\xi) \sum_{n=0}^{N} \frac{1}{n!} \mathcal{H}(\xi)^{(n)} : a_0^{(n)},
\]

(3.10)

where the column symbol “:\)” stands for the full index contraction, \( w(\xi) = \exp(-\xi^2/2) \),
\( \mathcal{H}^{(n)}, a^{(n)} \) and \( a^{(n)}_0 \), the Hermite polynomial and coefficients of \( f \) and \( f^{(0)} \) of degree \( n \) respectively. From now on, we will always omit the superscript \( N \) and assume that the distribution function (and its equilibrium counterpart) is represented by its approximate form in terms of Hermite polynomials up to an arbitrary order \( N \) except when explicitly stated otherwise. The equilibrium coefficients can easily be computed and are found to be up to order \( N = 4 \)

\[
\begin{align*}
 a^{(0)}_0 &= \rho, \\
 a^{(1)}_{0\alpha} &= \rho u_\alpha, \\
 a^{(2)}_{0\alpha\beta} &= \rho u_\alpha u_\beta + \rho(\theta - 1)\delta_{\alpha\beta}, \\
 a^{(3)}_{0\alpha\beta\gamma} &= \rho u_\alpha u_\beta u_\gamma + \rho(\theta - 1)(\delta_{\alpha\beta} u_\gamma + \delta_{\alpha\gamma} u_\beta + \delta_{\beta\gamma} u_\alpha), \\
 a^{(4)}_{0\alpha\beta\gamma\delta} &= \rho u_\alpha u_\beta u_\gamma u_\delta + \rho(\theta - 1)^2(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) \\
 &\quad + \rho(\theta - 1)(\delta_{\alpha\beta} u_\gamma u_\delta + \delta_{\alpha\gamma} u_\beta u_\delta + \delta_{\beta\gamma} u_\alpha u_\delta) \\
 &\quad + \rho(\theta - 1)^2(\delta_{\alpha\beta}\delta_{\gamma\delta} u_\epsilon + \delta_{\alpha\gamma} u_\delta u_\epsilon + \delta_{\beta\gamma} u_\alpha u_\epsilon).
\end{align*}
\]  

In order to recover the macroscopic equations of motion related with the BGK equation, one must take moments of Eq. (3.7). By taking the moments related with density (order zero), moment (order one) and energy (trace of order two) of this equation, one gets after some algebra and the use of Eqs. (3.2)-(3.6) and (3.11)-(3.13)

\[
\begin{align*}
 \partial_t \rho + \nabla \cdot (\rho u) &= 0, \\
 \partial_t (\rho u) + \nabla \cdot (\rho uu) + \nabla \cdot P &= 0, \\
 \rho (\partial_t \epsilon + u \cdot \nabla \epsilon) + P : (\nabla u) + \nabla \cdot q &= 0.
\end{align*}
\]  

These equations are only obtained under the assumption of mass, momentum and energy conservation respectively \( \int \Omega = \int \Omega = \int \Omega = 0 \), or in other terms

\[
\begin{align*}
 \int \Omega \int \xi (f - f^{(0)}) \, d\xi &= 0, & \text{Mass conservation} \\
 \int \Omega \int \xi (f - f^{(0)}) \, d\xi &= 0, & \text{Momentum conservation} \\
 \int \Omega \int \xi^2 (f - f^{(0)}) \, d\xi &= 0. & \text{Energy conservation}
\end{align*}
\]

The momentum and energy conservation still need to be closed (a constitutive equation must be found for \( P \) and \( q \)). In order to do so, one can use the Chapman–Enskog expansion (see Chapman & Cowling (1960); Huang (1987); Malaspinas (2009)). Although this expansion is not related with the Hermite expansion (and that the Hermite expansion is not a prerequisite we will discuss the Chapman–Enskog expansion in this frame here, because the polynomial expansion is used in Subsection 4.4 for discretization purposes).

The Chapman–Enskog expansion is based on the assumption that the distribution function \( f \) is assumed to be given by its equilibrium value \( f^{(0)} \) plus a small perturbation

\[
f = f^{(0)} + f^{(1)},
\]

where the equilibrium distribution is assumed to be given by Eq. (3.10), the perturbation, \( f^{(1)} \sim O(\text{Kn}) \ll 1 \), is of the order of the Knudsen number, \( \text{Kn} \). The derivation presented here is not the standard way that can be found in the literature and rather follows Huang (1987).

Replacing this Chapman–Enskog ansatz in Eq. (3.7), one obtains at the lowest order

\[
\partial_t f^{(0)} + (\xi \cdot \nabla) f^{(0)} = -\frac{1}{\tau} f^{(1)}. \tag{3.23}
\]
Multiplying this equation by 1, $\xi$ and $\xi^2/2$ and integrating over the microscopic velocity, and using the mass, momentum and energy conservation constrains on each equation respectively ($\int f^{(1)} = \int \xi f^{(1)} = \int \xi^2 f^{(1)} = 0$), one gets the inviscid Euler equations for mass, momentum and energy conservation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0,$$

(3.24)

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p = 0,$$

(3.25)

$$\rho (\partial_t \varepsilon + \mathbf{u} \cdot \nabla \varepsilon) + (p I) : (\nabla \mathbf{u}) = 0,$$

(3.26)

where $p = \rho \theta$ is the perfect gas law.

The stress tensor and the internal energy flux can be decomposed in their Chapman–Enskog counterparts

$$P = P^{(0)} + P^{(1)} = \rho \theta I + P^{(1)}, \quad q = q^{(0)} + q^{(1)} = \xi q^{(1)},$$

(3.27)

where $P^{(j)} = \int c c f^{(j)}$ and $q^{(j)} = \int c^2 c f^{(j)}/2$ for $j = 0, 1$ ($j$ corresponding to the Chapman–Enskog expansion order), and $q^{(0)} = 0$. Thus we are left with the computation of $P^{(1)}$ and $q^{(1)}$ which for simplicity are computed thanks to the Hermite expansion of the distribution function. Let us define $a^{(n)}_1$ the Hermite coefficient of order $n$ of the off-equilibrium distribution function $f^{(1)}$

$$f^{(1)} = \mathcal{H}(\xi) \sum_{n=0}^{N} \frac{1}{n!} \mathcal{H}(\xi)^{(n)} : a^{(n)}_1,$$

(3.28)

and express $P^{(1)}$ and $q^{(1)}$ in terms of these Hermite coefficients

$$P^{(1)}_{\alpha \beta} = a^{(2)}_{1 \alpha \beta},$$

(3.29)

$$q^{(n)} = \frac{1}{2} \left( a^{(3)}_{1 \alpha \beta \gamma} - 2 a^{(2)}_{1 \alpha \beta} u_\beta - a^{(2)}_{1 \beta \gamma} u_\alpha \right),$$

(3.30)

where we used that by construction $a^{(0)}_1 = a^{(1)} = 0$. Then projecting Eq. (3.23) on the Hermite basis, it follows that

$$\partial_t a^{(n)}_0 + \nabla \cdot a^{(n+1)}_0 + \left( \nabla a^{(n-1)}_0 + \text{perm} \right) = -\frac{1}{\tau} a^{(n)}_1,$$

(3.31)

where “perm” stands for all the cyclic index permutations. For $n = 2$ this equation becomes

$$\partial_t a^{(2)}_0 + \nabla \cdot a^{(3)}_0 + \left( \nabla a^{(1)}_0 + \text{perm} \right) = -\frac{1}{\tau} a^{(2)}_1,$$

$$\partial_t \left[ \rho \mathbf{u} u + \rho (\theta - 1) I \right] + \nabla \cdot \left[ \rho \mathbf{u} u + \rho (\theta - 1) (\mathbf{u} I + \text{perm}) \right]$$

(3.32)

$$+ \left[ \nabla (\rho \mathbf{u}) + (\nabla (\rho \mathbf{u}))^T \right] = -\frac{1}{\tau} a^{(2)}_1.$$

By using Eqs. (3.24)-(3.26) to eliminate the time derivative terms, this equation can be rewritten (after some tedious algebra that can be found in Malaspinas (2009)) as

$$a^{(2)}_1 = P^{(1)} = -2 \tau \rho \theta \Lambda,$$

(3.33)

where

$$\Lambda = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{D} I \nabla \cdot \mathbf{u} \right).$$

(3.34)

For the evaluation of $q^{(1)}$, one uses Eq. (3.31) with $n = 3$

$$\partial_t a^{(3)}_0 + \nabla \cdot a^{(4)}_0 + \left( \nabla a^{(2)}_0 + \text{perm} \right) = -\frac{1}{\tau} a^{(3)}_1.$$

(3.35)
By using again Eqs. (3.24)-(3.26) to eliminate the time derivatives in this equation (and even more tedious algebra than before that can also be found in Malaspinas (2009)) gives the constitutive equation for the internal energy flux

\[ q^{(1)} = -\tau \rho \theta \left( \frac{D+2}{2} \right) \nabla \theta. \]  

(3.36)

By comparing Eq. (3.33) and (3.36) with the Navier–Stokes equations, the transport coefficients \( \mu \) and \( \kappa \) (the thermal diffusivity) can be identified with the relaxation time through the following relations

\[ \mu = \kappa = \rho \theta \tau. \]  

(3.37)

Finally the motion equations obtained are the thermal, compressible Navier–Stokes equations

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0, \]  

(3.38)

\[ \partial_t (\rho u) + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot (2\mu \Lambda), \]  

(3.39)

\[ \rho \left( \partial_t \varepsilon + u \cdot \nabla \varepsilon \right) + (pI - 2\mu \Lambda) : (\nabla u) = \left( \frac{D+2}{2} \right) \nabla \cdot (\kappa \nabla \theta). \]  

(3.40)

This derivation has been done in the case where \( \tau \) is a constant, but all this remains valid even for a relaxation time is depending on space and time, as long as it is independent of \( \xi \) (the moments of the distribution is only performed in the microscopic velocity space). Furthermore, as can be seen from Eq. (3.37), only fluids with equal viscosity and diffusivity can be modelled, furthermore no bulk viscosity is present. This is easily understandable since the BGK model only contains one transport coefficient. To be able to circumvent this defect one can go to multiple relaxation time models such as the one presented in Shan & Chen (2007).

When one is interested in the Navier–Stokes limit of this truncated BGK equation, all these computations are exact as long as the distribution function is expanded in Hermite polynomials up to order \( N \geq 4 \). If \( N = 3 \), the general form of the energy equation is preserved, but the Hermite coefficient \( a^{(4)} \) in Eq. (3.35) vanishes and therefore spurious terms are introduced in \( q^{(1)} \) and it is not anymore proportional to the temperature gradient. Nevertheless the constitutive equation for the deviatoric stress remains unchanged. The macroscopic equations are therefore

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0, \]  

\[ \partial_t (\rho u) + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot (2\mu \Lambda). \]  

In the case where \( f \) is expanded up to order \( N = 2 \), the energy equation does not have the correct form anymore since \( a_0^{(3)} \) is null. The momentum conservation equation is still of the correct form, but the deviatoric stress tensor \( P^{(1)} \) will not be given by Eq. (3.34) but rather by

\[ P^{(1)} = -2\tau \rho \theta S, \]  

(3.41)

where \( S = (\nabla u + (\nabla u)^T)/2 \) and therefore this limit is valid only for weakly compressible flows where \( \nabla \cdot u \equiv 0 \) (the complete calculation of the error terms can be found in Malaspinas (2009)). Furthermore, in this case, the temperature is fixed a-priori at \( \theta = 1 \) and therefore the temperature is completely absent, but it is kept here for consistency, and finally one has the following macroscopic equation

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0, \]  

\[ \partial_t (\rho u) + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot (2\mu S). \]
Finally at the order \( N = 1 \) an approximate advection–diffusion is recovered if no momentum conservation is imposed \((\int \xi f \, d\xi \neq \int \xi f^{(0)} \, d\xi)\), and the associated macroscopic equation is found to be
\[
\partial_t \rho + \nabla \cdot (\rho u) = \nabla \cdot (\kappa \nabla \rho).
\]
(3.42)

All these macroscopic limits limits are summarized in Table 1 along with the conservation laws that are enforced in the computations.

The terms of order \( N > 3 \) in the Hermite series of the distribution function are relevant only when one is interested in having the viscous (diffusive) effects contained in these equations. When one only considers perfect fluids (Euler equations) going to a Hermite expansion order of \( N = 4 \) is not relevant as can be seen from Eqs. (3.24)-(3.26).

### 3.2. Heuristic eddy viscosity subgrid scale model

In order to include an eddy viscosity model in the BGK equation, a simple heuristic way (inspired by Navier–Stokes models, see Eq. (2.6)) consists of replacing the relaxation time \( \tau \) by its efficient counterpart \( \tau_{\text{eff}} \)
\[
\mu_{\text{eff}} = \mu + \mu_{\text{sgs}} = \rho \theta \tau + \rho \theta \tau_{\text{sgs}} = \rho \theta \tau_{\text{eff}},
\]
(3.43)

where in the second equality Eq. (3.37) was used. The SGS relaxation time is then straightforwardly computed through the relation
\[
\tau_{\text{sgs}} = \mu_{\text{sgs}} / (\rho \theta).
\]
(3.44)

Replacing \( \tau \) by \( \tau_{\text{eff}} \) in the BGK equation one therefore solves asymptotically the Navier–Stokes equations with an efficient viscosity model. This procedure is based on the assumption that the non-filtered BGK equation with an efficient relaxation time will represent correctly the filtered Navier–Stokes with the corresponding efficient viscosity. This statement is not true in general, but we will show in the Section 5 that up to a certain order of approximation this result is obtained by an \textit{a priori} analysis.

### 4. Consistent subgrid scale closure for the BGK equation

#### 4.1. The filtered BGK equation

Inspired by Leonard’s procedure for filtering the Navier–Stokes equations, one can write the filtered Boltzmann equation as
\[
\partial_t \overline{f} + (\xi \cdot \nabla) \overline{f} = \overline{\Omega(f)},
\]
(4.1)

where the filtering operation does not commute with the collision operator because of its non-linear character
\[
\overline{\Omega(f)} \neq \Omega(\overline{f}).
\]
(4.2)
Consistent subgrid scale modelling for LBM

The filtered Boltzmann equation can be rewritten as

$$\partial_t \tilde{f} + (\xi \cdot \nabla) \tilde{f} = \Omega(\tilde{f}) + \mathcal{R},$$  \hfill (4.3)

where $\mathcal{R} \equiv \overline{\Omega(f)} - \Omega(\tilde{f})$ corresponds to the subgrid term that has to be modelled.

Replacing $\Omega$ by the popular BGK collision operator, presented in the previous section (see Eq. (3.7)), one can rewrite this last equation as

$$\partial_t \tilde{f} + (\xi \cdot \nabla) \tilde{f} = -\frac{1}{\tau}(\tilde{f} - f^{(0)}(\tilde{f})) + \frac{1}{\tau}(\overline{f^{(0)}} - f^{(0)}(\tilde{f})),$$  \hfill (4.4)

where the constant $\tau$ is the relaxation time, $\overline{f^{(0)}}$ is the filtered Maxwell–Boltzmann equilibrium distribution and $f^{(0)}(\tilde{f})$ the equilibrium distribution function of the filtered macroscopic quantities. These computable macroscopic moments are discussed in more details in the next subsection.

Replacing $f^{(0)}$ by its Hermite expansion (see Eq. (3.10)) one can explicitly evaluate, order by order, the second term in the r.h.s. of Eq. (4.4)

$$\mathcal{R} = \frac{1}{\tau}(\tilde{f} - f^{(0)}(\tilde{f})) = \frac{w(\xi)}{\tau}\left\{\sum_{n=0}^{N} \frac{1}{n!} \mathcal{H}^{(n)} : \left[a_{0}^{(n)}(\rho, u, \theta) - a_{0}^{(n)}(\bar{\rho}, \tilde{u}, \tilde{\theta})\right]\right\},$$  \hfill (4.5)

where the “computable” velocity $\tilde{u}$ and temperature $\tilde{\theta}$ were defined as (see also Subsection 4.2 for a more detailed discussion of filtered moments evaluation)

$$\tilde{u} \equiv \frac{\bar{\rho} \tilde{u}}{\bar{\rho}},$$

$$\tilde{\theta} \equiv \frac{1}{\bar{\rho}} \left(\frac{1}{D} \int c^2 \tilde{f} \, dc\right),$$

with $c \equiv \xi - \tilde{u}$.

Defining $\mathcal{R}^{(n)} \equiv a_{0}^{(n)}(\rho, u, \theta) - a_{0}^{(n)}(\bar{\rho}, \tilde{u}, \tilde{\theta})$ we find up to order $N = 4$ (the order corresponding to compressible and thermal fluids)

$$\mathcal{R}^{(0)} = 0,$$  \hfill (4.6)

$$\mathcal{R}^{(1)} = 0,$$  \hfill (4.7)

$$\mathcal{R}^{(2)}_{\alpha \beta} = T_{\alpha \beta} + \chi \delta_{\alpha \beta},$$  \hfill (4.8)

$$\mathcal{R}^{(3)}_{\alpha \beta \gamma} = \sigma_{\alpha \beta \gamma} + \delta_{\alpha \gamma} q_{\beta} + \delta_{\beta \gamma} q_{\alpha},$$  \hfill (4.9)

$$\mathcal{R}^{(4)}_{\alpha \beta \gamma \delta} = \pi_{\alpha \beta \gamma \delta} + (\delta_{\alpha \beta} \delta_{\gamma \delta} + \delta_{\alpha \gamma} \delta_{\beta \delta} + \delta_{\alpha \delta} \delta_{\beta \gamma}) (\varphi + 2\chi) + \delta_{\alpha \beta} \psi_{\gamma \delta} + \delta_{\alpha \gamma} \psi_{\beta \delta} + \delta_{\alpha \delta} \psi_{\beta \gamma} + \delta_{\beta \gamma} \psi_{\alpha \delta} + \delta_{\beta \delta} \psi_{\alpha \gamma} + \delta_{\gamma \delta} \psi_{\alpha \beta} - \delta_{\alpha \beta} T_{\gamma \delta} - \delta_{\alpha \gamma} T_{\beta \delta} - \delta_{\alpha \delta} T_{\beta \gamma} - \delta_{\beta \gamma} T_{\alpha \delta} - \delta_{\beta \delta} T_{\alpha \gamma} - \delta_{\gamma \delta} T_{\alpha \beta}.$$  \hfill (4.10)

Here we defined seven different SGS quantities

$$T_{\alpha \beta} = \overline{\rho \bar{u}_\alpha \bar{u}_\beta} - \bar{\rho} \bar{\bar{u}}_\alpha \bar{u}_\beta,$$  \hfill (4.11)

$$\chi = \overline{\rho \bar{\theta} - \bar{\rho} \tilde{\theta}},$$  \hfill (4.12)

$$\sigma_{\alpha \beta \gamma} = \overline{\rho \bar{u}_\alpha \bar{u}_\beta \bar{u}_\gamma} - \bar{\rho} \bar{\bar{u}}_\alpha \bar{u}_\beta \bar{u}_\gamma,$$  \hfill (4.13)

$$q_{\alpha} = \overline{\rho \bar{u}_\alpha - \bar{\rho} \tilde{\bar{u}}_\alpha},$$  \hfill (4.14)
\[ \pi_{\alpha\beta\gamma\delta} = \overline{\rho u_{\alpha} u_{\beta} u_{\gamma} u_{\delta}} - \overline{\rho \tilde{u}_{\alpha} \tilde{u}_{\beta} \tilde{u}_{\gamma} \tilde{u}_{\delta}}, \quad (4.15) \]

\[ \varphi = \overline{\rho \theta^2} - \overline{\tilde{\rho} \tilde{\theta}^2}, \quad (4.16) \]

\[ \psi_{\alpha\beta} = \overline{\rho \theta u_{\alpha} u_{\beta}} - \overline{\tilde{\rho} \tilde{\theta} \tilde{u}_{\alpha} \tilde{u}_{\beta}}, \quad (4.17) \]

where \( T, \chi \) and \( q \), in particular, are respectively the subgrid stress, subgrid temperature density and subgrid heat flux. \( \sigma, \pi, \phi \) and \( \psi \) are related to cubic and quartic subgrid stress diffusion fluxes, subgrid temperature variance and subgrid heat flux diffusion, respectively. Depending on the truncation order \( N \), one needs to model up to order \( N \) the different subgrid quantities, \( R^{(n)} \). It is remarkable that all the subgrid terms to be modelled are also present in LES closures in the Navier–Stokes framework, but are here projected on the Hermite basis. Although the SGS quantities are very similar in both Boltzmann BGK and compressible Navier–Stokes equations their nature is completely different. In the case of the Boltzmann equation they are resulting from the collision operator, while they find their origin in the inertial term in the Navier–Stokes equations. This difference might open a different kind of modelling for the BGK equation.

It is also worth noting that applying the filtering procedure to BGK equations yields a unique mathematical model for large-eddy simulation (i.e. an unclosed set of filtered governing equations for LES), while an infinite set of possible governing equations is found in the case of compressible Navier-Stokes equations (see Garnier et al. (2009) for a comprehensive discussion). Therefore, the use of BGK equations as a starting point to derive LES governing equations for compressible flows seems better suited. This can be understood reminding that macroscopic variables such as internal energy are non-linear functions of the distribution function \( f \), and that filtering Navier-Stokes equations is equivalent to first applying a non-linear operator to BGK equations before applying the linear filter.

In order to make a link with the classical way of introducing LES closures in the BGK equation, we want to rewrite Eq. (4.4) using a single relaxation time

\[ \partial_t \mathcal{F} + (\boldsymbol{\xi} \cdot \nabla) \mathcal{F} = -\frac{1}{\tau} \left( \mathcal{F} - f^{(0)}(\mathcal{F}) \right) + \frac{w(\boldsymbol{\xi})}{\tau} \sum_{n=2}^{N} \frac{1}{n!} \mathcal{H}^{(n)} : R^{(n)}, \quad (4.18) \]

\[ \partial_t \mathcal{F} + (\boldsymbol{\xi} \cdot \nabla) \mathcal{F} = -\frac{1}{\tau_{\text{eff}}} \left( \mathcal{F} - f^{(0)}(\mathcal{F}) \right), \quad (4.19) \]

where

\[ \tau_{\text{eff}} \equiv \frac{\tau}{1 - \frac{\sum_{n=2}^{N} \mathcal{H}^{(n)} : R^{(n)}}{\tau}}. \quad (4.20) \]

This result will be used in the following subsections.

It must be noted that although \( \tau_{\text{eff}} \) is explicitly depending on the microscopic velocities, the relaxation time of the fluid still remains constant. This term is written in this form to shorten the notations. This notation is used in Section 5 in order to make a link with the classical way used in the literature to include eddy viscosity models in the lattice Boltzmann method. From our point of view, this notation might lead to confusion, since in general the SGS terms \( R^{(n)} \) are rather source terms that are acting on moments of order \( N \geq 2 \) of the filtered Boltzmann BGK equation, or in other terms, on the stress, on the internal energy and the internal energy flux. Furthermore the can go beyond eddy viscosity models and any model derived for the filtered Navier–Stokes equations for the subgrid scale stress tensor (or any other subgrid scale term) can be used.
Consistent subgrid scale modelling for LBM

4.2. The filtered macroscopic moments

The evaluation of the filtered moments is not trivial and is discussed here. Since the filtered equations are written at the $f$-level, the resulting macroscopic variables, which are of interest in practical applications, must be reconstructed via an adequate post-processing. Therefore, the question arises of the identification of an equivalent filter for the macroscopic variables. In this section we will make a crucial difference between the macroscopic filtered quantities (which in general cannot be evaluated from the filtered distribution function) and their computable counterpart. From the Eqs. (3.2)-(3.5) we can write the filtered macroscopic moments

\[ \tilde{\rho} = \int f \, d\xi = \int d\xi \, \tilde{f}, \]  
\[ \rho u = \int \xi f \, d\xi = \int \xi \tilde{f} \, d\xi, \]  
\[ \mathcal{P} = \int c c f \, d\xi = \int \xi \tilde{f} \, d\xi - \int u \xi f \, d\xi - \int \xi u f \, d\xi + \int \xi u f \, d\xi, \]  
\[ \tilde{p} = \rho \tilde{\theta} = \frac{1}{D} \int \epsilon^2 f \, d\epsilon = \frac{1}{D} \left( \int \xi^2 \tilde{f} \, d\xi - 2 \int \xi \cdot \tilde{u} \, f \, d\xi + \int \tilde{u}^2 \tilde{f} \, d\xi \right). \]  

From these relations one easily deduces that the filtered density, momentum and total energy can be computed directly from the filtered distribution function, which is not the case for the stress tensor, the pressure, the temperature or even the velocity. One can rather evaluate the following quantities (there exists different ways of approximating them, and here we propose one)

\[ \tilde{P} = \int \tilde{c} \tilde{c} \tilde{f} \, d\xi, \]  
\[ \tilde{p} = \frac{1}{D} \int \epsilon^2 \tilde{f} \, d\epsilon, \]  

where the “computable” filtered velocity $\tilde{\epsilon}$ is given by

\[ \tilde{\epsilon} = \int \xi \tilde{f} \, d\xi \neq \left( \frac{\int \xi f \, d\xi}{\int f \, d\xi} \right) = \epsilon, \]  

with $\hat{c} \equiv \xi - \hat{u}$. From Eq. (4.26) one can deduce that the temperature $\hat{\theta}$ can only be computed approximatively as

\[ \hat{\theta} = \rho / \tilde{\rho}. \]  

It is very difficult to evaluate the difference between the exact filtered quantities and the computable ones. The error made on the velocity field, is only due to the subgrid term

\[ \Delta \epsilon = \epsilon - \hat{\epsilon}. \]  

For the stress tensor things become even more difficult, because the error is not only depending on the subgrid scale stress, but also on the error made on the filtered velocity field. In general, one can say that for each higher order moment the errors are due to the corresponding subgrid scale term and on the errors of all the lower order moments errors.
4.3. The collisional invariants of the filtered BGK equation

As seen in the previous subsection, the computation of the macroscopic quantities can become problematic when dealing with the filtered quantities. Similar difficulties may arise with the collisional invariants and therefore they are discussed here.

For simplicity we use the collision operator written in the form of Eqs. (4.4) and (4.5)

\[ \Omega(f) = -\frac{1}{\tau} \left( \mathcal{J} - f^{(0)}(\mathcal{J}) \right) + \frac{w(\xi)}{\tau} \left\{ \sum_{n=0}^{N} \frac{1}{n!} \mathcal{H}^{(n)} : \left[ a^{(n)}_0 (\rho, u, \theta) - a^{(n)} (\bar{\rho}, \bar{u}, \bar{\theta}) \right] \right\} \]  

From the discussion of the previous subsection and thanks to orthogonality of the Hermite polynomials it is trivial to show that the zeroth and first order invariants corresponding to mass and momentum conservation are indeed verified. For the energy conservation things become more complicated. Similarly to the stress tensor and pressure computation, the filtered energy density \( \rho \varepsilon \), defined as

\[ \rho \varepsilon = \frac{D}{2} \int c^2 f \, d\xi, \]

cannot be computed directly but similarly to Eq. (4.25) one can use the following definition

\[ \tilde{\varepsilon} = \frac{1}{2} \int c^2 f \, d\xi. \]

We want now to compute the corresponding moment of the collision operator. Let us first rewrite \( ||\xi - \bar{u}|| \) in terms of Hermite polynomials in order to allow us to use their orthogonality properties

\[ ||\xi - \bar{u}||^2 = ||\mathcal{H}^{(2)}|| + D - 2\xi \cdot \bar{u} + \bar{u}^2. \]

The internal energy change due to the collision becomes

\[ \frac{1}{2} \int ||\xi - \bar{u}||^2 \Omega(f) = -\frac{1}{\tau} \left( \rho u^2 \varepsilon - \bar{\rho} u^2 + D \left( \rho \theta - \bar{\rho} \bar{\theta} \right) \right) - T_{\alpha\alpha} - D\chi = 0. \]  

This last relation is a consequence of the invariance of the trace of the moment of order 2 of the distribution function and shows that although the internal energy density is a non-linear quantity that cannot be evaluated exactly by using filtered quantities has an “equivalent” computable counterpart, which remains a collisional invariant.

4.4. Discretizing the BGK equation

In order to simulate the BGK equation on a computer, the first step is to discretize the microscopic velocity space. To do so, one uses the standard microscopic velocity discretization (following the procedure by Shan et al. (2006); Nie et al. (2008)) where the Gauss–Hermite quadrature is used. The basic idea is that the discrete velocity set is chosen such that the continuous polynomials can be integrated exactly up to a certain order. The “velocity discretized” BGK equation can be rewritten in terms of a discrete velocity set \( \{\xi_i\}_{i=0}^{q-1} \)

\[ \partial_t f_i + (\xi_i \cdot \nabla) f_i = -\frac{1}{\tau} \left( f_i - f_i^{(0)}(\mathcal{J}) \right) + \frac{1}{\tau} w_i \sum_{n=0}^{N} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)}, \]

\[ = -\frac{1}{\tau} \left( f_i - f_i^{(\text{eq})} \right), \]
Consistent subgrid scale modelling for LBM

where \( \bar{f}_i = \bar{f}(x, \xi_i, t) \) and \( f^{eq}_i = f^{(0)} - w_i \sum_{n=0}^{N} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)} \). The discretized efficient relaxation time \( \hat{\tau}_{i,eff}^{(N)} \) (corresponding to \( \tau_{eff} \) of Eq. (4.20)), which in the general case depends on both the discrete velocity \( i \) and the Hermite expansion truncation order \( N \), is found to be

\[
\hat{\tau}_{i,eff}^{(N)} = \frac{1}{1 - \frac{1}{\tau} \sum_{n=0}^{N} \frac{w_i}{n! c_s^n} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)}}
\]

where \( c_s \) is a constant depending on the lattice, which can be interpreted as the isentropic expansion factor \( \gamma \) of the lattice, and \( w_i \) are the weights related to the discrete velocities \( \xi_i \). As shown later, in certain cases the relaxation time might become again independent of the discrete velocities.

We are now left with the time–space integration of the (discretized in microscopic velocity space) BGK equation (4.36), which is done with the standard trapezoidal integration combined with a change of variables (see Dellar (2001); Malaspinas (2009) for example). The fully discrete lattice Boltzmann method reads (the temporal discretization step is chosen as \( \delta t = 1 \) for simplicity in the notations)

\[
\hat{f}_i(x + \xi_i, t + 1) = \hat{f}_i(x, t) - \frac{1}{\hat{\tau}} \left( \hat{f}_i(x, t) - f^{(0)}_i(x, t) \right) + \frac{w_i}{\hat{\tau}} \sum_{n=0}^{N} \frac{1}{n! c_s^n} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)},
\]

where the relaxation time \( \hat{\tau} = \tau + 1/2 \) the \( \hat{f}_i \) are given by

\[
\hat{f}_i = \bar{f}_i + \frac{1}{2\tau} \left( \bar{f}_i - f^{eq}_i \right),
\]

One can also rewrite Eq. (4.38) in a more standard way with a the fully discrete efficient relaxation time \( \hat{\tau}_{i,eff}^{(N)} \)

\[
\hat{f}_i(x + \xi_i, t + 1) = \hat{f}_i(x, t) - \frac{1}{\hat{\tau}_{i,eff}^{(N)}} \left( \hat{f}_i(x, t) - f^{(0)}_i(x, t) \right),
\]

with

\[
\hat{\tau}_{i,eff}^{(N)} = \frac{\hat{\tau}}{1 - \frac{\sum_{n=1}^{N} \frac{w_i}{n! c_s^n} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)}}{f_i - f^{(0)}_i}}
\]

\[
= \frac{2\mu_0 + c_s^2 \rho_0 \theta_0}{2c_s^2 \rho_0 \theta_0 \left( 1 - \frac{\sum_{n=1}^{N} \frac{w_i}{n! c_s^n} \mathcal{H}^{(n)}_i : \mathcal{R}^{(n)}}{f_i - f^{(0)}_i} \right)}.
\]

In the last equality we used that \( \mu_0 = c_s^2 \rho_0 \theta_0 (\hat{\tau} - 1/2) \) (the dynamic viscosity of the fluid at temperature \( \theta_0 \) and density \( \rho_0 \)). Eq. (4.38) along with Eq. (4.41) gives us a completely generic formula for implementing subgrid scale closures for any order of Hermite series truncation.

4.5. Implementation formulas

So far, in this section, we showed a consistent way of implementing subgrid scale closures in the BGK Boltzmann equation. Depending on the truncation order in Hermite polynomials of the equilibrium distribution function, there are up to seven different tensors that need to be modelled. These tensors are similar to those appearing in the classical compressible Navier–Stokes approaches, while their implementation is different since
they are, in our case, projected on the Hermite basis. Furthermore we also recovered, in the case of eddy viscosity closures, the classical way of introducing an efficient viscosity closure that we also added here the Hermite polynomials up to order four.

For implementation purposes, we write here explicitly the basic constitutive terms of the LBM scheme with a subgrid scale closure of order up to $N = 4$. The LBM scheme of Eq. (4.38) can be rewritten as

$$f_i(x + \xi, t + 1) = f_i(x, t) - \frac{1}{\tau} \left( \dot{f}_i(x, t) - f_i^{(0)}(x, t) \right) + R_i,$$  \hspace{1cm} (4.42)

with $\dot{\tau} = \tau + 1/2$ and $R_i$ is the discretized subgrid scale term corresponding to $R$. Hereafter the different terms of this equation are written explicitly. The equilibrium distribution function $f_i^{(0)}$ reads

$$f_i^{(0)} = \sum_{n=0}^{4} \frac{1}{c_n^2} \mathcal{H}_i^{(n)} : a_i^{(n)}$$

and the subgrid terms $R_i$, to be added in the collision term of the LBM, are given by

$$R_i = \sum_{n=0}^{4} \frac{1}{c_n^2} \mathcal{H}_i^{(n)} : R_i^{(n)}$$

The term $N = 1$ is not present for fluids but only for passive scalar transport. For completeness we also add here the Hermite polynomials up to order four

$$\mathcal{H}_i^{(0)} = 1,$$
$$\mathcal{H}_i^{(1)} = \xi_{i\alpha},$$
$$\mathcal{H}_i^{(2)} = \xi_{i\alpha} \xi_{i\beta} - c_2^2 \delta_{i\alpha\beta},$$
$$\mathcal{H}_i^{(3)} = \xi_{i\alpha} \xi_{i\beta} \xi_{i\gamma} - c_2^2 \left( \delta_{i\alpha\beta} \xi_{i\gamma} + \delta_{i\alpha\gamma} \xi_{i\beta} + \delta_{i\beta\gamma} \xi_{i\alpha} \right),$
5. Special truncation cases and Chapman–Enskog expansion

Going back to the continuous in time filtered BGK equation we now present three different truncations in Hermite polynomials, which lead to different macroscopic limits:

(a) $N = 1$, the advection–diffusion equation,
(b) $N = 2$, the weakly compressible Navier–Stokes equations,
(c) $N = 3, 4$, iso-thermal and thermal Navier–Stokes equations.

We propose a link with the classical way of introducing eddy viscosity (diffusivity) models (see Section 3) by performing a Chapman–Enskog-like expansion of Eq. (4.35). From Eq. (3.22), one can write the filtered $f_i$ in terms of the filtered equilibrium and non-equilibrium distribution functions as

$$f_i = f_i^{(0)} + f_i^{(1)}.$$

Unfortunately this form of expansion does not allow for an explicit evaluation of the filtered deviatoric stress tensor, $\mathbf{P}^{(1)}$, similar to what is done in Subsection 3.1. We rather assume that the filtered distribution function can be rewritten as

$$f_i \sim f_i^{(0)} (f_i) + f_i^{(1)} (f_i),$$

where

$$\mathbf{P}^{(N)}_{i, \text{eff}} = \frac{\tau_{i, \text{eff}}}{1 - \sum_{n=1}^{N} \frac{1}{c_s^2 n!} R_i^{(n)} : \tilde{a}_i^{(n)} (f_i)},$$

where $f_i^{(0)} (f_i)$ and $f_i^{(1)} (f_i)$ are respectively the equilibrium and non-equilibrium distribution functions evaluated with respect to the filtered density, velocity and temperature.

Furthermore, by using the Chapman–Enskog expansion formulation, one can rewrite $\tau_{i, \text{eff}}^{(N)}$ as

$$\tau_{i, \text{eff}}^{(N)} = \frac{\tau}{1 - \sum_{n=1}^{N} \frac{1}{c_s^2 n!} R_i^{(n)} : \tilde{a}_i^{(n)} (f_i)}.$$

We emphasise at this point that the Ansatz of Eq. (5.2) does not lead to the Chapman–Enskog expansion of the scheme. Nevertheless this formulation allows to perform computations similar that what is done in the non-filtered case and to make a link with classical LES models used in the LBM framework. Some details of this expansion can be found in Appendix A and the results obtained there are used in subsections 5.1-5.3.

5.1. Truncation at order $N = 1$ : the advection–diffusion case

This order of truncation is not representative of the Navier–Stokes limit, but rather is representing an advection–diffusion (AD) equation, which is particularly interesting in the passive scalar transport simulations (see Guo et al. (2002) for more information about the LBM advection–diffusion scheme). Nevertheless it is mentioned for the sake of completeness.

In this case, the Chapman–Enskog expansion of the “bare” BGK equation (3.7), with the additional assumption that the momentum is not a conserved quantity (or $\int \xi f \, d\xi \neq \int \xi f^{(0)} \, d\xi$), gives the following macroscopic limit

$$\partial_t \rho + \nabla \cdot (\rho u) = \nabla \cdot (\kappa \nabla \rho),$$

with $\kappa = c_s^2 \tau$. Furthermore, only $R^{(1)}$ and $\tilde{a}_i^{(1)}$ (the superscript (1) is referring to the Hermite truncation order) are considered in Eq. (4.37), and all higher order terms are neglected. The reader should be aware that both these terms are absent when considering
the Navier–Stokes limit of the BGK equation. Their presence actually reflects the fact that in the advection–diffusion of a scalar, no momentum conservation is imposed.

Inspired by classical advection–diffusion modelling, where the \( R^{(1)} \) vector is given by

\[
R^{(1)} = - \nabla \cdot (\kappa_{sgs} \nabla \rho),
\]

and by the Chapman–Enskog expansion of the AD-LBM which gives for \( \tilde{a}^{(1)}_1 \) (see Appendix A)

\[
\tilde{a}^{(1)}_1 = -c_s^2 (\tau + \tau_{sgs}) \nabla \rho,
\]

where \( \kappa_{sgs} = c_s^2 \tau_{sgs} \), one can write, using Eq. (5.4), the efficient relaxation time as

\[
\tau^{(1)}_{i,eff} = \frac{\tau}{1 - \left( -\frac{\kappa_{sgs} H^{(1)}_i (\nabla \rho)}{-c_s^2 (\tau + \tau_{sgs}) H^{(1)}_i (\nabla \rho)} \right)} = \frac{\tau}{1 - \frac{\tau_{sgs}}{\tau + \tau_{sgs}}} = \tau + \tau_{sgs},
\]

where the microscopic velocity terms vanished and thus \( \tau^{(1)}_{i,eff} \) is now independent of \( i \).

Finally, after time-space integration (presented shortly in Subsection 4.4), the efficient relaxation time \( \hat{\tau}^{(1)}_{i,eff} \) (see Eq. (4.41)) is given by (the Hermite truncation order is omitted for the sake of clarity)

\[
\hat{\tau}^{(1)}_{i,eff} = \hat{\tau} + \tau_{sgs},
\]

and the diffusivity \( \kappa_{eff} \) is found to be related to \( \hat{\tau} = \tau + 1/2 \) by

\[
\kappa_{eff} = \kappa + \kappa_{sgs} = c_s^2 (\hat{\tau} - 1/2 + \tau_{sgs}).
\]

5.2. Truncation at order \( N = 2 \) : the weakly compressible case

Let us now consider the truncation \( N = 2 \). As shown in Table 1, this limit corresponds to the a-thermal weakly compressible Navier–Stokes equations. Although, in this case, we have that \( \theta = 1 \), we keep it in the equations for consistency.

At this truncation order only \( R^{(2)} \) and \( \tilde{a}^{(2)}_1 \) remain in Eq. (4.41) and all the higher order terms can be neglected. As in the preceding subsection, let us focus only on the eddy viscosity assumption for modelling \( R^{(2)} \)

\[
R^{(2)} = -2 \mu_{sgs} \tilde{\nabla},
\]

Furthermore the Chapman–Enskog expansion gives us for \( \tilde{a}^{(2)}_1 \) (see Eq. (A14))

\[
\tilde{a}^{(2)}_1 = -2 c_s^2 (\tau + \tau_{sgs}) \tilde{\rho} \tilde{\theta} \tilde{\nabla},
\]

where we used \( \mu_{sgs} = 2 c_s^2 \tilde{\rho} \tilde{\theta} \tau_{sgs} \). Substituting these two last results in Eq. (5.4), the efficient relaxation time becomes

\[
\tau^{(2)}_{i,eff} = \frac{\tau}{1 - \left( -\frac{\tau_{sgs}}{\tau + \tau_{sgs}} \right)} = \tau + \tau_{sgs},
\]

where we point out that the relaxation time is again not depending on the microscopic velocity (as in the preceding subsection), since the terms depending on \( H^{(2)}_i \) cancelled out. Thus we recovered the classical way of incorporating eddy viscosity closures in the BGK equation (see Eq. (3.43)).

For implementation purposes, one needs to use the \( \hat{\tau}^{(2)}_{i,eff} \) relaxation time of Eq. (4.41).
As in the previous subsection, it is straightforward to find

\[ \hat{\tau}^{(2)}_{i, \text{eff}} = \hat{\tau} + \tau_{\text{sgs}}, \]  

(5.14)

where \( \hat{\tau} = \tau + 1/2 \).

5.3. Truncation at order \( N = 3, 4 \): the compressible cases

When keeping more terms in the compressible cases (\( N \geq 3 \) is the Hermite expansion of distribution function, see Table 1) the simplifications done in the previous section are not possible any more. To be more explicit let us consider the case \( N = 3 \) (i.e. the isothermal compressible Navier–Stokes approximation). In this case, the subgrid scale terms involved in Eq. (4.41) are \( R^{(2)} \) and \( R^{(3)} \), while only \( \tilde{a}^{(2)}_{i} \) is considered, since higher order terms do not enter the macroscopic physics of isothermal fluids (\( \tilde{a}^{(3)}_{i} \) is only relevant in the energy conservation equation). Then, Eq. (4.41) becomes

\[ \hat{\tau}^{(N)}_{i, \text{eff}} = 2\mu + \frac{c_s^2}{\rho \hat{\theta}} \left( \frac{1}{1 + \frac{H_{i,\alpha}\beta}{2}} \left( \frac{\hat{\tau}_{i,\alpha,\beta} - R^{(2)}_{i,\alpha,\beta}}{c_s^2} - R^{(3)}_{i,\alpha,\beta,\gamma} \right) \right), \]

(5.15)

where \( \hat{\tau}_{i,\alpha,\beta} = (\partial_{\alpha}\vec{u}_{\beta} + \partial_{\beta}\vec{u}_{\alpha} - 2\Delta \delta_{\alpha,\beta}\partial_{\gamma}\vec{u}_{\gamma}) \). Thus the approximation \( \tau^{(N)}_{\text{eff}} = \hat{\tau} + \tau_{\text{sgs}} \) does not hold any more for \( N \geq 3 \). In this case the efficient relaxation time now depends on the microscopic velocity. This can be explained by the fact that the subgrid terms stems from a mixing of subgrid heat fluxes and subgrid kinetic energy diffusion, which are not linearly fully correlated in the general case. Therefore, it is no possible to model both of them using a single modified relaxation time.

6. Computation of the strain rate

When using eddy viscosity models, in the weakly compressible limit (presented in Subsection 5.2), one often needs to locally access the value of the strain rate tensor. There exist two ways of computing it. Either from finite differences using the velocity field, or locally directly from the non-equilibrium \( \hat{f}_i \) distribution functions (for simplicity we use that \( \theta = 1 \) in this section)

\[ \sum_i H^{(2)}_{i} \hat{f}^{(1)}_i = \tilde{a}^{(2)}_i = -2c_s^2 \rho \hat{\theta} S. \]

(6.1)

Often, the \( \hat{\tau}_{\text{eff}} \) term depends on \( ||S|| \), which makes an exact computation of \( S \) in a local way more difficult. For example, in the case of the Smagorinsky model, the SGS viscosity is given by

\[ \mu_{\text{sgs}} = \bar{\rho}(C\Delta)^2 ||S|| \Rightarrow \tau_{\text{sgs}} = \frac{(C\Delta)^2}{c_s^2} ||S||, \]

(6.2)

where \( \Delta \) is the filter width and \( C \) the Smagorinsky constant. Thus, in order to compute \( S \) locally one must solve the system (Einstein’s summation convention is understood for repeated indexes)

\[ \tilde{a}^{(1)}_{i,\alpha,\beta} = -2\rho c_s^2 \left( \hat{\tau} + \frac{(C\Delta)^2}{c_s^2} \sqrt{2\gamma\delta S_{\gamma\delta}} \right) S_{\alpha,\beta}. \]

(6.3)
This equation admits four roots, which have the following form

$$\mathcal{S}_{\alpha\beta} = \zeta a^{(2)}_{\alpha\beta}, \quad (6.4)$$

where $\zeta$ is solution of the following equation

$$4\bar{\rho}^2(C\Delta)^4 \left| a^{(2)}_1 \right|^2 \zeta^4 - 4\bar{\rho}^2\bar{\tau}^2 c_s^4\zeta^2 - 4\bar{\rho}\bar{\tau} c_s^2 \zeta - 1 = 0. \quad (6.5)$$

The solutions of this equation are given by

$$\zeta_1 = \frac{1}{2} \frac{-\bar{\rho}\bar{\tau} c_s^2 + \sqrt{\bar{\rho}^2\bar{\tau}^2 c_s^4 - 2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}}{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}, \quad (6.6)$$

$$\zeta_2 = \frac{1}{2} \frac{-\bar{\rho}\bar{\tau} c_s^2 + \sqrt{\bar{\rho}^2\bar{\tau}^2 c_s^4 - 2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}}{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}, \quad (6.7)$$

$$\zeta_3 = \frac{1}{2} \frac{-\bar{\rho}\bar{\tau} c_s^2 + \sqrt{\bar{\rho}^2\bar{\tau}^2 c_s^4 + 2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}}{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}, \quad (6.8)$$

$$\zeta_4 = \frac{1}{2} \frac{-\bar{\rho}\bar{\tau} c_s^2 + \sqrt{\bar{\rho}^2\bar{\tau}^2 c_s^4 + 2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}}{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}. \quad (6.9)$$

While it is possible to exclude $\zeta_1$ and $\zeta_2$ because they might give complex solutions, it is impossible to chose a priori between $\zeta_3$ or $\zeta_4$. Nevertheless, for consistency, when $C \to 0$ (corresponding to the case where $\mu_{sgs} \to 0$), the strain rate tensor should be given by the standard CE result

$$\mathfrak{S} = -\frac{1}{\bar{\rho}\bar{\tau} c_s^2} \hat{a}^{(2)}_1 \leftrightarrow \zeta = \frac{1}{\bar{\rho}\bar{\tau} c_s^2}. \quad (6.10)$$

Replacing $\zeta_{3,4}$ by $\zeta_{\pm}$ for simplicity, one can expand Eqs. (6.8) and (6.9) in the limit $2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho} \ll \bar{\rho}^2\bar{\tau}^2 c_s^4$ at first order in Taylor series

$$\zeta_{\pm} = \frac{\bar{\rho}\bar{\tau} c_s^2}{2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}} \left( 1 \pm \sqrt{1 + \frac{2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}{\bar{\rho}^2\bar{\tau}^2 c_s^4}} \right), \quad (6.11)$$

$$\approx \frac{\bar{\rho}\bar{\tau} c_s^2}{2(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}} \left( 1 \pm \left( 1 + \frac{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}}{\bar{\rho}^2\bar{\tau}^2 c_s^4} \right) \right). \quad (6.12)$$

Finally we have that

$$\zeta_+ \approx \frac{\bar{\rho}\bar{\tau} c_s^2}{(C\Delta)^2 \left| a^{(2)}_1 \right|^2 \bar{\rho}} + \frac{1}{2\bar{\rho}\bar{\tau} c_s^2}, \quad (6.13)$$

$$\zeta_- \approx -\frac{1}{2\bar{\rho}\bar{\tau} c_s^2}. \quad (6.14)$$
Consistent subgrid scale modelling for LBM

Consistent strain
\[ -\left( \hat{\tau} + (C\Delta)^2/c_s^2||\mathbf{S}|| \right)^{-1} \left( \hat{f}_i - f_i^{(0)} \right) \]
\[ \mathbf{S} = \zeta_4 \hat{a}_1^{(2)} \]

Consistent smagorinsky
\[ -\left( \hat{\tau} + (C\Delta)^2/c_s^2||\mathbf{S}|| \right)^{-1} \left( \hat{f}_i - f_i^{(0)} \right) \]
\[ \mathbf{S} = \mathcal{R}_i S^{(2)}_{\alpha\beta} \]

Naive
\[ -\left( \hat{\tau} + (C\Delta)^2/c_s^2||\mathbf{S}|| \right)^{-1} \left( \hat{f}_i - f_i^{(0)} \right) \]
\[ \mathbf{S} = -\hat{a}_1^{(2)}/(\rho\tau c_s^2) \]

Table 2. Summary of the three different collision operators considered for numerical implementation

<table>
<thead>
<tr>
<th>SGS model</th>
<th>( \Omega )</th>
<th>Strain rate computation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Consistent strain</td>
<td>-\left( \hat{\tau} + (C\Delta)^2/c_s^2</td>
<td></td>
</tr>
<tr>
<td>Consistent smagorinsky</td>
<td>-\left( \hat{\tau} + (C\Delta)^2/c_s^2</td>
<td></td>
</tr>
<tr>
<td>Naive</td>
<td>-\left( \hat{\tau} + (C\Delta)^2/c_s^2</td>
<td></td>
</tr>
</tbody>
</table>

It is thus obvious that in the limit \( C \to 0 \), \( \zeta_+ \) must be discarded and that the only physically sound way to compute the strain rate locally is given by

\[ \mathbf{S}_{\alpha\beta} = \zeta_4 \hat{a}_1^{(2)}_{\alpha\beta}, \]  

7. Benchmark : the time developing mixing layer

In this section we test our implementation of the consistent way of adding a closure model in the LBM scheme on the time developing mixing layer. The tests are only performed in the weakly compressible limit of the Navier–Stokes equations. The results will be compared with the DNS of Rogers & Moser (1994).

The subgrid closure implemented is the Smagorinsky model. Three different closure formulas will be tested. The first one uses the approximation of Eq. (5.14), where

\[ \tau_{sgs} = \frac{(C\Delta)^2}{c_s^2} ||\mathbf{S}||, \]  

will be referred to as “consistent strain” hereafter. In this case the strain rate is computed locally according to Eq. (6.15). The second implements the exact formulation of Eq. (4.41), where

\[ \mathcal{R}_i = \frac{w_i}{\tau} \frac{(C\Delta)^2}{2c_s^2} ||\mathbf{S}|| \mathcal{H}^{(2)}_{i\alpha\beta} S_{\alpha\beta}, \]  

will be denoted “consistent smagorinsky” hereafter. Here the strain rate tensor is computed with a finite difference (FD) scheme, since we cannot rely on the Chapman–Enskog expansion theoretically. Finally the third is done using Eq. (5.14) but this time \( \mathbf{S} \) will be computed using the lower order approximation

\[ \mathbf{S} = -\frac{1}{\rho\tau c_s^2} \hat{a}_1^{(2)}, \]  

and will be referred to as “naive” in what follows. The different collision operators used are summarized in Table 2.

The simulation is initialized with a velocity field of (see Fig. 1)

\[ u_x = \frac{1}{2} \Delta U \text{erf} \left( \frac{y}{\sqrt{2\pi}\delta_0} \right), \quad u_y = 0, \quad u_z = 0. \]  

where \( \Delta U \) is the difference of velocity between the two layers, \( \delta_0 \) the initial momentum thickness, and erf the error function

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} \, dt. \]
The horizontal velocity profile with respect to $y$, for $\Delta U = 1$ and $\delta_m = 1$.

The momentum thickness $\delta_m$ is defined as

$$\delta_m = \int_{-\infty}^{\infty} \left( \frac{1}{4} - \frac{u^2}{\Delta U^2} \right) \, dy$$

and the initial Reynolds number based on the momentum thickness is $Re = \Delta U \delta_0 / \nu = 800$. The flow is periodic in the spanwise and streamwise directions, while a free-slip boundary condition is imposed on the $y$-boundaries. This flow exhibits an efficient behaviour after the appearance of a Kelvin–Helmholtz instability (see Rogers & Moser (1994)). When turbulence is well established, one has a self-similar behaviour of the flow and a constant growth of the momentum thickness $\delta_m$ with respect to the non-dimensional time, $\tau \equiv t \Delta U / \delta_m$, is expected. In order to trigger the Kelvin–Helmholtz instability a perturbation is superimposed on the initial velocity profile (see Terracol et al. (2003) for a detailed description of the perturbation). It consists of a dephased series of sines and cosines that will excite the first more unstable modes. This perturbation is modulated by a Gaussian centred on $y = 0$ within standard deviation of $\delta_0$. The amplitude of the perturbation is $0.1 \Delta U$.

The regular grid resolution used for the simulation presented hereafter is $[64 \times 64 \times 64]$ and $M = 1$ corresponding to the initial momentum thickness. The velocity difference in lattice units was chosen to be $\Delta U = 0.05$, the Smagorinsky constant was chosen to be $C = 0.14$ and the filter width $\Delta = 1$.

The lattice used is the standard D3Q19, which allows the exact integration of polynomials up to order five. In this case, the microscopic velocity set $\{\xi_i\}_{i=0}^{18}$ is

$$\begin{align*}
\xi_i & = \{ (0, 0, 0), \\
& (-1, 0, 0), (0, -1, 0), (0, 0, -1), \\
& (-1, -1, 0), (-1, +1, 0), (-1, 0, -1), (-1, 0, +1), (0, -1, -1), (0, -1, +1), \\
& (+1, 0, 0), (0, +1, 0), (0, 0, +1), \\
& (+1, +1, 0), (+1, -1, 0), (+1, 0, +1), (+1, 0, -1), (0, +1, +1), (0, +1, -1) \}. 
\end{align*}$$

and the weights $w_i$ and $c_i^2$ are given by

$$w_0 = 1/3, \quad w_{1,2,3,10,11,12} = 1/18, \quad w_{4,5,6,7,8,9,13,14,15,16,17,18} = 1/36, \quad c_i^2 = 1/3.$$
7.1. Results

As can be seen from Fig. 2 the both consistent smagorinsky, consistent strain and naive approaches give almost indistinguishable results and the self-similar behaviour is correctly recovered. The momentum thickness growth is of $d\delta_m/d\tau = 0.014$ and is in good agreement with the DNS of Rogers & Moser (1994) (note that the curve of Rogers & Moser has been slightly shifted in time in order for the momentum thickness growth to start at the same time). In the case of the “naive” way of computing the strain rate tensor, the momentum thickness growth rate is of lesser accuracy. Furthermore one can notice that the dissipation in this case is not constant as it is in the other two cases. These results show that our consistent way of introducing the subgrid scale stress tensor yields correct results. Furthermore an accurate way for the local evaluation of the strain rate is shown to be of crucial importance in order to obtain accurate results.

Although the growth rate of the momentum thickness with time is not accurately recovered, the results for the self-similarity of the average velocity and rms velocity are correctly recovered for all the three cases, as shown in Figs 3 and 4. The average and rms velocity curves all coincide when plotted with respect to the non-dimensional $y$-position, $\bar{y} = y/\delta_m$.

Finally we also plotted the 1D energy spectrum with respect to the $x$-component of the wave vector, $k_x$. One recovers qualitatively the expected $-5/3$ slope in good agreement with the theory. In this case also the implementation does not seem to have any great effect on the shape of the spectrum.
8. Conclusion

In this paper we showed how to theoretically include, in a consistent fashion, subgrid scale closures in the filtered BGK equation at any order in the Hermite polynomial expansion. This approach allows us to model closures for any kind of macroscopic limit, ranging from the advection–diffusion equation to the compressible thermal Navier–Stokes equations. It allows also use the models developed in the Navier–Stokes framework in a straightforward way.

In the weakly compressible limit, we showed that our approach is consistent with the standard closure for eddy viscosity models used so far in the literature, in the limit
where the Chapman–Enskog expansion and the filtering operation “commute” which is in general not the case.

We also derived a consistent way of computing the strain rate tensor from the velocity distribution functions and showed that the results obtained with this formula are more accurate than with a naive way of computing it.

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Appendix A. Chapman–Enskog expansion of the filtered BGK equation
In this appendix we do the Chapman–Enskog expansion of the filtered BGK equation. Two different cases are treated. The first is the advection–diffusion limit of the BGK equation and the second will be the Navier–Stokes limit where the mass, momentum and energy conservation equations (the procedure for the energy conservation is similar and therefore will not be done in details here). The filtered BGK equation (4.35) is given by

$$\partial_t \tilde{f}_i + (\xi_i \cdot \nabla) \tilde{f}_i = -\frac{1}{\tau} \left( \tilde{f}_i - f_i^{(0)}(\tilde{f}_i) \right) + \frac{1}{\tau} \sum_{n=0}^{N} \frac{1}{c_s^{2n} n!} H_n^{(n)} : \mathcal{R}^{(n)}.$$  \hspace{1cm} (A 1)

Replacing $\tilde{f}_i$ by their Chapman–Enskog expansion counterpart

$$\tilde{f}_i = f_i^{(0)}(\tilde{f}_i) + f_i^{(1)}(\tilde{f}_i), \quad f_i^{(1)} \ll f_i^{(0)},$$  \hspace{1cm} (A 2)

and taking the zeroth order moment of the filtered BGK equation, one gets

$$\partial_t \tilde{\rho} + \mathbf{\nabla} \cdot (\tilde{\rho} \tilde{u} + \tilde{a}_1^{(1)}) = 0,$$  \hspace{1cm} (A 3)

where we impose mass conservation ($\sum_i \tilde{f}_i^{(1)} = 0$), but momentum is not conserved ($\sum_i \xi_i \tilde{f}_i^{(1)} = \tilde{a}_1^{(1)} \neq 0$). We therefore need to compute $\tilde{a}_1^{(1)}$ (here the $\tilde{a}_0^{(n)}$ and $\tilde{a}_1^{(n)}$ stand for the coefficients related to $f_i^{(0)}(\tilde{f}_i)$ and $f_i^{(1)}(\tilde{f}_i)$). To this aim, we project the filtered BGK equation (Eq. (4.4)) on the Hermite polynomial of order $n$, and keeping only the lower order terms, one finds (omitting the overline for simplicity in the notations)

$$\partial_t \tilde{a}_0^{(n)} + \mathbf{\nabla} \cdot \tilde{a}_0^{(n+1)} + c_s^2 (\mathbf{\nabla} \tilde{a}_0^{(n-1)} + \text{perm}) = -\frac{1}{\tau} \tilde{a}_1^{(n)} + \frac{1}{\tau} \mathcal{R}^{(n)},$$  \hspace{1cm} (A 4)

where “perm” stands for all cyclic index permutations. In the case of the advection diffusion limit, we only need to truncate the Hermite series of the equilibrium distribution up to order $N = 1$. For $n = 0$, the l.h.s. of this equation is null because of mass and momentum conservation and one obtains

$$\partial_t \tilde{\rho} + \mathbf{\nabla} \cdot (\tilde{\rho} \tilde{u}) = 0.$$  \hspace{1cm} (A 5)

For $n = 1$, Eq. (A 4) becomes (remember that $\tilde{a}_0^{(2)} = 0$ because $f_i^{(0)}$ is truncated at order $N = 1$)

$$\partial_t (\tilde{\rho} \tilde{u}) + c_s^2 \mathbf{\nabla} \tilde{\rho} = -\frac{1}{\tau} \tilde{a}_1^{(1)} + \frac{1}{\tau} \mathcal{R}^{(1)},$$  \hspace{1cm} (A 6)
Using Eqs. (A 5) and after some algebra, one gets

\[ \tilde{a}_1^{(1)} = -c_s^2 \tau \nabla \tilde{p} + \mathcal{R}^{(1)} + \tau (\tilde{u} \nabla \cdot (\tilde{\rho} \tilde{u}) - \tilde{\rho} \partial_t \tilde{u}), \]  

(A 7)

where \( \mathcal{E} \) is an error term which is usually neglected. Finally replacing this relation in Eq. (A 3) one finds

\[ \partial_t \tilde{\rho} + \nabla \cdot (\tilde{\rho} \tilde{u}) = \nabla \cdot \left( \kappa \nabla \tilde{\rho} - \mathcal{R}^{(1)} \right), \]  

(A 8)

with \( \kappa = c_s^2 \tau \).

In the case of fluids we apply the same procedure as made above on the filtered BGK equation (4.4), but further assume momentum conservation \( (\sum \xi_i f_i^{(1)} = \tilde{a}_1^{(1)} = 0) \).

Thus taking zeroth and first order moments of the filtered BGK equation, one obtains

\[ \partial_t \tilde{\rho} + \nabla \cdot (\tilde{\rho} \tilde{u}) = 0, \]  

(A 9)

\[ \partial_t (\tilde{\rho} \tilde{u}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{u}) + \nabla \cdot (\tilde{P}^{(0)} + \tilde{P}^{(1)}) = 0, \]  

(A 10)

where \( \tilde{P}^{(0)} = \sum c_i \tilde{c}_i f_i^{(1)} (T_i) = c_s^2 \tilde{\rho} \tilde{p} I \) and \( \tilde{P}^{(1)} = \sum c_i \tilde{c}_i f_i^{(1)} \). We therefore need to compute \( \tilde{P}^{(1)} \). To this aim, we use Eq. (A 4). For \( n = 0 \) and \( n = 1 \), the l.h.s. of this equation is null because of mass and momentum conservation and one obtains

\[ \partial_t \tilde{\rho} + \nabla \cdot \tilde{\rho} \tilde{u} = 0, \]  

(A 11)

\[ \partial_t (\tilde{\rho} \tilde{u}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{u}) = -\nabla \tilde{p}, \]  

(A 12)

where \( \tilde{p} = c_s^2 \tilde{\rho} \tilde{\theta} \). For \( n = 2 \), Eq. (A 4) becomes

\[ \partial_t (\tilde{\rho} \tilde{u} \tilde{u}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{u} \tilde{u} + \tilde{\rho} \tilde{\theta} - 1) (\tilde{u} + \text{perm}) \]

\[ -c_s^2 \left( \nabla (\tilde{\rho} \tilde{u}) + \left( \nabla (\tilde{\rho} \tilde{u}) \right)^T \right) = -\frac{1}{\tau} \tilde{a}_1^{(2)} + \frac{1}{\tau} \mathcal{R}^{(2)}, \]  

(A 13)

with the superscript “T” standing for the transpose operation. Using Eqs. (A 11) and (A 12) and after some tedious algebra, one gets

\[ \tilde{a}_1^{(2)} = -2c_s^2 \tau \tilde{\rho} \tilde{\theta} \lambda + \mathcal{R}^{(2)}, \]  

(A 14)

where \( \lambda = \frac{\nabla \tilde{u} + (\nabla \tilde{u})^T}{2} = \mathcal{S} \) for \( N = 2 \) and \( \lambda = \frac{\nabla \tilde{u} + (\nabla \tilde{u})^T - \frac{2}{\beta} I \nabla \cdot \tilde{u}}{2} \) for \( N \geq 3 \). This result is exact if the equilibrium distribution is expanded at least up to order \( N = 3 \). In the weakly compressible limit where \( N = 2 \) there are error terms of order \( \tilde{\rho}^3 \) that are neglected. Using this last relation one can compute \( \tilde{P}^{(1)} \) and one gets for the momentum conservation equation

\[ \partial_t (\tilde{\rho} \tilde{u}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{u}) = -\nabla \tilde{p} + \nabla \cdot \left( 2 \mu \tilde{\lambda} \right) - \nabla \cdot \mathcal{R}^{(2)}, \]  

(A 15)

where \( \mu = c_s^2 \tilde{\rho} \tilde{\theta} \).

To obtain the energy equation, one takes half the trace of the second moment of Eq. (A 1) and doing some algebra one gets

\[ \tilde{\rho} (\partial_t \tilde{\varepsilon} + u \cdot \nabla \tilde{\varepsilon}) + \left( \tilde{P}^{(0)} + \tilde{P}^{(1)} \right) : (\nabla \tilde{u}) + \nabla \cdot \left( \tilde{q}^{(0)} + \tilde{q}^{(1)} \right) = 0, \]  

(A 16)

where \( \tilde{q} = \int c_i^2 \tilde{c}_i \tilde{f}_i d\tilde{c} \). A straightforward computation gives that \( \tilde{q}^{(0)} = 0 \) and we are left with the evaluation of the heat flux. To compute it one must first use the trace of Eq. (A 13), that is given by

\[ \partial_t (\tilde{\rho} \tilde{\varepsilon}) - \tilde{u} \cdot \nabla (\tilde{\rho} \tilde{\theta}) + \left( \frac{D + 2}{2} \right) \nabla \cdot (\tilde{\rho} \tilde{\theta} \tilde{u}) = 0. \]  

(A 17)
Then using Eq. (A.4) where \( n = 3 \) and take the trace of this equation and by using Eqs. (A.11), (A.12) and (A.17), one finds

\[
a_{\alpha\beta\beta}^{(3)} = -c_s^2 \rho \theta \left( 2 \bar{\Lambda}_{\alpha\beta} u_{\beta} + (D + 2) \partial_{\alpha} \theta \right) + R_{\alpha\beta\beta}^{(3)},
\]

(A.18)

Since \( q_\alpha^{(1)} = (a_{\alpha\beta\beta}^{(3)} - 2 u_{\beta} a_{\alpha\beta}^{(2)})/2 \) it is straightforward to deduce that the filtered heat flux is given by

\[
q_\alpha^{(1)} = -c_s^2 \rho \theta \left( \frac{D + 2}{2} \right) \partial_{\alpha} \theta + R_{\alpha\beta\beta}^{(3)}
\]

(A.19)

Finally the filtered energy equation is

\[
\bar{\rho} \left( \partial_t \varepsilon + \mathbf{u} \cdot \nabla \varepsilon \right) + \left( \bar{\rho} l - \mu \bar{\Lambda} \right) : (\nabla \mathbf{u}) = \left( \frac{D + 2}{2} \right) \nabla \cdot (\kappa \nabla \theta) - \nabla \cdot \text{tr} \left( R^{(3)} \right),
\]

(A.20)

where \( \kappa = c_s^2 \rho \theta \tau \) and \( \text{tr}(R^{(3)}) \) stands for the contraction of the two last indices of \( R_{\alpha\beta\gamma}^{(3)} \).

REFERENCES


26

O. Malaspinas and P. Sagaut


