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Toward advanced subgrid models for Lattice-Boltzmann-based Large-eddy simulation: Theoretical formulations

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ABSTRACT

This paper addresses the issue of developing advanced subgrid model for large-eddy simulations (LES) of turbulent flows based on Lattice Boltzmann methods (LBM). Most of already existing subgrid closures used in LES-LBM are straightforward extensions of the most crude model developed within the Navier–Stokes equations, namely the Smagorinsky eddy-viscosity model. In a first part, it is shown how to obtain an improved eddy-viscosity subgrid model for LBM. The original implementation of the Inertial-Range Consistent Smagorinsky model proposed by Dong and Sagaut for the D3Q19 scheme is used as an illustration. In a second step, an original extension of the Approximate Deconvolution Method proposed by Adams and Stolz for Navier–Stokes simulation is proposed. This new LBM-LES approach does not rely on the eddy-viscosity concept and is written directly within the LBM framework. It is shown that it can be implemented thanks to a trivial modification of the existing LBM solvers for Direct Numerical Simulation.

1. Introduction

Turbulent flows exhibit a very wide range of scales. The rapid growth of the range of excited scales of motion versus the Reynolds number renders the Direct Numerical Simulation (i.e., the direct capturing of all scales of motion) of almost all turbulent flows of practical interest impossible, due to the limitation of available computing facilities. In order to describe the unsteady behavior of turbulent flows at a much lower cost, the Large-Eddy Simulation (LES, cf. [1] for a general presentation) has been developed after the publication of Smagorinsky's seminal paper in 1963 [2]. The LES strategy consists in removing the smallest turbulent scales of the flow, whose contribution to global features of the flow is assumed to be small, therefore allowing for the use of a much coarser grid resolution and a significant reduction in the number of degrees of freedom of the computational model. Because of the intrinsic nonlinearity of turbulence dynamics, the influence of the small removed scales on the large resolved ones must be taken into account via a subgrid model. Such models have been developed within the Navier–Stokes framework for many different purposes and flow regimes, including compressible flows [3,4], heat transfer [5] and generation of noise by turbulence [6], and many modelling strategies have been proposed, including multiscale and multiresolution approaches [7,8].

While the Navier–Stokes model has been almost exclusively used during almost two centuries to describe hydrodynamic turbulence, Lattice Boltzmann Methods receive a rapidly growing interest because of their computational efficiency. These methods, which rely on the Boltzmann equation, allow for the prediction of the macroscopic quantities found in continuum mechanics, such as velocity and pressure. Although it has been proved several years ago that hydrodynamic turbulence can be accurately described using these methods, the development of Large-Eddy Simulation within the LBM framework is still at a very early stage. The reader is referred to [9–18] and the references given therein for a description of the use of LBM for computational fluid dynamics and turbulent flow simulation.

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Starting from the following generic governing equation for LBM:

$$\underbrace{\frac{\partial}{\partial t}f + v \cdot \nabla f}_{\frac{Df}{Dt}} = C(f), \tag{1}$$

where $f(x, v, t)$, v and $C(f)$ are the single-particle distribution function that represents the density of kinetic particles in the phase space (x, v) at time t, density distribution, the velocity and the collision operator, respectively, LBM-LES equations are usually obtained applying a low-pass filter in the frequency/wavenumber space to (1). Considering the convolution filter kernel G, and denoting $\bar{f} \equiv G \star f$ the filtered solution, one obtains

$$\frac{\partial}{\partial t}\bar{f} + v \cdot \nabla \bar{f} = \frac{D\bar{f}}{Dt} = \overline{C(f)} = G \star C(f), \tag{2}$$

which can be recast as follows

$$\frac{D\bar{f}}{Dt} - C(\bar{f}) = \underbrace{G \star C(f) - C(\bar{f})}_{R}, \tag{3}$$

in which all computable terms have been put on the left-hand side. The right-hand-side term R is referred to as the subgrid term, which cannot be directly computed and must therefore be modelled. The local macroscopic density $\rho(x, t)$ and momentum $\rho u(x, t)$ are recovered computing the moments of the density distribution function:

$$\rho(x, t) = \int f(x, v, t)\mathrm{d}v, \qquad \rho u(x, t) = \int v f(x, v, t)\mathrm{d}v. \tag{4}$$

In LES-LBM, the filtered macroscopic quantities are computed as follows:

$$\bar{\rho}(x, t) = \int \bar{f}(x, v, t)\mathrm{d}v, \qquad \overline{\rho u}(x, t) = \int v\bar{f}(x, v, t)\mathrm{d}v. \tag{5}$$

The rest of the paper is organized as follows. Section 2 is devoted to the use of eddy-viscosity closures inspired from existing Navier–Stokes subgrid model. The possibility to develop 'user-friendly' advanced subgrid eddy-viscosity for LBM-LES is illustrated thanks to the recent work by Dong and Sagaut [19,20]. A new way to obtain an efficient LBM-LES method is presented in Section 3. It relies on the Approximate Deconvolution Method (ADM) introduced by Stolz and Adams in the late 1990s [21–23], leading to a fully general procedure that can be coupled with almost all LBM schemes in a trivial way and which is not based on the eddy-viscosity paradigm.

2. Inertial-range consistent subgrid models for LBM-BGK methods

2.1. General formulation for eddy-viscosity closures

Among the different closure strategies used to derive subgrid models, the eddy-viscosity approach is certainly the most popular, since related models can be easily implemented and that they have stabilizing numerical properties. We will now present this approach for the LBM-LES case. To this end, we will consider the Boltzmann equation with the Bhatnagar–Gross–Krook (1954) collision model:

$$\frac{Df}{Dt} = -\frac{1}{\tau}(f - f^{eq}), \qquad f^{eq}(x, v, t) = \frac{\rho}{(2\pi \mathcal{R}T(x, t))^{d/2}} \exp\left(-\frac{(v - u(x, t))^2}{2\mathcal{R}T(x, t)}\right), \tag{6}$$

where f^{eq}, T, $\mathcal{R}$ and d are the local kinetic equilibrium distribution function associated with the Maxwell–Boltzmann theory, the temperature, the perfect gas constant and the dimension of the momentum space, respectively. The relaxation time scale τ and the fluid molecular viscosity ν are tied by the relation $\nu \propto T\tau$. The corresponding form for LES-LBM is (space and time dependencies are omitted for the sake of brevity)

$$\frac{D\bar{f}}{Dt} = -\frac{1}{\tau^*}(\bar{f} - \tilde{f}^{eq}), \qquad \tilde{f}^{eq} = \frac{\rho}{(2\pi \mathcal{R}T)^{d/2}} \exp\left(-\frac{(v - \bar{u})^2}{2\mathcal{R}T}\right) \neq G \star f^{eq}, \tag{7}$$

where it is important to note that the computable equilibrium distribution function $\tilde{f}^{eq}$ is not equal to the filtered equilibrium distribution function $\bar{f}^{eq}$ in the general case. τ^* is the relaxation time scale related to the filtered problem.

Following the eddy-viscosity approach, the subgrid scale motion is taken into account using an eddy-viscosity model, as classically done for the Navier–Stokes equations. Denoting ν_t the eddy-viscosity, which is usually evaluated using a model derived for the Navier–Stokes equations, the LES relaxation time τ^* must be expressed as $\mathcal{F}(\nu, \nu_t) \propto T\tau^*$, where the function $\mathcal{F}$ is to be defined.

2.2. Concept of inertial-range consistency and IRC Smagorinsky model

The concept of inertial-range consistent subgrid model has been recently proposed by Meyers and colleagues [24–26]. It relies on the idea that the subgrid model for the unresolved scales must be designed in such a way that the correct resolved turbulent kinetic energy balance is recovered during the simulation. Therefore, a mandatory requirement is that the Reynolds number effects must be taken into account, along with the position of the cutoff wavenumber within the kinetic energy spectrum of the exact turbulent solution. This location is known to have a deep impact on the magnitude of the kinetic energy transfer across the cutoff between resolved and subgrid modes of motion.

We exemplify the discussion using the Smagorinsky eddy-viscosity model [2], which is the most popular eddy-viscosity subgrid model. It is defined as follows

$$\nu_t = (C_S h)^2 \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}, \qquad \bar{S}_{ij} \equiv \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \tag{8}$$

where h and C_S are the cutoff length scale associated with the LES cutoff and an arbitrary parameter referred to as the Smagorinsky constant, respectively. The problem consists in tuning the C_S parameter in an adequate way. In the case of isotropic turbulence, Meyers et al. [24–26] have shown that a universal value for that parameter cannot be defined, since its exact expression takes the form of a filtered and kinetic energy spectrum dependent function:

$$C_S = \frac{C_\infty}{\Phi^{3/4}} \sqrt{1 - \left(\frac{C_\infty}{\gamma\eta}\right)^{4/3} \frac{\Phi}{\gamma}}, \tag{9}$$

where $C_\infty \approx 0.17 \sim 0.18$ is the asymptotic value obtained considering and infinite Reynolds number and that the LES filter G is a sharp cutoff filter in wavenumber space. η is the Kolmogorov scale. The two functions γ and Φ are defined as

$$\gamma = \frac{1}{\pi h}\frac{4}{3}\int_0^{+\infty} k^{1/3}\left(\hat{G}(k)\right)^2 \mathrm{d}k, \tag{10}$$

where $\hat{G}(k)$ is the transfer function of the filter kernel G, and

$$\Phi = \frac{\int_0^{+\infty} k^{1/3}\left(\hat{G}(k/L)\right)^2 f_L(k) f_\eta(k Re_L^{-3/4}) \mathrm{d}k}{\int_0^{+\infty} k^{1/3}\left(\hat{G}(k/L)\right)^2 \mathrm{d}k}, \tag{11}$$

where L, Re_L, f_L and f_η are the turbulent integral scale, the integral scale-based Reynolds number, the low- and the high-wavenumber kinetic energy spectrum shape function, respectively. Explicit expressions of the spectrum shape functions can be found in many references, including Pope's book [27]. With the constant defined by (9), the Smagorinsky model becomes inertial-range consistent in the sense that the induced kinetic energy dissipation will be exact.

2.3. An example: D3Q19 implementation

The subgrid model defined by Eqs. (8) and (9) is exact, but does not lead to tractable simulations since the computation of the constant is computationally too demanding. Meyers and Sagaut found that, leaving the definition of the Smagorinsky constant unchanged (i.e., using Eq. (8) along with $C_S \approx 0.17 \sim 0.18$), inertial-range consistency is closely mimicked changing the total viscosity definition, i.e., considering the harmonic average $\sqrt{\nu^2 + \nu_t^2}$ instead of the sum of the molecular and subgrid viscosities. The remapping-based approach suggested by Meyers has been recently extended to the D3Q19 scheme by Dong and colleagues [19,20]. The D3Q19 model can be interpreted as a particular discretization of the Boltzmann-BGK equation (cf. [28] for an exhaustive discussion). The associated Inertial-Range consistent model for LBM-LES is

$$\bar{f}_\alpha(x + v_\alpha \delta t, t + \delta t) - \bar{f}_\alpha(x, t) = \frac{1}{\tau_w}\left(\bar{f}_\alpha(x, t) - \tilde{f}_\alpha^{eq}(x, t)\right), \quad \alpha = 0\text{–}18, \tag{12}$$

where δt is the time step and

$$\tau_w = \frac{1}{2} + \frac{3}{2\delta t}\sqrt{\nu^2 + \nu_t^2}, \tag{13a}$$

$$\tilde{f}_\alpha^{eq} = \omega_\alpha \bar{\rho}\left\{1 + 3\left(\frac{v_\alpha \cdot \bar{u}}{c^2} + 3\frac{(v_\alpha \cdot \bar{u})^2}{2c^4} - \frac{\bar{u}^2}{2c^2}\right)\right\}, \tag{13b}$$

where $c = \delta t/h$ is a reference velocity taken equal to 1 on a uniform lattice. The discrete velocities v_α and the weighting coefficients ω_α are defined as follows:

$$v_\alpha = \begin{cases} (0,0,0), & \alpha = 0, \\ (\pm 1,0,0)c,\ (0,\pm 1,0)c,\ (0,0,\pm 1)c, & \alpha = 1\text{–}6, \\ (\pm 1,\pm 1,0)c,\ (\pm 1,0,\pm 1)c,\ (0,\pm 1,\pm 1)c, & \alpha = 7\text{–}18, \end{cases} \tag{14a}$$

$$\omega_\alpha = \begin{cases} 1/3, & \alpha = 0, \\ 1/18, & \alpha = 1\text{–}6, \\ 1/36, & \alpha = 7\text{–}18. \end{cases} \tag{14b}$$

3. Approximate deconvolution methods for LBM-LES

The previous developments are based on the eddy-viscosity assumption, which is based on a simplified view of inter-scale kinetic energy transfers at asymptotically high Reynolds numbers deduced from the Navier–Stokes equations. Let us emphasize that the subgrid closure problem originates in the lack of commutativity of the LES filter and nonlinear terms. Since nonlinearities in LBM equations differ from those of the Navier–Stokes equations, the use of an eddy-viscosity model can be interpreted as a convenient trick but not as an optimal way to close the LBM-LES equations. In order to get a much more general LBM-LES method, we now propose to extend the Approximate Deconvolution Method (ADM) originally developed by Stolz and Adams within the Navier–Stokes framework [21–23]. An advantage of this approach is that it can be applied to LBM governing equations, without resorting to some extrapolation of Navier–Stokes closures. The ADM approach relies on the introduction of an easily computable operator Q which approximates the inverse of the LES filter G, i.e., one has $(Q \star G) = I + O(h^l)$, where I is the identity operator, h a measure of the grid resolution and $l \geq 1$ the order of the reconstruction.

3.1. High-order deconvolution method

The most general deconvolution approach was proposed by Mathew et al. [29] for compressible Navier–Stokes equations. It is based on the following splitting of the subgrid term that appear in the filtered LBM equation (3):

$$\begin{aligned} R &\equiv G \star C(f) - C(\bar{f}) \\ &= \underbrace{\left[G \star C(f^*) - C(\bar{f})\right]}_{R_1} + \underbrace{\left[G \star C(f) - G \star C(f^*)\right]}_{R_2}, \end{aligned} \tag{15}$$

where $f^* = Q \star \bar{f}$ is an approximate reconstruction of the unfiltered field f. The term R_1 is computable. On the contrary, the term R_2 needs to be modelled. Such a model is recovered using a first-order Taylor series expansion:

$$\begin{aligned} R_2 &= G \star \left[C(f) - C(f^*)\right] = G \star \left[\left.\frac{\partial C}{\partial f}\right|_f (f - f^*) + O(f - f^*)^2 \right] \\ &\simeq G \star \left[\left.\frac{\partial C}{\partial f}\right|_{f^*} (I - Q \star G) \star f^* \right]. \end{aligned} \tag{16}$$

Inserting this truncated expression and R_1 into (3), one obtains the following closed equation:

$$\frac{D\bar{f}}{Dt} - G \star C(f^*) = G \star \left[\left.\frac{\partial C}{\partial f}\right|_{f^*} (I - Q \star G) \star f^* \right], \tag{17}$$

from which we find

$$G \star \left(\frac{Df^*}{Dt} - C(f^*) \right) = G \star \left[\left.\frac{\partial C}{\partial f}\right|_{f^*} (I - Q \star G) \star f^* \right]. \tag{18}$$

Eq. (18) shows that the associated LES-LBM method can be implemented using a three-step procedure:

(1) Deconvolution step: $f^{*(n)} = Q \star \bar{f}^{(n)}$,
(2) Compute $f^{*(n+1)}$ starting from $f^{*(n)}$ and solving the following equation for 1 time step,

$$\frac{Df^*}{Dt} - C(f^*) = \left.\frac{\partial C}{\partial f}\right|_{f^*} (I - Q \star G) \star f^*,$$

(3) Filtering step: $\bar{f}^{(n+1)} = G \star f^{*(n+1)}$.

Looking at the three-step procedure, it is seen that the first and third steps can be combined in a single filtering step with filter $(Q \star G)$, which can be applied at the end of the time step integration:

Two-step procedure

(1) Compute $f^{*(n+1)}$ starting from $f^{*(n)}$ solving the following equation for 1 time step,

$$\frac{Df^*}{Dt} - C(f^*) = \left.\frac{\partial C}{\partial f}\right|_{f^*} (I - Q \star G) \star f^*,$$

(2) Filtering step: $f^{*(n+1)} = (Q \star G) \star f^{*(n+1)}$.

Let us emphasize that $(Q \star G)$ is a high-pass filter in physical space, i.e., a low-pass filter in wavenumber space. It can be implemented in many different ways, among which two popular approaches are observed. The first solution consists in choosing Q and G, then finding the transfer function of $(Q \star G)$ and finally implementing a linear filter in physical space with the required transfer function. The second solution is to implement Q and to compute $(Q \star G)$ explicitly. A common way to implement Q is based on the Van Cittert iterative procedure: $Q = \sum_{p=0}^{l} (I - G)^p$.

3.2. Simplified procedure

All available numerical experiments carried out using Navier–Stokes equations have shown that the R_2 term can be neglected without corrupting the accuracy of the results [29]. Neglecting this term in the LBM case, one obtains the following governing equation:

$$G \star \left(\frac{Df^*}{Dt} - C(f^*) \right) = 0. \tag{19}$$

The corresponding two-step procedure is

(1) Compute $f^{*(n+1)}$ starting from $f^{*(n)}$ solving the basic LBM equation for DNS (1) for 1 time step,

$$\frac{Df^*}{Dt} - C(f^*) = 0,$$

(2) Filtering step: $f^{*(n+1)} = (Q \star G) \star f^{*(n+1)}$.

The very interesting point here is that the equation which is solved is identical to the original LBM equation (1) for DNS. Therefore, an LBM-LES solver is obtained by simply implementing the explicit filtering step at the end of each time step of the time-integration procedure in every LBM-DNS solver. The advantage of the simplified procedure with respect to the previous one is twofold: the computational cost is dramatically reduced, since the computation of the right-hand-side term which involves the gradient $\left.\frac{\partial C}{\partial f}\right|_{f^*}$ is no longer needed, and the implementation in a DNS-LBM solver is trivial. As reported by Mathew and colleagues, numerical stability can be improved by iterating the filtering step. A non-iterative way to implement it is to directly consider $(Q \star G)^p$, with $p \geq 1$, as the basic filter kernel.

4. Conclusions

The present paper was devoted to the presentation of advanced turbulent closures for LBM-LES. After deriving the governing equations for LBM-LES considering the convolution filter paradigm for scale separation, the key features of the recently proposed inertial-range consistent LBM-LES method have been recalled. In a second step, a totally new approach was introduced. This new approach relies on the approximate defiltering approach. Both a high-order and a more tractable leading order method have been proposed. A very interesting property of this new approach is that it does not rely on the eddy-viscosity concept and is therefore more general, since it involves no implicit assumption on the subgrid scale dynamics. Another important feature of the two-step procedure derived from the simplified deconvolution procedure is that it can be implemented in a straightforward way by implementing an explicit filtering step in any LBM solver. Writing boundary conditions for LBM-LES remains an open issue. This is the same as for the Navier–Stokes-based LES method: instead of deriving boundary conditions by filtering the DNS conditions, the latter are used for LES also, without filtering. The most difficult case to treat is the no-slip condition at solid walls. The usual solution is to decrease the LES cutoff length in the vicinity of solid walls to recover a DNS-like resolution, leading to a natural use of DNS boundary conditions.

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