J. Fluid Mech. (2012), *vol.* 700, *pp.* 514–542. © Cambridge University Press 2012
doi:10.1017/jfm.2012.155

Consistent subgrid scale modelling for lattice Boltzmann methods

Orestis Malaspinas† and Pierre Sagaut

Institut Jean le Rond d'Alembert, UMR 7190, Université Pierre et Marie Curie - Paris 6,
4 place Jussieu - case 162, F-75252, France

(Received 7 May 2011; revised 13 February 2012; accepted 22 March 2012;
first published online 30 April 2012)

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 and 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: turbulence modelling, turbulence simulation

1. Introduction

Turbulent flows are present in many engineering applications, such as flows past cars or aircraft, 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, Deck & Terracol 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 (Meyers, Sagaut & Geurts 2006; Meyers & Sagaut 2006), and also numerical discretization (Meyers, Sagaut & Geurts 2007). Multiphysics models have been developed during the past decades, e.g. to account for heat transfer

† Email address for correspondence: malaspinas@lmm.jussieu.fr

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

(Labbé, Montreuil & Sagaut 2002) or noise generation (Seror *et al.* 2001). Increasing efficiency of the LES by combining it with multiresolution techniques (e.g. Quéméré, Sagaut & Couaillier 2001, 2002) is still a very active research topic. 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 Eggels 1996; Hou *et al.* 1996; Filippova *et al.* 2001; Krafczyk, Tölke & Luo 2003; Kerimo & Girimaji 2007; Dong, Sagaut & Marié 2008; Chen 2009; Premnath, Pattison & Banerjee 2009; Weickert *et al.* 2010, among others), by simply adding an efficient relaxation time in the collision operator. All of these models are only valid in the weakly compressible limit, while the LBM can in principle also be applied to fully compressible flows (see Nie, Shan & Chen 2008; Chikatamarla *et al.* 2010; Scagliarini *et al.* 2010*a*,*b*).

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

In the present paper we propose a consistent *a priori* approach for including SGS closures to the LBM (see Chen & Doolen 1998; Wolf-Gladrow 2000; Succi 2001; Shan, Yuan & Chen 2006; Aidun & Clausen 2010, for complete references on the LBM), by applying the filtering procedure proposed by Leonard (1974). This approach allows us to explicitly express the SGS tensors to be modelled and provide a formula to include them into the model. We also show that the standard approach, which consists of 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 direct numerical simulation (DNS) results of Rogers & Moser (1994).

We point out that although our paper is focused on LES in the LBM 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 § 2 we introduce the notation to be used in the paper by shortly recalling 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 § 3. In § 4 the consistent inclusion of subgrid closures is described. The link between our approach and the classical existing ‘eddy relaxation time’ is made in § 5. Then an accurate way of computing the strain rate tensor from the distribution function for Smagorinsky-like models is shown in § 6. In § 7 the

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

developments of §§ 4–6 are validated on the time developing mixing layer benchmark. Finally, this work is concluded in § 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 recall the filtering techniques inspired by the work of Leonard (1974) for the Navier–Stokes equations, in order to introduce the notation and understand the procedure that will be applied to the BGK equation afterwards.

With $\mathscr{G}$ a homogeneous convolution filter kernel, and denoting the filtered counterpart of any quantity, a, as

$$\overline{a} \equiv \mathscr{G} * a = \int_{-\infty}^{\infty} \mathscr{G}(\boldsymbol{x} - \boldsymbol{y}) a(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}, \tag{2.1}$$

one can write the filtered incompressible Navier–Stokes equations as

$$\nabla \cdot \overline{\boldsymbol{u}} = 0, \tag{2.2}$$

$$\rho(\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}}) = -\nabla \overline{p} + 2\nabla \cdot (\mu \overline{\boldsymbol{S}}) - \nabla \cdot \boldsymbol{T}, \tag{2.3}$$

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

$$\boldsymbol{T} \equiv \overline{\boldsymbol{u}\boldsymbol{u}} - \overline{\boldsymbol{u}}\,\overline{\boldsymbol{u}}. \tag{2.4}$$

The appearance of the SGS stress tensor is due to the fact that the filtering operation does not commute with the nonlinear 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 SGS stress tensor consists of assuming that $\boldsymbol{T} = -2\mu_{sgs}\overline{\boldsymbol{S}}$ (Boussinesq approximation), where μ_{sgs} is the SGS viscosity which for example in Smagorinsky (1963) is proportional to the norm of the filtered strain rate tensor, $\left\|\overline{\boldsymbol{S}}\right\| \equiv \sqrt{2\mathrm{tr}\left(\overline{\boldsymbol{S}} \cdot \overline{\boldsymbol{S}}\right)}$ and is given by $\mu_{sgs} = \rho\,(C\Delta)^2 \left\|\overline{\boldsymbol{S}}\right\|$ (C being the Smagorinsky constant and Δ the filter width).

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

$$\rho(\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}}) = -\nabla \overline{p} + 2\nabla \cdot (\mu_{eff} \overline{\boldsymbol{S}}), \tag{2.5}$$

where μ_{eff} is the efficient viscosity defined as

$$\mu_{eff} \equiv \mu + \mu_{sgs}. \tag{2.6}$$

3. SGS 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, Gross & Krook 1954). Then we provide the basic steps used in the lattice Boltzmann framework in order to recover the

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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 $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ of finding a particle with velocity $\boldsymbol{\xi}$ at position $\boldsymbol{x}$ and time t in terms of particle collisions only, and reads in absence of a force as

$$\partial_t f(\boldsymbol{x}, \boldsymbol{\xi}, t) + (\boldsymbol{\xi} \cdot \nabla) f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \Omega(f), \tag{3.1}$$

where Ω is the collision operator. The macroscopic fields such as the density ρ, the velocity $\boldsymbol{u}$, the stress tensor $\boldsymbol{P}$, the temperature θ (actually the temperature times the Boltzmann constant), the internal energy ε and the internal energy flux $\boldsymbol{q}$ are given by the following moments of the distribution function

$$\rho = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{\xi}, \tag{3.2}$$

$$\rho \boldsymbol{u} = \int \boldsymbol{\xi} f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{\xi}, \tag{3.3}$$

$$\boldsymbol{P} = \int \boldsymbol{c}\boldsymbol{c} f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{c}, \tag{3.4}$$

$$\rho\theta = \frac{2}{D}\rho\varepsilon = \frac{1}{D}\int \boldsymbol{c}^2 f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{c}, \tag{3.5}$$

$$\boldsymbol{q} = \frac{1}{2}\int \boldsymbol{c}^2 \boldsymbol{c} f(\boldsymbol{x}, \boldsymbol{\xi}, t)\, \mathrm{d}\boldsymbol{c}, \tag{3.6}$$

where $\boldsymbol{c} = \boldsymbol{\xi} - \boldsymbol{u}$ 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

$$\partial_t f(\boldsymbol{x}, \boldsymbol{\xi}, t) + (\boldsymbol{\xi} \cdot \nabla) f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}(f(\boldsymbol{x}, \boldsymbol{\xi}, t) - f^{(0)}(\rho, \boldsymbol{u}, \theta)), \tag{3.7}$$

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

$$f^{(0)} = \frac{\rho(\boldsymbol{x}, t)}{(2\pi\theta(\boldsymbol{x}, t))^{D/2}} \exp\left(-\frac{(\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{\xi})^2}{2\theta(\boldsymbol{x}, t)}\right). \tag{3.8}$$

Here, our approach stops following kinetic theory textbooks. Since we are interested in numerically solving (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 (1949*b*) (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 (1949*a*) for a summary on

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

Hermite polynomials)

$$f^N = w(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{\mathcal{H}}\,(\boldsymbol{\xi})^{(n)} : \boldsymbol{a}^{(n)}, \tag{3.9}$$

$$f^{(0)N} = w(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{\mathcal{H}}\,(\boldsymbol{\xi})^{(n)} : \boldsymbol{a}_0^{(n)}, \tag{3.10}$$

where the column symbol ':' stands for the full index contraction, $w(\boldsymbol{\xi}) = \exp(-\boldsymbol{\xi}^2/2)$, $\boldsymbol{\mathcal{H}}^{(n)}$, $\boldsymbol{a}^{(n)}$ and $\boldsymbol{a}_0^{(n)}$, 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 $N = 4$

$$a_0^{(0)} = \rho, \tag{3.11}$$

$$a_{0\alpha}^{(1)} = \rho u_\alpha, \tag{3.12}$$

$$a_{0\alpha\beta}^{(2)} = \rho u_\alpha u_\beta + \rho(\theta - 1)\delta_{\alpha\beta}, \tag{3.13}$$

$$a_{0\alpha\beta\gamma}^{(3)} = \rho u_\alpha u_\beta u_\gamma + \rho(\theta - 1)(\delta_{\alpha\beta}u_\gamma + \delta_{\alpha\gamma}u_\beta + \delta_{\beta\gamma}u_\alpha), \tag{3.14}$$

$$\begin{aligned} a_{0\alpha\beta\gamma\delta}^{(4)} = {} & \rho u_\alpha u_\beta u_\gamma u_\delta + \rho\,(\theta - 1)^2(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) \\ & + \rho(\theta - 1)(\delta_{\alpha\beta}u_\gamma u_\delta + \delta_{\alpha\gamma}u_\beta u_\delta + \delta_{\alpha\delta}u_\beta u_\gamma \\ & + \delta_{\beta\gamma}u_\alpha u_\delta + \delta_{\beta\delta}u_\alpha u_\gamma + \delta_{\gamma\delta}u_\alpha u_\beta). \end{aligned} \tag{3.15}$$

In order to recover the macroscopic equations of motion related with the BGK equation, one must take moments of (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 (3.2)–(3.6) and (3.11)–(3.13)

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0, \tag{3.16}$$

$$\partial_t(\rho \boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \boldsymbol{\nabla} \cdot \boldsymbol{P} = 0, \tag{3.17}$$

$$\rho(\partial_t \varepsilon + \boldsymbol{u} \cdot \boldsymbol{\nabla}\varepsilon) + \boldsymbol{P} : (\boldsymbol{\nabla}\boldsymbol{u}) + \boldsymbol{\nabla} \cdot \boldsymbol{q} = 0. \tag{3.18}$$

These equations are only obtained under the assumption of mass, momentum and energy conservation, respectively ($\int \Omega = \int \boldsymbol{\xi}\Omega = \int \boldsymbol{\xi}^2\Omega = 0$), or in other terms

$$\int (f - f^{(0)})\,\mathrm{d}\boldsymbol{\xi} = 0, \quad \text{Mass conservation} \tag{3.19}$$

$$\int \boldsymbol{\xi}(f - f^{(0)})\,\mathrm{d}\boldsymbol{\xi} = 0, \quad \text{Momentum conservation} \tag{3.20}$$

$$\int \boldsymbol{\xi}^2(f - f^{(0)})\,\mathrm{d}\boldsymbol{\xi} = 0. \quad \text{Energy conservation.} \tag{3.21}$$

The momentum and energy conservation still need to be closed (a constitutive equation must be found for $\boldsymbol{P}$ and $\boldsymbol{q}$). 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 § 4.4 for discretization purposes).

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$f = f^{(0)} + f^{(1)}, \tag{3.22}$$

where the equilibrium distribution is assumed to be given by (3.10), the perturbation, $f^{(1)} \sim O(Kn) \ll 1$, is of the order of the Knudsen number, 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 (3.7), one obtains at the lowest order

$$\partial_t f^{(0)} + (\boldsymbol{\xi} \cdot \boldsymbol{\nabla}) f^{(0)} = -\frac{1}{\tau} f^{(1)}. \tag{3.23}$$

Multiplying this equation by 1, $\boldsymbol{\xi}$ and $\boldsymbol{\xi}^2/2$ and integrating over the microscopic velocity, and using the mass, momentum and energy conservation constrains on each equation, respectively ($\int f^{(1)} = \int \boldsymbol{\xi} f^{(1)} = \int \boldsymbol{\xi}^2 f^{(1)} = 0$), one obtains the inviscid Euler equations for mass, momentum and energy conservation

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0, \tag{3.24}$$

$$\partial_t (\rho \boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \boldsymbol{\nabla} p = 0, \tag{3.25}$$

$$\rho \left(\partial_t \varepsilon + \boldsymbol{u} \cdot \boldsymbol{\nabla} \varepsilon\right) + (p\boldsymbol{I}) : (\boldsymbol{\nabla} \boldsymbol{u}) = 0, \tag{3.26}$$

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

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

$$\boldsymbol{P} = \boldsymbol{P}^{(0)} + \boldsymbol{P}^{(1)} = \rho\theta \boldsymbol{I} + \boldsymbol{P}^{(1)}, \quad \boldsymbol{q} = \boldsymbol{q}^{(0)} + \boldsymbol{q}^{(1)} = \boldsymbol{q}^{(1)}, \tag{3.27}$$

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

$$f^{(1)} = w(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{\mathcal{H}}(\boldsymbol{\xi})^{(n)} : \boldsymbol{a}_1^{(n)}, \tag{3.28}$$

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

$$\boldsymbol{P}^{(1)}_{\alpha\beta} = a^{(2)}_{1\alpha\beta}, \tag{3.29}$$

$$q^{(n)}_{\alpha} = \tfrac{1}{2}(a^{(3)}_{1\alpha\beta\beta} - 2a^{(2)}_{1\alpha\beta} u_\beta - a^{(2)}_{1\beta\beta} u_\alpha), \tag{3.30}$$

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

$$\partial_t \boldsymbol{a}_0^{(n)} + \boldsymbol{\nabla} \cdot \boldsymbol{a}_0^{(n+1)} + (\boldsymbol{\nabla} \boldsymbol{a}_0^{(n-1)} + \text{perm}) = -\frac{1}{\tau} \boldsymbol{a}_1^{(n)}, \tag{3.31}$$

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

$$\partial_t \boldsymbol{a}_0^{(2)} + \boldsymbol{\nabla} \cdot \boldsymbol{a}_0^{(3)} + (\boldsymbol{\nabla} \boldsymbol{a}_0^{(1)} + \text{perm}) = -\frac{1}{\tau} \boldsymbol{a}_1^{(2)}, \tag{3.32}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

$$\partial_t\left[\rho\boldsymbol{uu}+\rho(\theta-1)\boldsymbol{I}\right]+\boldsymbol{\nabla}\cdot\left[\rho\boldsymbol{uuu}+\rho(\theta-1)(\boldsymbol{uI}+\text{perm})\right]$$
$$+\left[\boldsymbol{\nabla}(\rho\boldsymbol{u})+(\boldsymbol{\nabla}(\rho\boldsymbol{u}))^{\mathrm{T}}\right]=-\frac{1}{\tau}\boldsymbol{a}_1^{(2)}. \tag{3.33}$$

By using (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

$$\boldsymbol{a}_1^{(2)}=\boldsymbol{P}^{(1)}=-2\tau\rho\theta\boldsymbol{\Lambda}, \tag{3.34}$$

where

$$\boldsymbol{\Lambda}=\frac{1}{2}\left(\boldsymbol{\nabla u}+(\boldsymbol{\nabla u})^{\mathrm{T}}-\frac{2}{D}\boldsymbol{I}\boldsymbol{\nabla}\cdot\boldsymbol{u}\right). \tag{3.35}$$

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

$$\partial_t\boldsymbol{a}_0^{(3)}+\boldsymbol{\nabla}\cdot\boldsymbol{a}_0^{(4)}+\left(\boldsymbol{\nabla a}_0^{(2)}+\text{perm}\right)=-\frac{1}{\tau}\boldsymbol{a}_1^{(3)}. \tag{3.36}$$

By using again (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

$$\boldsymbol{q}^{(1)}=-\tau\rho\theta\left(\frac{D+2}{2}\right)\boldsymbol{\nabla}\theta. \tag{3.37}$$

By comparing (3.34) and (3.37) with the Navier–Stokes equations, the transport coefficients μ and κ (the thermal diffusivity) can be identified with the relaxation time through the following relations

$$\mu=\kappa=\rho\theta\tau. \tag{3.38}$$

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

$$\partial_t\rho+\boldsymbol{\nabla}\cdot(\rho\boldsymbol{u})=0, \tag{3.39}$$
$$\partial_t(\rho\boldsymbol{u})+\boldsymbol{\nabla}\cdot(\rho\boldsymbol{uu})=-\boldsymbol{\nabla}p+\boldsymbol{\nabla}\cdot(2\mu\boldsymbol{\Lambda}), \tag{3.40}$$
$$\rho(\partial_t\varepsilon+\boldsymbol{u}\cdot\boldsymbol{\nabla}\varepsilon)+(p\boldsymbol{I}-2\mu\boldsymbol{\Lambda}):(\boldsymbol{\nabla u})=\left(\frac{D+2}{2}\right)\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla}\theta). \tag{3.41}$$

This derivation has been done in the case where τ is a constant, but all of this remains valid even for a relaxation time is depending on space and time, as long as it is independent of $\boldsymbol{\xi}$ (the moments of the distribution is only performed in the microscopic velocity space). Furthermore, as can be seen from (3.38), 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 that presented in Shan & Chen (2007).

When one is interested in the Navier–Stokes limit of this truncated BGK equation, all of these computations are exact as long as the distribution function is expanded in Hermite polynomials up to order $N\geqslant 4$. If $N=3$, the general form of the energy equation is preserved, but the Hermite coefficient $\boldsymbol{a}^{(4)}$ in (3.36) vanishes and therefore spurious terms are introduced in $\boldsymbol{q}^{(1)}$ and it is not anymore proportional to the temperature gradient. Nevertheless the constitutive equation for the deviatoric stress

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

N	Conservation laws	Macroscopic limit
1	Mass only	Advection–diffusion
2	Mass and momentum	Weakly compressible, athermal Navier–Stokes ($\theta = 1$)
3	Mass and momentum	Compressible, isothermal Navier–Stokes
4	Mass, momentum and energy	Compressible, thermal Navier–Stokes

TABLE 1. The macroscopic limit for small Knudsen number of the BGK Boltzmann equation depending on the truncation order N and the associated conservation laws.

remains unchanged. The macroscopic equations are therefore

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{3.42}$$

$$\partial_t (\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot (2\mu \boldsymbol{\Lambda}). \tag{3.43}$$

In the case where f is expanded up to order $N = 2$, the energy equation does not have the correct form anymore since $\boldsymbol{a}_0^{(3)}$ is null. The momentum conservation equation is still of the correct form, but the deviatoric stress tensor $\boldsymbol{P}^{(1)}$ will not be given by (3.35) but rather by

$$\boldsymbol{P}^{(1)} = -2\tau\rho\theta \boldsymbol{S}, \tag{3.44}$$

where $\boldsymbol{S} = (\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\mathrm{T}})/2$ and therefore this limit is valid only for weakly compressible flows where $\nabla \cdot \boldsymbol{u} \cong 0$ (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

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{3.45}$$

$$\partial_t (\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot (2\mu \boldsymbol{S}). \tag{3.46}$$

Finally at the order $N = 1$ an approximate advection–diffusion is recovered if no momentum conservation is imposed ($\int \boldsymbol{\xi} f \,\mathrm{d}\boldsymbol{\xi} \neq \int \boldsymbol{\xi} f^{(0)} \,\mathrm{d}\boldsymbol{\xi}$), and the associated macroscopic equation is found to be

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = \nabla \cdot (\kappa \nabla \rho). \tag{3.47}$$

All of these macroscopic 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 (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 (2.6), consists of replacing the relaxation time τ by its efficient counterpart τ_{eff}

$$\mu_{eff} = \mu + \mu_{sgs} = \rho\theta\tau + \rho\theta\tau_{sgs} = \rho\theta\tau_{eff}, \tag{3.48}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

where in the second equality (3.38) was used. The SGS relaxation time is then straightforwardly computed through the relation

$$\tau_{sgs} = \mu_{sgs}/(\rho\theta). \tag{3.49}$$

Replacing τ by τ_{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 § 5 that up to a certain order of approximation this result is obtained by an *a priori* analysis.

4. Consistent SGS 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

$$\partial_t \bar{f} + (\boldsymbol{\xi}\cdot\nabla)\bar{f} = \overline{\Omega(f)}, \tag{4.1}$$

where the filtering operation does not commute with the collision operator because of its nonlinear character

$$\overline{\Omega(f)} \neq \Omega(\bar{f}). \tag{4.2}$$

The filtered Boltzmann equation can be rewritten as

$$\partial_t \bar{f} + (\boldsymbol{\xi}\cdot\nabla)\bar{f} = \Omega(\bar{f}) + \mathscr{R}, \tag{4.3}$$

where $\mathscr{R} \equiv \overline{\Omega(f)} - \Omega(\bar{f})$ corresponds to the subgrid term that has to be modelled. Replacing Ω by the popular BGK collision operator, presented in the previous section (see (3.7)), on can rewrite this last equation as

$$\partial_t \bar{f} + (\boldsymbol{\xi}\cdot\nabla)\bar{f} = -\frac{1}{\tau}(\bar{f} - f^{(0)}(\bar{f})) + \underbrace{\frac{1}{\tau}(\overline{f^{(0)}} - f^{(0)}(\bar{f}))}_{=\mathscr{R}}, \tag{4.4}$$

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

Replacing $f^{(0)}$ by its Hermite expansion (see (3.10)) one can explicitly evaluate, order by order, the second term in the right-hand side of (4.4)

$$\begin{aligned}\mathscr{R} &= \frac{1}{\tau}\left(\overline{f^{(0)}} - f^{(0)}(\bar{f})\right) \\ &= \frac{w(\boldsymbol{\xi})}{\tau}\left\{\sum_{n=0}^{N}\frac{1}{n!}\boldsymbol{\mathcal{H}}^{(n)} : [\overline{\boldsymbol{a}_0^{(n)}(\rho,\boldsymbol{u},\theta)} - \boldsymbol{a}^{(n)}(\bar{\rho},\tilde{\boldsymbol{u}},\tilde{\theta})]\right\},\end{aligned} \tag{4.5}$$

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

$$\tilde{\boldsymbol{u}} \equiv \frac{\overline{\rho\boldsymbol{u}}}{\bar{\rho}}, \tag{4.6}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

$$\tilde{\theta} \equiv \frac{1}{\bar{\rho}} \left(\frac{1}{D} \int \tilde{\boldsymbol{c}}^2 \overline{f} \, \mathrm{d}\tilde{\boldsymbol{c}} \right), \tag{4.7}$$

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

Defining $\mathscr{R}^{(n)} \equiv \overline{\boldsymbol{a}_0^{(n)}(\rho, \boldsymbol{u}, \theta)} - \boldsymbol{a}_0^{(n)}(\bar{\rho}, \tilde{\boldsymbol{u}}, \tilde{\theta})$ we find up to order $N = 4$ (the order corresponding to compressible and thermal fluids)

$$\mathscr{R}^{(0)} = 0, \tag{4.8}$$

$$\mathscr{R}^{(1)}_{\alpha} = 0, \tag{4.9}$$

$$\mathscr{R}^{(2)}_{\alpha\beta} = T_{\alpha\beta} + \chi \delta_{\alpha\beta}, \tag{4.10}$$

$$\mathscr{R}^{(3)}_{\alpha\beta\gamma} = \sigma_{\alpha\beta\gamma} + \delta_{\alpha\beta} q_{\gamma} + \delta_{\alpha\gamma} q_{\beta} + \delta_{\beta\gamma} q_{\alpha}, \tag{4.11}$$

$$\begin{aligned} \mathscr{R}^{(4)}_{\alpha\beta\gamma\delta} = {} & \pi_{\alpha\beta\gamma\delta} + (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})(\varphi + 2\chi) \\ & + \delta_{\alpha\beta}\psi_{\gamma\delta} + \delta_{\alpha\gamma}\psi_{\beta\delta} + \delta_{\alpha\delta}\psi_{\beta\gamma} + \delta_{\beta\gamma}\psi_{\alpha\delta} + \delta_{\beta\delta}\psi_{\alpha\gamma} + \delta_{\gamma\delta}\psi_{\alpha\beta} \\ & - \delta_{\alpha\beta} T_{\gamma\delta} - \delta_{\alpha\gamma} T_{\beta\delta} - \delta_{\alpha\delta} T_{\beta\gamma} - \delta_{\beta\gamma} T_{\alpha\delta} - \delta_{\beta\delta} T_{\alpha\gamma} - \delta_{\gamma\delta} T_{\alpha\beta}. \end{aligned} \tag{4.12}$$

Here we defined seven different SGS quantities

$$T_{\alpha\beta} = \overline{\rho u_{\alpha} u_{\beta}} - \bar{\rho} \tilde{u}_{\alpha} \tilde{u}_{\beta}, \tag{4.13}$$

$$\chi = \overline{\rho\theta} - \bar{\rho}\tilde{\theta}, \tag{4.14}$$

$$\sigma_{\alpha\beta\gamma} = \overline{\rho u_{\alpha} u_{\beta} u_{\gamma}} - \bar{\rho} \tilde{u}_{\alpha} \tilde{u}_{\beta} \tilde{u}_{\gamma}, \tag{4.15}$$

$$q_{\alpha} = \overline{\rho\theta u_{\alpha}} - \bar{\rho}\tilde{\theta}\tilde{u}_{\alpha}, \tag{4.16}$$

$$\pi_{\alpha\beta\gamma\delta} = \overline{\rho u_{\alpha} u_{\beta} u_{\gamma} u_{\delta}} - \bar{\rho} \tilde{u}_{\alpha} \tilde{u}_{\beta} \tilde{u}_{\gamma} \tilde{u}_{\delta}, \tag{4.17}$$

$$\varphi = \overline{\rho\theta^2} - \bar{\rho}\tilde{\theta}^2, \tag{4.18}$$

$$\psi_{\alpha\beta} = \overline{\rho\theta u_{\alpha} u_{\beta}} - \bar{\rho}\tilde{\theta}\tilde{u}_{\alpha}\tilde{u}_{\beta}, \tag{4.19}$$

where $\boldsymbol{T}$, χ and $\boldsymbol{q}$, in particular, are the subgrid stress, subgrid temperature density and subgrid heat flux, respectively, and σ, π, ϕ and ψ 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, $\mathscr{R}^{(n)}$. 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 LES (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, Adams & Sagaut (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 by recalling that macroscopic variables such as internal energy are nonlinear functions of the distribution function f, and that filtering Navier–Stokes equations is equivalent to first applying a nonlinear operator to BGK equations before applying the linear filter.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$\partial_t \bar{f} + (\boldsymbol{\xi} \cdot \boldsymbol{\nabla})\bar{f} = -\frac{1}{\tau}(\bar{f} - f^{(0)}(\bar{f})) + \frac{w(\boldsymbol{\xi})}{\tau}\sum_{n=2}^{N}\frac{1}{n!}\boldsymbol{\mathcal{H}}^{(n)} : \mathscr{R}^{(n)}, \tag{4.20}$$

$$\partial_t \bar{f} + (\boldsymbol{\xi} \cdot \boldsymbol{\nabla})\bar{f} = -\frac{1}{\tau_{eff}}(\bar{f} - f^{(0)}(\bar{f})), \tag{4.21}$$

where

$$\tau_{eff} \equiv \frac{\tau}{\dfrac{\sum_n \boldsymbol{\mathcal{H}}^{(n)} : \mathscr{R}^{(n)}/n!}{(\bar{f} - f^{(0)}(\bar{f}))}}. \tag{4.22}$$

This result will be used in the following subsections.

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

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 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 equations (3.2)–(3.5) we can write the filtered macroscopic moments

$$\bar{\rho} = \overline{\int f \,\mathrm{d}\boldsymbol{\xi}} = \int \mathrm{d}\boldsymbol{\xi}\, \bar{f}, \tag{4.23}$$

$$\overline{\rho \boldsymbol{u}} = \overline{\int \boldsymbol{\xi} f \,\mathrm{d}\boldsymbol{\xi}} = \int \boldsymbol{\xi}\bar{f}\,\mathrm{d}\boldsymbol{\xi}, \tag{4.24}$$

$$\overline{\boldsymbol{P}} = \overline{\int \boldsymbol{c}\boldsymbol{c} f \,\mathrm{d}\boldsymbol{c}} = \int \boldsymbol{\xi}\boldsymbol{\xi}\bar{f}\,\mathrm{d}\boldsymbol{\xi} - \int \overline{\boldsymbol{u}f}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\xi} - \int \boldsymbol{\xi}\overline{\boldsymbol{u}f}\,\mathrm{d}\boldsymbol{\xi} + \int \overline{\boldsymbol{u}\boldsymbol{u}f}\,\mathrm{d}\boldsymbol{\xi}, \tag{4.25}$$

$$\bar{p} = \overline{\rho\theta} = \frac{1}{D}\overline{\int \boldsymbol{c}^2 f \,\mathrm{d}\boldsymbol{c}} = \frac{1}{D}\left(\int \boldsymbol{\xi}^2\bar{f}\,\mathrm{d}\boldsymbol{\xi} - 2\int \boldsymbol{\xi}\cdot\overline{\boldsymbol{u}f}\,\mathrm{d}\boldsymbol{\xi} + \int \overline{\boldsymbol{u}^2 f}\,\mathrm{d}\boldsymbol{\xi}\right). \tag{4.26}$$

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 exist different ways of

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

approximating them, and here we propose one)

$$\tilde{\boldsymbol{P}} = \int \tilde{\boldsymbol{c}}\tilde{\boldsymbol{c}}\overline{f}\,\mathrm{d}\boldsymbol{\xi}, \tag{4.27}$$

$$\tilde{p} = \frac{1}{D}\int \tilde{\boldsymbol{c}}^2\overline{f}\,\mathrm{d}\boldsymbol{\xi}, \tag{4.28}$$

where the 'computable' filtered velocity $\tilde{\boldsymbol{u}}$ is given by

$$\tilde{\boldsymbol{u}} = \frac{\int \boldsymbol{\xi}\overline{f}\,\mathrm{d}\boldsymbol{\xi}}{\bar{\rho}} \neq \overline{\left(\frac{\int \boldsymbol{\xi} f\,\mathrm{d}\boldsymbol{\xi}}{\int f\,\mathrm{d}\boldsymbol{\xi}}\right)} = \overline{\boldsymbol{u}}, \tag{4.29}$$

with $\tilde{\boldsymbol{c}} \equiv \boldsymbol{\xi} - \tilde{\boldsymbol{u}}$. From (4.28) one can deduce that the temperature $\tilde{\theta}$ can only be computed approximatively as

$$\tilde{\theta} = \tilde{p}/\bar{\rho}. \tag{4.30}$$

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

$$\Delta\overline{\boldsymbol{u}} = \overline{\boldsymbol{u}} - \tilde{\boldsymbol{u}}. \tag{4.31}$$

For the stress tensor things become even more difficult, because the error is not only depending on the SGS 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 SGS term and on the errors of all of 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 (4.4) and (4.5)

$$\overline{\Omega(f)} = -\frac{1}{\tau}(\overline{f} - f^{(0)}(\bar{f})) + \frac{w(\boldsymbol{\xi})}{\tau}\left\{\sum_{n=0}^{N}\frac{1}{n!}\boldsymbol{\mathcal{H}}^{(n)} : [\overline{\boldsymbol{a}_0^{(n)}(\rho,\boldsymbol{u},\theta)} - \boldsymbol{a}^{(n)}(\bar{\rho},\tilde{\boldsymbol{u}},\tilde{\theta})]\right\}. \tag{4.32}$$

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 $\overline{\rho\epsilon}$, defined as

$$\overline{\rho\varepsilon} = \frac{D}{2}\overline{p} = \frac{1}{2}\overline{\int \boldsymbol{c}^2 f\,\mathrm{d}\boldsymbol{\xi}}, \tag{4.33}$$

cannot be computed directly but similarly to (4.27) one can use the following definition

$$\widetilde{\epsilon} = \frac{1}{2}\frac{1}{\bar{\rho}}\int \tilde{\boldsymbol{c}}^2\overline{f}\,\mathrm{d}\boldsymbol{\xi}. \tag{4.34}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$\|\boldsymbol{\xi} - \tilde{\boldsymbol{u}}\|^2 = \|\boldsymbol{\mathcal{H}}^{(2)}\| + D - 2\boldsymbol{\xi} \cdot \tilde{\boldsymbol{u}} + \tilde{\boldsymbol{u}}^2. \tag{4.35}$$

The internal energy change due to the collision becomes

$$\frac{1}{2}\int \|\boldsymbol{\xi} - \tilde{\boldsymbol{u}}\|^2 \overline{\Omega(f)} = -\frac{1}{2\tau}((\overline{\rho \boldsymbol{u}^2} - \bar{\rho}\tilde{\boldsymbol{u}}^2 + D(\overline{\rho\theta} - \bar{\rho}\tilde{\theta})) - T_{\alpha\alpha} - D\chi) = 0. \tag{4.36}$$

This last relation is a consequence of the invariance of the trace of the moment of order two of the distribution function and shows that although the internal energy density is a nonlinear 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) and 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 $\{\boldsymbol{\xi}_i\}_{i=0}^{q-1}$

$$\partial_t \bar{f}_i + (\boldsymbol{\xi}_i \cdot \nabla)\bar{f}_i = -\frac{1}{\tau}(\bar{f}_i - f_i^{(0)}) + \frac{1}{\tau} w_i \sum_{n=0}^{N} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}/(n! c_s^{2n}), \tag{4.37}$$

$$= -\frac{1}{\tau}\left(\bar{f}_i - f_i^{eq}\right), \tag{4.38}$$

where $\bar{f}_i = \bar{f}(\boldsymbol{x}, \boldsymbol{\xi}_i, t)$ and $f_i^{eq} = f^{(0)} - w_i \sum_{n=0}^{N} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}/(n! c_s^{2n})$. The discretized efficient relaxation time $\tau_{i,eff}^{(N)}$ (corresponding to τ_{eff} of (4.22)), which in the general case depends on both the discrete velocity i and the Hermite expansion truncation order N, is found to be

$$\tau_{i,eff}^{(N)} = \frac{\tau}{1 - \dfrac{1}{(\bar{f}_i - f_i^{(0)})} \displaystyle\sum_{n=0}^{N} \frac{w_i}{n! c_s^{2n}} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}}, \tag{4.39}$$

where c_s is a constant depending on the lattice, which can be interpreted as the isentropic expansion factor γ of the lattice, and w_i are the weights related to the discrete velocities $\boldsymbol{\xi}_i$. 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 (4.38), which is done with the standard trapezoidal integration combined with a change of variables (see Dellar 2001; Malaspinas 2009, for example). The fully discrete LBM reads (the temporal discretization step is chosen

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

as $\delta t = 1$ for simplicity in the notation)

$$\hat{f}_i(\boldsymbol{x}+\boldsymbol{\xi}_i, t+1) = \hat{f}_i(\boldsymbol{x}, t) - \frac{1}{\hat{\tau}}(\hat{f}_i(\boldsymbol{x}, t) - f_i^{(0)}(\boldsymbol{x}, t)) + \frac{w_i}{\hat{\tau}} \sum_{n=0}^{N} \frac{1}{n! c_s^{2n}} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}, \quad (4.40)$$

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

$$\hat{f}_i = \bar{f}_i + \frac{1}{2\tau}(\bar{f}_i - f_i^{eq}), \quad (4.41)$$

One can also rewrite (4.40) in a more standard way with a the fully discrete efficient relaxation time $\hat{\tau}_{i,eff}^{(N)}$

$$\hat{f}_i(\boldsymbol{x}+\boldsymbol{\xi}_i, t+1) = \hat{f}_i(\boldsymbol{x}, t) - \frac{1}{\hat{\tau}_{i,eff}^{(N)}}(\hat{f}_i(\boldsymbol{x}, t) - f_i^{(0)}(\boldsymbol{x}, t)), \quad (4.42)$$

with

$$\begin{aligned} \hat{\tau}_{i,eff}^{(N)} &\equiv \frac{\hat{\tau}}{\left(1 - \dfrac{\displaystyle\sum_{n=1}^{N} \frac{w_i}{n! c_s^{2n}} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}}{\hat{f}_i - f_i^{(0)}}\right)} \\ &= \frac{2\mu_0 + c_s^2 \rho_0 \theta_0}{2c_s^2 \rho_0 \theta_0 \left(1 - \dfrac{\displaystyle\sum_{n=1}^{N} \frac{w_i}{n! c_s^{2n}} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}}{\hat{f}_i - f_i^{(0)}}\right)}. \end{aligned} \quad (4.43)$$

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 θ_0 and density ρ_0). Equation (4.40) along with (4.43) gives us a completely generic formula for implementing SGS closures for any order of Hermite series truncation.

4.5. *Implementation formulae*

So far, in this section, we showed a consistent way of implementing SGS 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 in the LBM.

For implementation purposes, we write here explicitly the basic constitutive terms of the LBM scheme with a SGS closure of order up to $N = 4$. The LBM scheme of (4.40) can be rewritten as

$$\hat{f}_i(\boldsymbol{x}+\boldsymbol{\xi}_i, t+1) = \hat{f}_i(\boldsymbol{x}, t) - \frac{1}{\hat{\tau}}(\hat{f}_i(\boldsymbol{x}, t) - f_i^{(0)}(\boldsymbol{x}, t)) + \mathscr{R}_i, \quad (4.44)$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$
\begin{aligned}
f_i^{(0)} &= w_i \sum_{n=0}^{4} \frac{1}{c_s^{2n} n!} \boldsymbol{\mathcal{H}}_i^{(n)} : \boldsymbol{a}_0^{(n)} \\
&= w_i \Bigg\{ \bar{\rho} && (N=0) \\
&\quad + \frac{1}{c_s^2} \xi_{i\alpha} \bar{\rho} \tilde{u}_\alpha && (N=1) \\
&\quad + \frac{1}{2c_s^4} \boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)} (\bar{\rho} \tilde{u}_\alpha \tilde{u}_\beta + c_s^2 \bar{\rho} (\tilde{\theta} - 1) \delta_{\alpha\beta}) && (N=2) \\
&\quad + \frac{1}{6c_s^6} \boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma}^{(3)} (\bar{\rho} \tilde{u}_\alpha \tilde{u}_\beta \tilde{u}_\gamma + c_s^2 \bar{\rho} (\tilde{\theta} - 1) \\
&\quad \times (\delta_{\alpha\beta} \tilde{u}_\gamma + \delta_{\alpha\gamma} \tilde{u}_\beta + \delta_{\beta\gamma} \tilde{u}_\alpha) && (N=3) \\
&\quad + \frac{1}{24c_s^8} \boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma\delta}^{(4)} [\bar{\rho} \tilde{u}_\alpha \tilde{u}_\beta \tilde{u}_\gamma \tilde{u}_\delta + c_s^4 \bar{\rho} \, (\tilde{\theta} - 1)^2 \\
&\quad \times (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \\
&\quad + c_s^2 \bar{\rho} (\tilde{\theta} - 1) (\delta_{\alpha\beta} \tilde{u}_\gamma \tilde{u}_\delta + \delta_{\alpha\gamma} \tilde{u}_\beta \tilde{u}_\delta + \delta_{\alpha\delta} \tilde{u}_\beta \tilde{u}_\gamma)] \Bigg\} && (N=4)
\end{aligned}
\tag{4.45}
$$

and the subgrid terms $\mathscr{R}_i$, to be added in the collision term of the LBM, are given by

$$
\begin{aligned}
\mathscr{R}_i &= \frac{w_i}{\hat{\tau}} \sum_{n=0}^{4} \frac{1}{c_s^{2n} n!} \boldsymbol{\mathcal{H}}_i^{(n)} : \boldsymbol{\mathscr{R}}^{(n)} \\
&= w_i \Bigg\{ && (N=0) \\
&\quad + \frac{1}{c_s^2} \xi_{i\alpha} (\overline{\rho u}_\alpha - \bar{\rho} \tilde{u}_\alpha) && (N=1) \\
&\quad + \frac{1}{2c_s^4} \boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)} (T_{\alpha\beta} + \chi \delta_{\alpha\beta}) && (N=2) \\
&\quad + \frac{1}{6c_s^6} \boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma}^{(3)} (\sigma_{\alpha\beta\gamma} + \delta_{\alpha\beta} q_\gamma + \delta_{\alpha\gamma} q_\beta + \delta_{\beta\gamma} q_\alpha) && (N=3) \\
&\quad + \frac{1}{24c_s^8} \boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma\delta}^{(4)} \big[\pi_{\alpha\beta\gamma\delta} + (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})(\varphi + 2\chi) \\
&\quad + \delta_{\alpha\beta} \psi_{\gamma\delta} + \delta_{\alpha\gamma} \psi_{\beta\delta} + \delta_{\alpha\delta} \psi_{\beta\gamma} + \delta_{\beta\gamma} \psi_{\alpha\delta} + \delta_{\beta\delta} \psi_{\alpha\gamma} + \delta_{\gamma\delta} \psi_{\alpha\beta} \\
&\quad - \delta_{\alpha\beta} T_{\gamma\delta} - \delta_{\alpha\gamma} T_{\beta\delta} - \delta_{\alpha\delta} T_{\beta\gamma} - \delta_{\beta\gamma} T_{\alpha\delta} - \delta_{\beta\delta} T_{\alpha\gamma} - \delta_{\gamma\delta} T_{\alpha\beta}] \Bigg\} && (N=4).
\end{aligned}
\tag{4.46}
$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$\mathcal{H}_i^{(0)} = 1, \tag{4.47}$$

$$\mathcal{H}_{i\alpha}^{(1)} = \xi_{i\alpha}, \tag{4.48}$$

$$\mathcal{H}_{i\alpha\beta}^{(2)} = \xi_{i\alpha}\xi_{i\beta} - c_s^2\delta_{\alpha\beta}, \tag{4.49}$$

$$\mathcal{H}_{i\alpha\beta\gamma}^{(3)} = \xi_{i\alpha}\xi_{i\beta}\xi_{i\gamma} - c_s^2(\delta_{\alpha\beta}\xi_{i\gamma} + \delta_{\alpha\gamma}\xi_{i\beta} + \delta_{\beta\gamma}\xi_{i\alpha}), \tag{4.50}$$

$$\begin{aligned}\mathcal{H}_{i\alpha\beta\gamma\delta}^{(4)} = {} & \xi_{i\alpha}\xi_{i\beta}\xi_{i\gamma}\xi_{i\delta} - c_s^2(\delta_{\alpha\beta}\xi_{i\gamma}\xi_{i\delta} + \delta_{\alpha\gamma}\xi_{i\beta}\xi_{i\delta} + \delta_{\alpha\delta}\xi_{i\beta}\xi_{i\gamma} \\ & + \delta_{\beta\gamma}\xi_{i\alpha}\xi_{i\delta} + \delta_{\beta\delta}\xi_{i\alpha}\xi_{i\gamma} + \delta_{\gamma\delta}\xi_{i\alpha}\xi_{i\beta}) \\ & + c_s^4(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}).\end{aligned} \tag{4.51}$$

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*) $N = 3, 4$, isothermal and thermal Navier–Stokes equations.

We propose a link with the classical way of introducing eddy viscosity (diffusivity) models (see § 3) by performing a Chapman–Enskog-like expansion of (4.37). From (3.22), one can write the filtered f_i in terms of the filtered equilibrium and non-equilibrium distribution functions as

$$\bar{f}_i = \overline{f_i^{(0)}} + \overline{f_i^{(1)}}. \tag{5.1}$$

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

$$\bar{f}_i \cong f_i^{(0)}(\bar{f}_i) + f_i^{(1)}(\bar{f}_i), \tag{5.2}$$

$$= \sum_{n=0}^{N} \frac{w_i}{c_s^{2n} n!} \mathcal{H}_i^{(n)} : (\tilde{\boldsymbol{a}}_0^{(n)}(\bar{f}_i) + \tilde{\boldsymbol{a}}_1^{(n)}(\bar{f}_i)) \tag{5.3}$$

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

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

$$\tau_{i,eff}^{(N)} = \frac{\tau}{1 - \dfrac{\displaystyle\sum_{n=1}^{N} \frac{1}{c_s^{2n} n!} \mathcal{H}_i^{(n)} : \mathscr{R}^{(n)}}{\displaystyle\sum_{n=1}^{N} \frac{1}{c_s^{2n} n!} \mathcal{H}_i^{(n)} : \tilde{\boldsymbol{a}}_1^{(n)}(\bar{f})}}. \tag{5.4}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

We emphasize at this point that the Ansatz of (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 and the results obtained there are used in §§ 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, Shi & Zheng (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 $\int \boldsymbol{\xi} f \,\mathrm{d}\boldsymbol{\xi} \neq \int \boldsymbol{\xi} f^{(0)} \,\mathrm{d}\boldsymbol{\xi}$), gives the following macroscopic limit

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} \rho), \tag{5.5}$$

with $\kappa = c_s^2 \tau$. Furthermore, only $\mathscr{R}^{(1)}$ and $\tilde{\boldsymbol{a}}_1^{(1)}$ (the superscript (1) is referring to the Hermite truncation order) are considered in (4.39), and all higher-order terms are neglected. The reader should be aware that both of 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 $\mathscr{R}^{(1)}$ vector is given by

$$\mathscr{R}^{(1)} = -\boldsymbol{\nabla} \cdot (\kappa_{sgs} \boldsymbol{\nabla} \bar{\rho}), \tag{5.6}$$

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

$$\tilde{\boldsymbol{a}}_1^{(1)} = -c_s^2 (\tau + \tau_{sgs}) \boldsymbol{\nabla} \bar{\rho}, \tag{5.7}$$

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

$$\begin{aligned} \tau_{i,eff}^{(1)} &= \frac{\tau}{1 - \left(\dfrac{-\kappa_{sgs} \boldsymbol{\mathcal{H}}_i^{(1)} \cdot (\boldsymbol{\nabla} \bar{\rho})}{-c_s^2 (\tau + \tau_{sgs}) \boldsymbol{\mathcal{H}}_i^{(1)} \cdot (\boldsymbol{\nabla} \bar{\rho})} \right)} \\ &= \frac{\tau}{1 - \dfrac{\tau_{sgs}}{\tau + \tau_{sgs}}} = \tau + \tau_{sgs}, \end{aligned} \tag{5.8}$$

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

Finally, after time–space integration (presented shortly in § 4.4), the efficient relaxation time $\hat{\tau}_{i,eff}^{(1)}$ (see (4.43)) is given by (the Hermite truncation order is omitted for the sake of clarity)

$$\hat{\tau}_{i,eff} = \hat{\tau} + \tau_{sgs} \tag{5.9}$$

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

$$\kappa_{eff} = \kappa + \kappa_{sgs} = c_s^2 (\hat{\tau} - 1/2 + \tau_{sgs}). \tag{5.10}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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 athermal 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 $\mathscr{R}^{(2)}$ and $\tilde{\boldsymbol{a}}_1^{(2)}$ remain in (4.43) and all of the higher-order terms can be neglected. As in the preceding subsection, let us focus only on the eddy viscosity assumption for modelling $\mathscr{R}^{(2)}$

$$\mathscr{R}^{(2)} = -2\mu_{sgs}\overline{\mathbf{S}}. \tag{5.11}$$

Furthermore the Chapman–Enskog expansion gives us for $\tilde{\boldsymbol{a}}_1^{(2)}$ (see (A 14))

$$\tilde{\boldsymbol{a}}_1^{(2)} = -2c_s^2(\tau + \tau_{sgs})\bar{\rho}\tilde{\theta}\,\overline{\mathbf{S}}, \tag{5.12}$$

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

$$\tau_{i,eff}^{(2)} = \frac{\tau}{\left(1 - \dfrac{\tau_{sgs}}{(\tau + \tau_{sgs})}\right)} = \tau + \tau_{sgs} \tag{5.13}$$

where we point out that the relaxation time is again not dependent on the microscopic velocity (as in the preceding subsection), since the terms depending on $\boldsymbol{\mathcal{H}}_i^{(2)}$ are cancelled out. Thus, we recovered the classical way of incorporating eddy viscosity closures in the BGK equation (see (3.48)).

For implementation purposes, one needs to use the $\hat{\tau}_{i,eff}^{(2)}$ relaxation time of (4.43). As in the previous subsection, it is straightforward to find

$$\hat{\tau}_{i,eff}^{(2)} = \hat{\tau} + \tau_{sgs}, \tag{5.14}$$

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 ($N \geqslant 3$ is the Hermite expansion of distribution function, see table 1) the simplifications done in the previous section are no longer possible. To be more explicit let us consider the case $N = 3$ (i.e. the isothermal compressible Navier–Stokes approximation). In this case, the SGS terms involved in (4.43) are $\mathscr{R}^{(2)}$ and $\mathscr{R}^{(3)}$, while only $\tilde{\boldsymbol{a}}_1^{(2)}$ is considered, since higher-order terms do not enter the macroscopic physics of isothermal fluids ($\tilde{\boldsymbol{a}}_1^{(3)}$ is only relevant in the energy conservation equation). Then, (4.43) becomes

$$\begin{aligned}\hat{\tau}_{i,eff}^{(N)} &= \frac{2\mu + c_s^2\bar{\rho}\tilde{\theta}}{2c_s^2\bar{\rho}\tilde{\theta}} \frac{1}{1 + \dfrac{\boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)}\mathscr{R}_{\alpha\beta}^{(2)} + \dfrac{1}{3c_s^4}\boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma}^{(3)}R_{\alpha\beta\gamma}^{(3)}}{\left(\boldsymbol{\mathcal{H}}_{\alpha\beta}^{(2)}\left(\tau\bar{\rho}\tilde{\theta}\cdot\overline{\Lambda}_{\alpha\beta} - \mathscr{R}_{\alpha\beta}^{(2)}\right)\right)}}, \\ &= \hat{\tau}\left(\frac{\boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)}(2\tau\bar{\rho}\tilde{\theta}\cdot\overline{\Lambda}_{\alpha\beta} - \mathscr{R}_{\alpha\beta}^{(2)})}{2\tau\bar{\rho}\tilde{\theta}\boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)}\overline{\Lambda}_{\alpha\beta} + \dfrac{1}{3c_s^4}\boldsymbol{\mathcal{H}}_{i\alpha\beta\gamma}^{(3)}\mathscr{R}_{\alpha\beta\gamma}^{(3)}}\right),\end{aligned} \tag{5.15}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

where $\overline{\Lambda}_{\alpha\beta} = \left(\partial_\alpha \overline{u}_\beta + \partial_\beta \overline{u}_\alpha - (2/D)\delta_{\alpha\beta}\partial_\gamma \overline{u}_\gamma\right)$. Thus, the approximation $\hat{\tau}_{eff}^{(N)} = \hat{\tau} + \tau_{sgs}$ no longer holds for $N \geqslant 3$. 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 not 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 § 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)

$$\sum_i \boldsymbol{\mathcal{H}}_i^{(2)} \hat{f}_i^{(1)} = \hat{\boldsymbol{a}}_1^{(2)} = -2c_s^2 \bar{\rho} \hat{\tau}_{eff} \overline{\boldsymbol{S}}. \tag{6.1}$$

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

$$\mu_{sgs} = \bar{\rho}\,(C\Delta)^2 \left\|\overline{\boldsymbol{S}}\right\| \Rightarrow \tau_{sgs} = \frac{(C\Delta)^2}{c_s^2} \left\|\overline{\boldsymbol{S}}\right\|, \tag{6.2}$$

where Δ is the filter width and C the Smagorinsky constant. Thus, in order to compute $\overline{\boldsymbol{S}}$ locally one must solve the system (Einstein's summation convention is understood for repeated indexes)

$$\hat{a}_{1\alpha\beta}^{(1)} = -2\bar{\rho}c_s^2 \left(\hat{\tau} + \frac{(C\Delta)^2}{c_s^2}\sqrt{2\overline{S}_{\gamma\delta}\overline{S}_{\gamma\delta}}\right)\overline{S}_{\alpha\beta}. \tag{6.3}$$

This equation admits four roots, which have the following form

$$\overline{S}_{\alpha\beta} = \zeta \hat{a}_{1\alpha\beta}^{(2)}, \tag{6.4}$$

where ζ is solution of the following equation

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

The solutions of this equation are given by

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

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

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

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

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

While it is possible to exclude ζ_1 and ζ_2 because they might give complex solutions, it is impossible to chose *a priori* between ζ_3 and ζ_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 Chapman–Enskog result

$$\overline{\boldsymbol{S}} = -\frac{1}{\bar{\rho}\hat{\tau}c_s^2}\hat{\boldsymbol{a}}_1^{(2)} \Leftrightarrow \zeta = -\frac{1}{\bar{\rho}\hat{\tau}c_s^2}. \tag{6.10}$$

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

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

$$\cong \frac{\bar{\rho}\hat{\tau}c_s^2}{2\,(C\Delta)^2\,\|\hat{\boldsymbol{a}}_1^{(2)}\|\bar{\rho}}\left(1 \pm \left(1 + \frac{(C\Delta)^2\,\|\hat{\boldsymbol{a}}_1^{(2)}\|\bar{\rho}}{\bar{\rho}^2\hat{\tau}^2c_s^4}\right)\right). \tag{6.12}$$

Finally, we have that

$$\zeta_+ \cong \frac{\bar{\rho}\hat{\tau}c_s^2}{(C\Delta)^2\,\|\hat{\boldsymbol{a}}_1^{(2)}\|\bar{\rho}} + \frac{1}{2\bar{\rho}\hat{\tau}c_s^2}, \tag{6.13}$$

$$\zeta_- \cong -\frac{1}{2\bar{\rho}\hat{\tau}c_s^2}. \tag{6.14}$$

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

$$\overline{S}_{\alpha\beta} = \zeta_4\hat{a}_{1\alpha\beta}^{(2)}. \tag{6.15}$$

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 formulae will be tested. The first one uses the approximation of (5.14), where

$$\tau_{sgs} = \frac{(C\Delta)^2}{c_s^2}\left\|\overline{\boldsymbol{S}}\right\|, \tag{7.1}$$

will be referred to as 'consistent strain' hereafter. In this case the strain rate is computed locally according to (6.15). The second implements the exact formulation of (4.43), where

$$\mathscr{R}_i = \frac{w_i}{\hat{\tau}}\frac{(C\Delta)^2}{2c_s^4}\left\|\overline{\boldsymbol{S}}\right\|\boldsymbol{\mathcal{H}}_{i\alpha\beta}^{(2)}\overline{S}_{\alpha\beta}, \tag{7.2}$$

will be denoted as the '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 (5.14) but

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

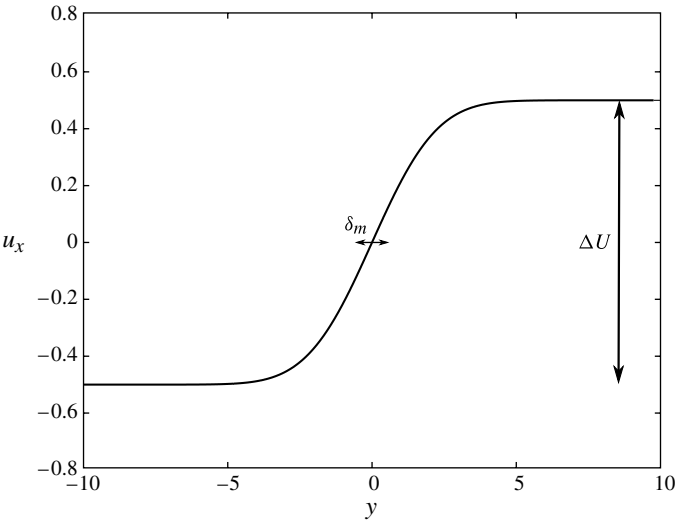


FIGURE 1. The horizontal velocity profile with respect to y, for $\Delta U = 1$ and $\delta_m = 1$.

SGS model	Ω	Strain rate computation
Consistent strain	$-\left(\hat{\tau} + (C\Delta)^2/c_s^2\|\overline{\boldsymbol{S}}\|\right)^{-1}(\hat{f}_i - f_i^{(0)})$	$\overline{\boldsymbol{S}} = \zeta_4 \hat{a}_1^{(2)}$
Consistent Smagorinsky	$-\frac{1}{\hat{\tau}}(\hat{f}_i - f_i^{(0)}) + \frac{w_i (C\Delta)^2}{2c_s^4 \hat{\tau}}\|\overline{\boldsymbol{S}}\|\mathscr{H}_i^{(2)} : \overline{\boldsymbol{S}}$	$\overline{\boldsymbol{S}} = (\nabla\tilde{\boldsymbol{u}} + (\nabla\tilde{\boldsymbol{u}})^{\mathrm{T}})/2$, FD
Naive	$-\left(\hat{\tau} + (C\Delta)^2\|\overline{\boldsymbol{S}}\|/c_s^2\right)^{-1}(\hat{f}_i - f_i^{(0)})$	$\overline{\boldsymbol{S}} = -\hat{a}_1^{(2)}/(\rho\hat{\tau}c_s^2)$

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

this time $\overline{\boldsymbol{S}}$ will be computed using the lower-order approximation

$$\overline{\boldsymbol{S}} = -\frac{1}{\rho\hat{\tau}c_s^2}\hat{\boldsymbol{a}}_1^{(2)}, \tag{7.3}$$

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 figure 1)

$$u_x = \frac{1}{2}\Delta U erf\left(\frac{y}{\sqrt{2\pi}\delta_0}\right), \quad u_y = 0, \quad u_z = 0. \tag{7.4}$$

where ΔU is the difference of velocity between the two layers, δ_0 the initial momentum thickness, and erf the error function

$$erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,\mathrm{d}t. \tag{7.5}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

The momentum thickness δ_m is defined as

$$\delta_m = \int_{-\infty}^{\infty} \left(\frac{1}{4} - \frac{u_x^2}{\Delta U^2} \right) \mathrm{d}y \tag{7.6}$$

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 δ_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, Sagaut & Basdevant (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 δ_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 $\{\boldsymbol{\xi}_i\}_{i=0}^{18}$ is

$$\begin{aligned} \boldsymbol{\xi}_i = \{&(0,0,0),\\ &(-1,0,0),(0,-1,0),(0,0,-1),\\ &(-1,-1,0),(-1,+1,0),(-1,0,-1),(-1,0,+1),\\ &(0,-1,-1),(0,-1,+1),\\ &(+1,0,0),(0,+1,0),(0,0,+1),\\ &(+1,+1,0),(+1,-1,0),(+1,0,+1),(+1,0,-1),\\ &(0,+1,+1),(0,+1,-1)\}. \end{aligned} \tag{7.7}$$

and the weights w_i and c_s^2 are given by

$$w_0 = 1/3, \quad w_{1,2,3,10,11,12} = 1/18, \quad w_{4,5,6,7,8,9,13,14,15,16,17,18} = 1/36, \quad c_s^2 = 1/3. \tag{7.8}$$

7.1. *Results*

As can be seen from figure 2 the 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 $\mathrm{d}\delta_m/\mathrm{d}\tau = 0.014$ and is in good agreement with the DNS of Rogers & Moser (1994) (note that the curve of Rogers and 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 note 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 SGS 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.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

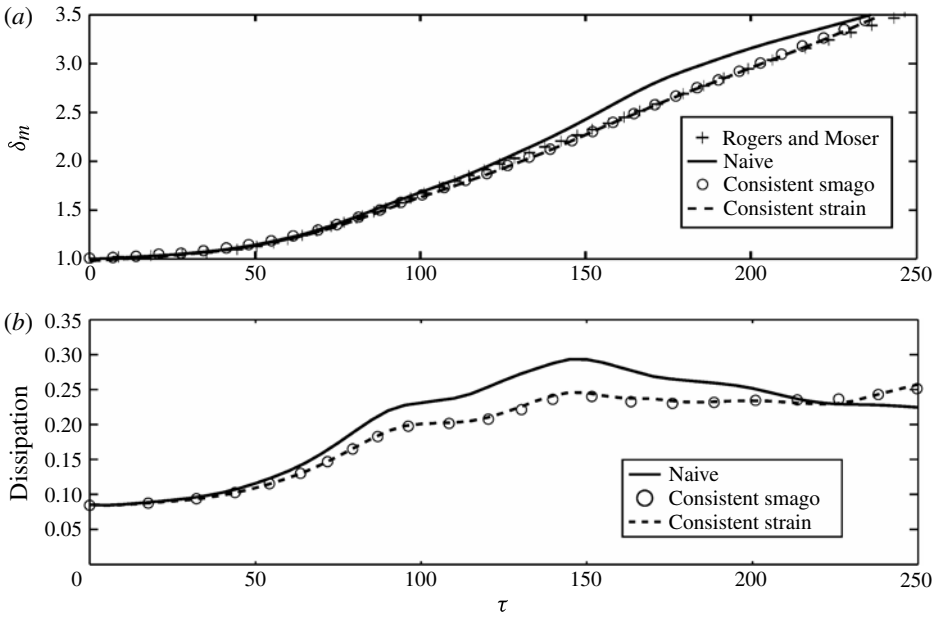


FIGURE 2. Momentum thickness (a) and dissipation (b) with respect to the non-dimensional time $\tau = t\Delta U/\delta_m$.

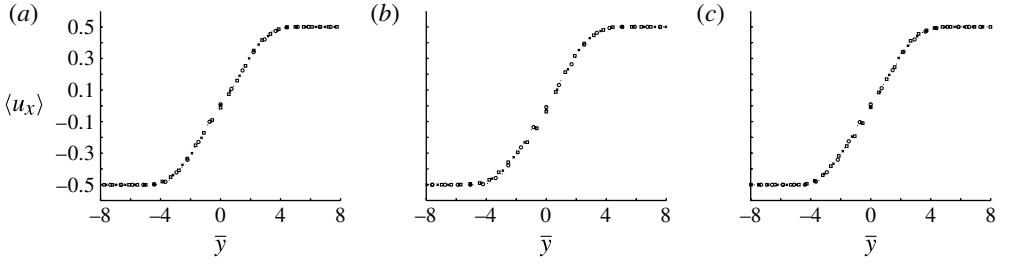


FIGURE 3. Average velocity with respect to the non-dimensional position $\overline{y} = y/\delta_m$ for the 'naive' (a), 'consistent Smagorinsky' (b) and the 'consistent strain' (c) cases for five instantaneous times during the self-similar period.

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 root mean square (r.m.s.) velocity are correctly recovered for all of the three cases, as shown in figures 3 and 4. The average and r.m.s. velocity curves all coincide when plotted with respect to the non-dimensional y-position, $\overline{y} \equiv y/\delta_m$.

Finally we also plotted the one-dimensional 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.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

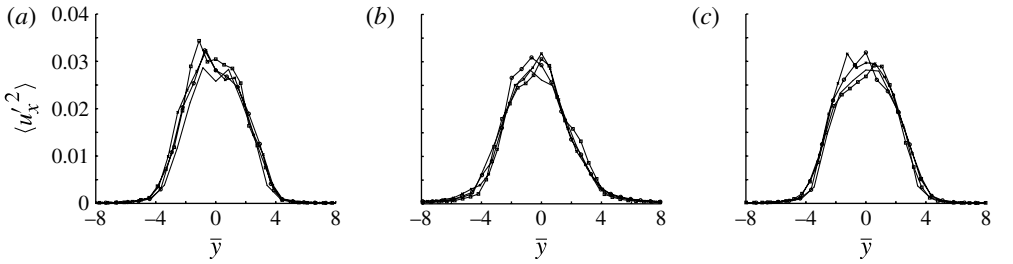


FIGURE 4. Average r.m.s. velocity with respect to the non-dimensional position $\bar{y} = y/\delta_m$ for the 'naive' (*a*), 'consistent Smagorinsky' (*b*) and the 'consistent strain' (*c*) cases for five instantaneous times during the self-similar period.

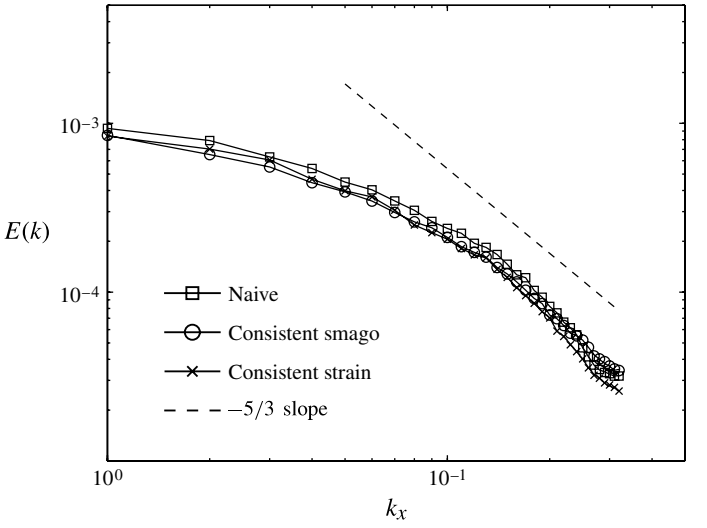


FIGURE 5. One-dimensional energy spectrum with respect to k_x.

8. Conclusion

In this paper we showed how to theoretically include, in a consistent fashion, SGS 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 also allows us to 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.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

Acknowledgement

O.M. would like to thankfully acknowledge the support of the Swiss National Science Foundation SNF (Award PBELP2-133356).

Appendix. Chapman–Enskog expansion of the filtered BGK equation

In this appendix we perform 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 shown in detail here). The filtered BGK equation (4.37) is given by

$$\partial_t \bar{f}_i + (\boldsymbol{\xi}_i \cdot \nabla)\bar{f}_i = -\frac{1}{\tau}(\bar{f}_i - f_i^{(0)}(\bar{f}_i)) + \frac{1}{\tau}\sum_{n=0}^{N} \frac{1}{c_s^{2n} n!} \boldsymbol{\mathcal{H}}_i^{(n)} : \mathscr{R}^{(n)}. \tag{A 1}$$

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

$$\bar{f}_i = f_i^{(0)}(\bar{f}_i) + f_i^{(1)}, \quad f_i^{(1)} \ll f_i^{(0)}, \tag{A 2}$$

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

$$\partial_t \bar{\rho} + \nabla \cdot \left(\bar{\rho}\tilde{\boldsymbol{u}} + \tilde{\boldsymbol{a}}_1^{(1)}\right) = 0, \tag{A 3}$$

where we impose mass conservation ($\sum_i f_i^{(1)} = 0$), but momentum is not conserved ($\sum_i \boldsymbol{\xi}_i f_i^{(1)} = \tilde{\boldsymbol{a}}_1^{(1)} \neq 0$). We therefore need to compute $\tilde{\boldsymbol{a}}_1^{(1)}$ (here the $\tilde{\boldsymbol{a}}_0^{(n)}$ and $\tilde{\boldsymbol{a}}_1^{(n)}$ stand for the coefficients related to $f_i^{(0)}(\bar{f}_i)$ and $f_i^{(1)}(\bar{f}_i)$). To this aim, we project the filtered BGK equation (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 notation)

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

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 left-hand side of this equation is null because of mass and momentum conservation and one obtains

$$\partial_t \bar{\rho} + \nabla \cdot (\bar{\rho}\tilde{\boldsymbol{u}}) = 0. \tag{A 5}$$

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

$$\partial_t(\bar{\rho}\tilde{\boldsymbol{u}}) + c_s^2 \nabla \bar{\rho} = -\frac{1}{\tau}\tilde{\boldsymbol{a}}_1^{(1)} + \frac{1}{\tau}\mathscr{R}^{(1)}, \tag{A 6}$$

Using (A 5) and after some algebra, one obtains

$$\tilde{\boldsymbol{a}}_1^{(1)} = -c_s^2 \tau \nabla \bar{\rho} + \mathscr{R}^{(1)} + \underbrace{\tau\left(\tilde{\boldsymbol{u}}\nabla \cdot (\rho\tilde{\boldsymbol{u}}) - \rho\partial_t \tilde{\boldsymbol{u}}\right)}_{\mathscr{E}}, \tag{A 7}$$

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

$$\partial_t \bar{\rho} + \nabla \cdot (\bar{\rho}\tilde{\boldsymbol{u}}) = \nabla \cdot \left(\kappa \nabla \bar{\rho} - \mathscr{R}^{(1)}\right), \tag{A 8}$$

with $\kappa = c_s^2 \tau$.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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 ($\sum_i \boldsymbol{\xi}_i f_i^{(1)} = \tilde{\boldsymbol{a}}_1^{(1)} = 0$). Thus, taking zeroth and first-order moments of the filtered BGK equation, one obtains

$$\partial_t \bar{\rho} + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}) = 0, \tag{A 9}$$

$$\partial_t (\bar{\rho}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\tilde{\boldsymbol{P}}^{(0)} + \tilde{\boldsymbol{P}}^{(1)}) = 0, \tag{A 10}$$

where $\tilde{\boldsymbol{P}}^{(0)} = \sum_i \tilde{\boldsymbol{c}}_i \tilde{\boldsymbol{c}}_i f_i^{(0)}(\bar{f}_i) = c_s^2 \bar{\rho}\tilde{\theta}\boldsymbol{I}$ and $\tilde{\boldsymbol{P}}^{(1)} = \sum_i \tilde{\boldsymbol{c}}_i \tilde{\boldsymbol{c}}_i f_i^{(1)}$. We therefore need to compute $\tilde{\boldsymbol{P}}^{(1)}$. To this aim, we use (A 4). For $n = 0$ and $n = 1$, the left-hand side of this equation is null because of mass and momentum conservation and one obtains

$$\partial_t \bar{\rho} + \boldsymbol{\nabla} \cdot \bar{\rho}\tilde{\boldsymbol{u}} = 0, \tag{A 11}$$

$$\partial_t (\bar{\rho}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) = -\boldsymbol{\nabla}\tilde{p}, \tag{A 12}$$

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

$$\begin{aligned} &\partial_t (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}} + \bar{\rho}(\tilde{\theta} - 1)(\boldsymbol{I}\tilde{\boldsymbol{u}} + \text{perm})) \\ &\quad - c_s^2 (\boldsymbol{\nabla}(\bar{\rho}\tilde{\boldsymbol{u}}) + (\boldsymbol{\nabla}(\bar{\rho}\tilde{\boldsymbol{u}}))^{\mathrm{T}}) = -\frac{1}{\tau}\tilde{\boldsymbol{a}}_1^{(2)} + \frac{1}{\tau}\mathscr{R}^{(2)}, \end{aligned} \tag{A 13}$$

with the superscript 'T' denoting the transpose operation. Using (A 11) and (A 12) and after some tedious algebra, one obtains

$$\tilde{\boldsymbol{a}}_1^{(2)} = -2c_s^2 \tau \bar{\rho}\tilde{\theta}\tilde{\boldsymbol{\Lambda}} + \mathscr{R}^{(2)}, \tag{A 14}$$

where $\tilde{\boldsymbol{\Lambda}} = (\boldsymbol{\nabla}\tilde{\boldsymbol{u}} + (\boldsymbol{\nabla}\tilde{\boldsymbol{u}})^{\mathrm{T}})/2 = \overline{\boldsymbol{S}}$ for $N = 2$ and $\tilde{\boldsymbol{\Lambda}} = (\boldsymbol{\nabla}\tilde{\boldsymbol{u}} + (\boldsymbol{\nabla}\tilde{\boldsymbol{u}})^{\mathrm{T}} - (2/D)\boldsymbol{I}\boldsymbol{\nabla} \cdot \tilde{\boldsymbol{u}})$ for $N \geqslant 3$. 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 $\tilde{u}^3$ that are neglected. Using this last relation one can compute $\tilde{\boldsymbol{P}}^{(1)}$ and one gets for the momentum conservation equation

$$\partial_t (\bar{\rho}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) = -\boldsymbol{\nabla}\tilde{p} + \boldsymbol{\nabla} \cdot (2\mu\tilde{\boldsymbol{\Lambda}}) - \boldsymbol{\nabla} \cdot \mathscr{R}^{(2)}, \tag{A 15}$$

where $\mu = c_s^2 \bar{\rho}\tilde{\theta}\tau$.

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

$$\bar{\rho}(\partial_t \tilde{\varepsilon} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\tilde{\varepsilon}) + (\tilde{\boldsymbol{P}}^{(0)} + \tilde{\boldsymbol{P}}^{(1)}) : (\boldsymbol{\nabla}\tilde{\boldsymbol{u}}) + \boldsymbol{\nabla} \cdot (\tilde{\boldsymbol{q}}^{(0)} + \tilde{\boldsymbol{q}}^{(1)}) = 0, \tag{A 16}$$

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

$$\partial_t (\bar{\rho}\tilde{\varepsilon}) - \tilde{\boldsymbol{u}} \cdot \boldsymbol{\nabla}(\bar{\rho}\tilde{\theta}) + \left(\frac{D+2}{2}\right) \boldsymbol{\nabla} \cdot (\bar{\rho}\tilde{\theta}\tilde{\boldsymbol{u}}) = 0. \tag{A 17}$$

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

$$a_{1\alpha\beta\beta}^{(3)} = -c_s^2 \tau \bar{\rho}\tilde{\theta}(2\tilde{\Lambda}_{\alpha\beta}u_\beta + (D+2)\partial_\alpha \tilde{\theta}) + \mathscr{R}_{\alpha\beta\beta}^{(3)}. \tag{A 18}$$

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

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

$$\tilde{q}_\alpha^{(1)} = -c_s^2 \tau \bar{\rho}\tilde{\theta}\left(\frac{D+2}{2}\right)\partial_\alpha \tilde{\theta} + \mathscr{R}_{\beta\beta\alpha}^{(3)}. \tag{A 19}$$

Finally the filtered energy equation is

$$\bar{\rho}(\partial_t \tilde{\varepsilon} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\tilde{\varepsilon}) + (\tilde{p}\boldsymbol{I} - \mu\tilde{\boldsymbol{\Lambda}}) : (\boldsymbol{\nabla}\tilde{\boldsymbol{u}}) = \left(\frac{D+2}{2}\right)\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla}\tilde{\theta}) - \boldsymbol{\nabla}\cdot\mathrm{tr}(\mathscr{R}^{(3)}), \tag{A 20}$$

where $\kappa = c_s^2\bar{\rho}\tilde{\theta}\tau$ and $\mathrm{tr}(\mathscr{R}^{(3)})$ stands for the contraction of the two last indices of $\mathscr{R}_{\alpha\beta\gamma}^{(3)}$.

REFERENCES

AIDUN, C. K. & CLAUSEN, R. J. 2010 Lattice-Boltzmann method for complex flows. *Annu. Rev. Fluid Mech.* **42** (1), 439–472.

ANSUMALI, S., KARLIN, I. V., ILIYA, V. & SUCCI, S. 2004 Kinetic theory of turbulence modeling: smallness parameter, scaling and microscopic derivation of Smagorinsky model. *Physica* A: *Statist. Mech. Appl.* **338** (3–4), 379–394.

BHATNAGAR, P. L., GROSS, E. P. & KROOK, M. 1954 A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems. *Phys. Rev.* **94** (3), 511–525.

CHAPMAN, S. & COWLING, T. G. 1960 *The Mathematical Theory of Non-uniform Gases*. Cambridge University Press.

CHEN, S. 2009 A large-eddy-based lattice Boltzmann model for turbulent flow simulation. *Appl. Maths Comput.* **215** (2), 591–598.

CHEN, S. & DOOLEN, G. D. 1998 Lattice Boltzmann method for fluid flows. *Annu. Rev. Fluid Mech.* **30** (1), 329–364.

CHEN, H., KANDASAMY, S., ORSZAG, S., SHOCK, R., SUCCI, S. & YAKHOT, V. 2003 Extended Boltzmann kinetic equation for turbulent flows. *Science* **301** (5633), 633–636.

CHEN, H., ORSZAG, S. A., STAROSELSKY, I. & SUCCI, S. 2004 Expanded analogy between Boltzmann kinetic theory of fluids and turbulence. *J. Fluid Mech.* **519**, 301–314.

CHEN, H., SUCCI, S. & ORSZAG, S. 1999 Analysis of subgrid scale turbulence using the Boltzmann Bhatnagar–Gross–Krook kinetic equation. *Phys. Rev.* E **59** (3), R2527–R2530.

CHIKATAMARLA, S. S., FROUZAKIS, C. E., KARLIN, I. V., TOMBOULIDES, A. G. & BOULOUCHOS, K. B. 2010 Lattice Boltzmann method for direct numerical simulation of turbulent flows. *J. Fluid Mech.* **656**, 298–308.

DELLAR, P. J. 2001 Bulk and shear viscosities in lattice Boltzmann equations. *Phys. Rev.* E **64** (3), 031203.

DONG, Y.-H., SAGAUT, P. & MARIÉ, S. 2008 Inertial consistent subgrid model for large-eddy simulation based on the lattice Boltzmann method. *Phys. Fluids* **20** (3), 035104.

EGGELS, J. G. M. 1996 Direct and large-eddy simulation of turbulent fluid flow using the lattice-Boltzmann scheme. *Intl J. Heat Fluid Flow* **17** (3), 307–323.

FILIPPOVA, O., SUCCI, S., MAZZOCCO, F., ARRIGHETTI, C., BELLA, G. & HÄNEL, D. 2001 Multiscale lattice Boltzmann schemes with turbulence modelling. *J. Comput. Phys.* **170** (2), 812–829.

GARNIER, E., ADAMS, N. & SAGAUT, P. 2009 *Large-eddy Simulation for Compressible Flows*. Springer.

GIRIMAJI, S. S. 2007 Boltzmann kinetic equation for filtered fluid turbulence. *Phys. Rev. Lett.* **99** (3), 034501.

GRAD, H. 1949*a* Note on the *N*-dimensional Hermite polynomials. *Commun. Pure Appl. Maths* **9**, 325.

GRAD, H. 1949*b* On the kinetic theory of rarefied gases. *Commun. Pure Appl. Maths* **9**, 331.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

GUO, Z., SHI, B. & ZHENG, C. 2002 A coupled lattice BGK model for the Boussinesq equations. *Intl J. Numer. Meth. Fluids* **39**, 325–342.

HOU, S., STERLING, J., CHEN, S. & DOOLEN, G. D. 1996 A lattice Boltzmann subgrid model for high Reynolds number flows. *Fields Inst. Comm.* **6**, 151-66.

HUANG, K. 1987 *Statistical Mechanics*. John Wiley & Sons.

KERIMO, J. & GIRIMAJI, S. 2007 Boltzmann-BGK approach to simulating weakly compressible 3D turbulence: comparison between lattice Boltzmann and gas kinetic methods. *J. Turbul.* **8**.

KRAFCZYK, M., TÖLKE, J. & LUO, L.-S. 2003 Large-eddy simulations with a multiple-relaxation-time LBE model. *Intl J. Mod. Phys. B* **17** (1–2), 33–39.

LABBÉ, O., MONTREUIL, E. & SAGAUT, P. 2002 Large-eddy simulation of heat transfer over a backward facing step. *Intl J. Numer. Heat Transfer, Part* A **42** (1–2), 73–90.

LEONARD, A. 1974 Energy cascade in large-eddy simulations of turbulent fluid flows. *Adv. Geophys.* A **18**, 237–248.

MALASPINAS, O. 2009 Lattice Boltzmann method for the simulation of viscoelastic fluid flows. PhD dissertation, EPFL, Lausanne, Switzerland.

MALASPINAS, O. & SAGAUT, P. 2011 Advanced large-eddy simulation for lattice Boltzmann methods: the approximate deconvolution model. *Phys. Fluids* **23**.

MEYERS, J. & SAGAUT, P. 2006 On the model coefficients for the standard and the variational multi-scale Smagorinsky model. *J. Fluid Mech.* **569**, 287–319.

MEYERS, J., SAGAUT, P. & GEURTS, B. J. 2006 Optimal model parameters for multi-obective large-eddy simulations. *Phys. Fluids* **18** (9), 095103.

MEYERS, J., SAGAUT, P. & GEURTS, B. J. 2007 A computational error assessment of central finite-volume discretizations in large-eddy simulation using a Smagorinsky model. *J. Comput. Phys.* **227** (1), 156–173.

NIE, X. B., SHAN, X. & CHEN, H. 2008 Galilean invariance of lattice Boltzmann models. *Europhys. Lett.* **81** (3), 34005.

PREMNATH, K. N., PATTISON, M. J. & BANERJEE, S. 2009 Dynamic subgrid scale modeling of turbulent flows using lattice-Boltzmann method. *Physica* A: *Statist. Mech. Appl.* **388** (13), 2640–2658.

QUÉMÉRÉ, P., SAGAUT, P. & COUAILLIER, V. 2001 A new multidomain/multiresolution method for large-eddy simulation. *Intl J. Numer. Meth. Fluids* **36** (4), 391–416.

QUÉMÉRÉ, P., SAGAUT, P. & COUAILLIER, V. 2002 Zonal multi-domain RANS/LES simulations of turbulent flows. *Intl J. Numer. Meth. Fluids* **40** (7), 903–925.

ROGERS, M. M. & MOSER, R. D. 1994 Direct simulation of a self-similar turbulent mixing layer. *Phys. Fluids* **6** (2), 903–923.

SAGAUT, P. 2005 *Large Eddy Simulation for Incompressible Flows: An Introduction*. Springer.

SAGAUT, P. 2010 Toward advanced subgrid models for lattice-Boltzmann-based large-eddy simulation: theoretical formulations. In *Mesoscopic Methods in Engineering and Science, International Conferences on Mesoscopic Methods in Engineering and Science*, *Comput. Maths Applics.* **59** (7), 2194–2199.

SAGAUT, P., DECK, S. & TERRACOL, M. 2006 *Multiscale and Multiresolution Approaches in Turbulence*. Imperial College Press.

SCAGLIARINI, A., BIFERALE, L., SBRAGAGLIA, M., SUGIYAMA, K. & TOSCHI, F. 2010*a* Lattice Boltzmann methods for thermal flows: Continuum limit and applications to compressible Rayleigh–Taylor systems. *Phys. Fluids* **22** (5), 055101.

SCAGLIARINI, A., BIFERALE, L., SBRAGAGLIA, M., SUGIYAMA, K. & TOSCHI, F. 2010*b* Numerical simulations of compressible Rayleigh–Taylor turbulence in stratified fluids. *Phys. Scr.* **2010** (T142), 014017.

SEROR, C., SAGAUT, P., BAILLY, C. & JUVÉ, D. 2001 On the radiated noise computed by large-eddy simulation. *Phys. Fluids* **13** (2), 476–487.

SHAN, X. & CHEN, H. 2007 A general multiple-relaxation-time Boltzmann collision model. *Intl J. Mod. Phys.* C **18**, 635.

SHAN, X., YUAN, X.-F. & CHEN, H. 2006 Kinetic theory representation of hydrodynamics: a way beyond the Navier–Stokes equation. *J. Fluid Mech.* **550**, 413–441.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press

SMAGORINSKY, J. 1963 General circulation experiments with the primitive equations: I. The basic equations. *Mon. Weath. Rev.* **91**, 99–164.

SUCCI, S. 2001 *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*. Oxford University Press.

TERRACOL, M., SAGAUT, P. & BASDEVANT, C. 2003 A time self-adaptive multilevel algorithm for large-eddy simulation. *J. Comput. Phys.* **184** (2), 339–365.

WEICKERT, M., TEIKE, G., SCHMIDT, O. & SOMMERFELD, M. 2010 Investigation of the LES WALE turbulence model within the lattice Boltzmann framework. *Comput. Maths Applic.* **59** (7), 2200–2214.

WOLF-GLADROW, D. A. 2000 *Lattice-Gas Cellular Automata and Lattice Boltzmann Models: An Introduction*. Springer.

https://doi.org/10.1017/jfm.2012.155 Published online by Cambridge University Press