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Challenges in Lattice Boltzmann Computing

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Some of the most urgent challenges facing the lattice Boltzmann equation (LBE) to rival state-of-the-art computer fluid dynamics (CFD) techniques are discussed. A novel LBE scheme for k–ε turbulence modeling is proposed.

KEY WORDS: Fluid dynamics; turbulence; channel flow; lattice Boltzmann equation; numerical simulation; finite volume; k–ε turbulence model.

1. INTRODUCTION

Lattice Boltzmann methods have known a rapid expansion in the late 1980s. Originally motivated by the need to beat the statistical noise plaguing its ancestor (the lattice gas automata method),[1] the lattice Boltzmann method has undergone a series of progressive refinements and extensions which have taken it to the point where it can be used as a competitive technique to compute a variety of nontrivial flows.[2] Yet, as compared to state-of-the-art computational fluid dynamics (CFD) techniques, it appears that the gap to be bridged is still rather wide. Among te most urgent developments which are called for, we note the following two:

1. Ability to deal with complex geometries.
2. Ability to incorporate turbulence models.

In this paper we briefly review some recent developments pertaining to 1 and 2 and make few suggestions for further improvements.

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2. COMPLEX GEOMETRY

In what follows, we shall refer to the lattice Boltzmann equation (LBE) in its "Chapman–Eksong" form,[2]

$$f_i(\mathbf{x}+\mathbf{c}_i, t+1)-f_i(\mathbf{x}, t)=\sum_{j=1}^{b} A_{ij}(f_j-f_j^{eq}), \qquad i=1, b \tag{1}$$

where $f_i(\mathbf{x}, t)$ represents the particle population at time t on the node $\mathbf{x}$ along direction $\mathbf{c}_i$. The velocity variable $\mathbf{c}_i$ is discretized on a suitable discrete lattice, ensuring isotropy on a macroscopic level. For three-dimensional simulations we need a four-dimensional lattice (face-centered hypercube, FCHC), in which 24 distinct values of $\mathbf{c}_i$ are defined. The r.h.s. of (1) represents the effects of particle collisions: the matrix A_{ij} is symmetric and fulfills the sum rules imposed by mass and momentum conservation. The f_j^{eq} represents the local equilibrium distribution function, expanded to the second order in the local flow field $\mathbf{u}$ in order to retain convective effects:

$$f_i^{eq}=Q_{i\alpha\beta}u_\alpha u_\beta, \qquad Q_{i\alpha\beta}=c_{i\alpha}c_{i\beta}-\frac{c^2}{D}\delta_{\alpha\beta}; \qquad \alpha, \beta=1, 2, 3$$

where $D=4$ is the dimension of the lattice. It can be shown that in the continuum limit Eq. (1) converges to the Navier–Stokes equation for an incompressible fluid.

Equation (1) can be regarded as a first-order Lagrangian scheme for the following set of partial differential equations:

$$\partial_t f_i(\mathbf{x}, t)+\mathbf{c}_i\cdot\partial_x f_i(\mathbf{x}, t)=\sum_j A_{ij}(f_j-f_j^{eq})\equiv C_i \tag{2}$$

in which the collision term is treated fully explicitly and the streaming term is integrated along the characteristics $\Delta\mathbf{x}_i=\mathbf{c}_i\,\Delta t$. In order for Eq. (1) to reproduce the Navier–Stokes equations in the hydrodynamic limit, stringent conditions are imposed on the lattice topology. In particular, since all discrete speeds have the same magnitude $|\mathbf{c}_i|=c$, the characteristics give rise to a forcedly regular and uniform spatial mesh. This is the key to the simplicity of the scheme, and also to its amenability to massive parallel computing on both SIMD and MIMD architectures.

On the other hand, it also sets a serious obstacle to the ability of the method to handle complex geometries such as those commonly encountered in most CFD engineering applications. It appears therefore that removing this obstacle is important to raising the competitiveness of the

LBE in the CFD arena. This problem has been addressed[2–4] in the recent past. In particular, in Ref. 5 it is shown that by borrowing some standard ideas from the finite-volume method, the original LBE can be extended in such a way as to handle Cartesian nonuniform geometries. Directing the reader to the original reference for a detailed description, here we shall content ourselves with a reminder.

The basic idea is to start from the differential form of LBE, Eq. (2), and apply Gauss" theorem to a set of macrocells (finite volumes) covering the spatial domain. For each cell, with a volume V_p, a corresponding "coarse-grain" distribution F_{ip} is defined as

$$F_{ip} \equiv \frac{1}{V_p} \int_{V_p} f_i \, dV \tag{3}$$

The mean value of the r.h.s. of Eq. (2) becomes

$$\begin{aligned} \langle C_i(F_{ip}) \rangle &= \frac{1}{V_p} \int_{V_p} C_i(f_i) \, dV \\ &= \frac{1}{V_p} \int_{V_p} \sum_j A_{ij}(f_j - f_j^{\text{eq}}) \, dV \end{aligned}$$

This can be rewritten as

$$\langle C_i(F_{ip}) \rangle = \sum_j A_{ij}[(F_{jp} - F_{jp}^{\text{eq}} - F_{jp}^{\text{neq}})] \tag{4}$$

where

$$F_{jp}^{\text{eq}} \equiv Q_{j\alpha\beta} U_{\alpha p} U_{\beta p}, \qquad F_{jp}^{\text{neq}} \equiv Q_{j\alpha\beta} \langle u'_{\alpha p} u'_{\beta p} \rangle$$

Here

$$U_{\alpha p} \equiv \frac{1}{V_p} \int_{V_p} u_\alpha \, dV, \qquad \alpha = x, y, z$$

represents the mean velocity over a macrocell and $u'_{\alpha p}$ is the velocity fluctuation at the macrocell scale. The kinetic term of the l.h.s. of Eq. (2), using the Gauss theorem, becomes

$$\begin{aligned} \Phi_{ip} &= \frac{1}{V_p} \int_{V_p} (\mathbf{c}_i \cdot \nabla f_i) \, dV \\ &= \frac{1}{V_p} \int_{\partial V_p} (\mathbf{c}_i \cdot \hat{n}) f_i \, d\sigma \end{aligned}$$

This term is naturally interpreted as the balance of the probability density passing through the boundaries of the macrocell V_p. In order to compute Φ_{ip}, we need to specify the surface values f_i as a function of the nodal values F_i. This requires an interpolation procedure within the neighborhood of the cell V_p. We have studied two interpolation schemes based on a piecewise constant (PWC) and piecewise linear (PWL) representation of the function f_i, respectively. It has been shown that at least piecewest linear interpolation is required for the streaming operator in order to avoid serious problems of numrical diffusion.[6]

The PWC and PWL schemes are shown in Figs. 1 and 2, respectively, for the case of one-dimensional propagation along the z axis. In both cases the time variation of the mean population of cell p is given by

$$\frac{\Delta F_{ip}}{\Delta t} = \Phi_{\text{in}} - \Phi_{\text{out}} = \Phi_{ip}$$

where Φ_{in}, Φ_{out} respect the income and the outcome fluxes per unit volume, respectively. For instance, in the case of Fig. 1,

$$\Phi_{\text{in}} = F(k-1)\frac{\Delta x\, \Delta y\, \Delta t}{V(k)}$$

$$\Phi_{\text{out}} = F(k)\frac{\Delta x\, \Delta y\, \Delta t}{V(k)}$$

where $V(k) = \Delta x\, \Delta y\, \Delta z(k)$ is the volume of the kth cell.

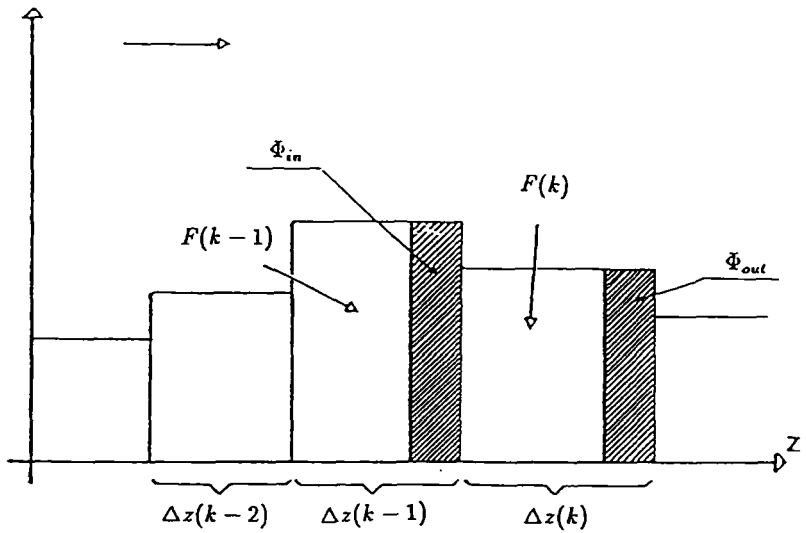

Fig. 1. An example of piecewise constant interpolation: the arrow denotes the propagation direction.

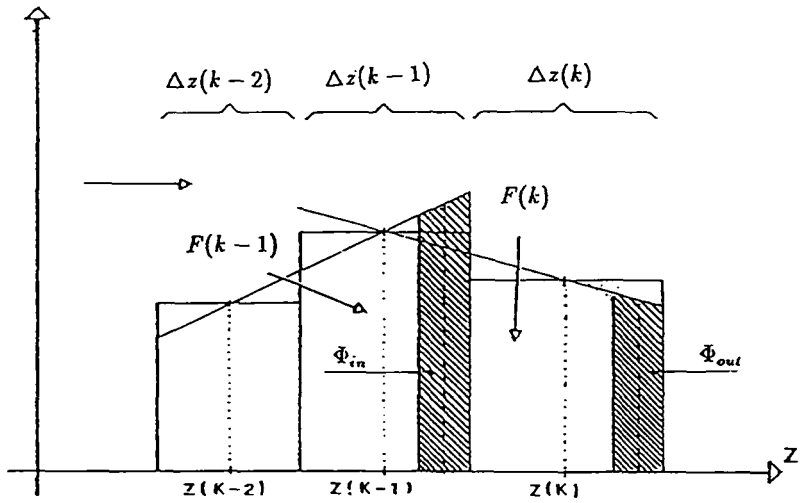

Fig. 2. An example of piecewise linear interpolation: the arrow denotes the propagation direction.

In Fig. 2, $z^+(k)$ is a free term which is adjusted in such a way as to minimize numerical diffusion. Equation (2) for a nonuniform lattice becomes

$$\hat{F}_{ip} = F_{ip} + \Delta t \left[\sum_j A_{ij}(F_{jp} - F_{jp}^{\text{eq}}) - \Phi_{ip} \right] \tag{5}$$

where $\hat{F}_{ip}$ is the population at time $t + \Delta t$. Note that the velocity fluctuations at the cell scale have been neglected in the collision operator ($F_{ip}^{\text{neq}} = 0$). This corresponds to a PWC approximation of the collision operator, as opposed to the PWL interpolation used for the streaming operator. The rationale behind this choice is that the collision operator, being local, i.e., no space derivatives, can be consistently discretized by a zeroth-order polynomial interpolation.

Equation (5) has been successfully employed in two dimensions for the calculation of low-Reynolds-number flows past bluff bodies. More recently the FVLBE has been extended to three dimensions with stretched grid size along z and successfully employed for the simulation of turbulent channel flow.[7] A typical mean-velocity profile in a turbulent channel flow is shown in Fig. 3 and compared with the theoretical velocity profile.[8] Similarly, in Fig. 4 we report the stress tensor $\tau_{xz} = \langle u_x u_z \rangle$. This calculation was performed on a $64 * 64 * 128$ nonuniform mesh covering a domain size of

$512*960*192$ physical units. This calculation takes about 5 sec/step on a IBM RS/6000, model 580, corresponding to roughly $100\,\mu$sec/grid point. This is about three times higher than the corresponding figure for uniform LBE (about $30\,\mu$sec/grid point), an overhead that is largely overcompensated by the savings in terms of number of grid points, about a factor 165. As a matter of fact, this calculation would have been just *unfeasible* with a conventional uniform LBE (83 GB of memory and 2000 sec/step!). The present FVLBE compares well also with state-of-the-art CFD calculations based on Spectral-Chebitsev expansion.[9] The three-dimensional FVLBE scheme implemented so far is restricted to a Cartesian streched mesh of the form

$$x_i = \Delta x * i$$
$$y_j = \Delta y * j$$
$$z_k = \Delta z(k) * k$$

This simplifies the interpolation procedure and consequently the form of the streaming term Φ_{ip} to a considerable extent. Besides the obvious gains in computational efficiency, this also permits us to control (partially) the numerical viscosity of the scheme beforehand. However, in principle

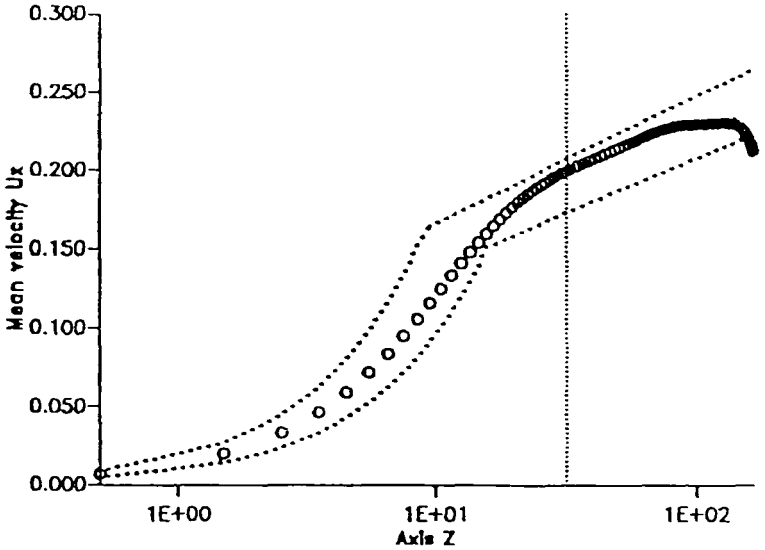

Fig. 3. Mean velocity profile for a turbulent channel flow; the dotted lines represent the maximum and the minimum values of the theoretical velocity profile, computed with the viscosity derived by the numerical experiment: Reynolds number $R \approx 3000$, viscosity $\nu = 0.013 \pm 0.002$, typical velocity $v_* = 0.014 \pm 0.001$.

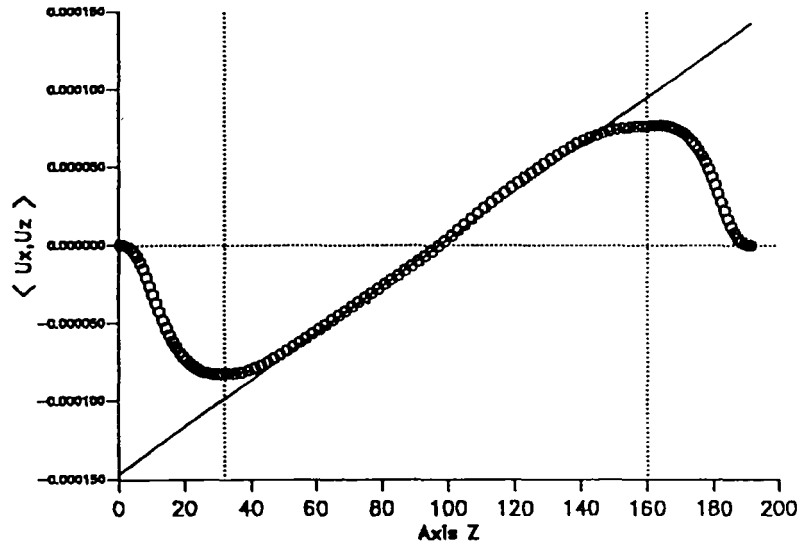

Fig. 4. Stress tensor $\tau_{xz} \equiv \langle u_x u_z \rangle$ vs. z, for the same condition as in Fig. 3. As a consistency check, we computed $v_* = (\tau/\rho)^{1/2}|_{z=0}$ and obtained $v_* = 0.012$.

there are no conceptual obstacles which prevent the present FVLBE formulation from being extended to arbitrarily structured geometries based on hexahedral cell shapes. A similar argument would equally apply to a finite-element implementation of LBE, which would open the way to even more complex (unstructured) geometries. The question which comes about is then: what would we gain with respect to existing finite-volume of finite-element methods?

In our view a possible advantage is the fact that within LBE diffusion effects *do not* involve second-order spatial derivatives: in fact, second-order spatial derivatives emerge from adiabatic relaxation of the stress tensor to its equilibrium form.[2] This results in a handier treatment of the diffusive fluxes in the interpolation procedure. Only future experimenation, however, can tell us whether this potential advantage translates into a higher efficiency on parallel computers.

3. TURBULENCE MODELING

Another must for any competitive CFD method aiming at the description of high-Reynolds-number flows of engineering interest is the ability to incorporate some form of turbulence modeling, i.e., some mathematical representation of small (unresolved, subgrid) scales on the large (resolved)

ones. The task is a very difficult one and constitutes one of the major open problems in CFD. In the absence of a complete theory (which might well not exist!) several semiempirical approaches have been worked out over the years. In this context, a keystone idea is the concept of "eddy viscosity" ν_t as a synthetic indicator of the damping effects exerted by small scales on the large ones. In the most common turbulence models, the eddy viscosity provides the link between the deviatoric component of the turbulent stress tensor $\tau_{\alpha\beta} \equiv \langle u'_\alpha u'_\beta \rangle$ and the large-scale strain tensor $S_{\alpha\beta} = \frac{1}{2}(\partial_\alpha U_\beta + \partial_\beta U_\alpha)$:

$$\tau_{\alpha\beta} - \tfrac{1}{3}\tau_{\gamma\gamma}\delta_{\alpha\beta} = -\nu_t S_{\alpha\beta}$$

In these expressions U_α represents the large-scale field, while u'_α is the small-scale fluctuating velocity (Greek indices denote spatial components). The simplest form of eddy viscosity is due to Smagorinski,[10] and reads as

$$\nu_t = C_s \Delta^2 |S| \tag{6}$$

where Δ is the typical linear mesh size, and $|S| = (S_{\alpha\beta} S_{\alpha\beta})^{1/2}$, and C_s is an empirical constant ($C_s > 0$). Turbulence models in the Smagorinski class, i.e., in which ν_t is a algebraic function of the local strain tensor, are quite naturally included within the LBE formalism. This is because the strain tensor is available locally at each lattice site, being in fact an independent variable treated by the LBE exactly on the same footing as fluid density ρ and velocity **u**. This was realized very early by the LBE community, although, to the best of our knownledge, the first actual application appeared only as late as 1992.[11] In practice, all that is needed is to let the leading eigenvalue λ of the scattering matrix A_{ij}, the one controlling the fluid viscosity via the relation

$$\nu = \frac{1}{3}\left(\frac{1}{|\lambda|} - \frac{1}{2}\right) \tag{7}$$

to become an appropriate function of $|S|$. By inverting (7), one gets

$$|\lambda(S)| = \frac{2}{6\nu(S) + 1}$$

which is straightforwardlyy implemented in any LBE code at virtually zero extra cost. On the next level of complexity in the hierarchy of turbulence models one finds the two-equation k–ε turbulence model, where k is the mean turbulent kinetic energy and ε the mean turbulent kinetic energy dissipation:

$$k \equiv \sum_\alpha \frac{1}{2}\langle u'_\alpha u'_\alpha \rangle, \qquad \varepsilon \equiv \frac{dk}{dt} = \left\langle \frac{1}{2} |\nabla u'|^2 \right\rangle$$

The k–ε model is again based on the notion of effective eddy viscosity, but, at variance with Smagorinski, it responds to the variance of small scales, via k and ε,

$$\nu_t \approx \frac{k^2}{\varepsilon} \tag{8}$$

As a result, to close Navier–Stokes, two dynamical equations for k and ε are needed. Typically they take the following form:

$$\begin{aligned} \frac{\partial k}{\partial t} + \mathbf{u} \cdot \frac{\partial k}{\partial \mathbf{x}} &= \alpha_k \nu_t \Delta k - \varepsilon - \tau_{\alpha\beta} S_{\alpha\beta} \\ \frac{\partial \varepsilon}{\partial t} + \mathbf{u} \cdot \frac{\partial \varepsilon}{\partial \mathbf{x}} &= \alpha_\varepsilon \nu_t \Delta \varepsilon - C_1 \frac{\varepsilon}{k} \tau_{\alpha\beta} S_{\alpha\beta} - C_2 \frac{\varepsilon^2}{k} \end{aligned} \tag{9}$$

where α_ε, α_k, C_1, C_2 are calibration constants.[12]

An interesting question arises as to whether an LBE scheme can be found which generates Eq. (9). In the next section we will argue for a positive answer to this question.

4. A TENTATIVE LBE SCHEME FOR k–ϵ TURBULENCE MODEL

The first step is to interpret k and ε as densities of two additional populations χ_i and η_i:

$$k = \sum_{i=1}^{2d} \chi_i, \qquad \varepsilon = \sum_{i=1}^{2d} \eta_i \tag{10}$$

living in a simple d-dimensional nearest neighbor lattice (four populations in two dimensions and six in three dimensions). The advective and the diffusive terms in Eq. (9) are standard for LBE scheme and do not need any special ingredient. Similarly, the terms $-\varepsilon$, ε^2/k, and $k^2 S^2/\varepsilon$, being local, can be modeled as nonlinear volume mass production sources by terms of the form

$$\frac{1}{2d}\varepsilon \equiv \sum_i \frac{\eta_i}{2d}, \qquad \frac{1}{2d}\frac{\varepsilon^2}{k} \equiv \frac{1}{2d}\frac{\sum_{ij} \eta_i \eta_j}{\sum_k \chi_k}$$

$$\tau_{\alpha\beta} S_{\alpha\beta} = -\frac{k^2}{\varepsilon} S^2 + \frac{2k}{d} S$$

respectively.

The final form of the k–ε LBE scheme is

$$\chi_i(\mathbf{x}+\mathbf{c}_i, t+1)-\chi_i(\mathbf{x}, t)=\lambda(\chi_i-\chi_i^{eq})-\frac{1}{2d}\left(\varepsilon-\frac{2k}{d}S+\frac{k^2}{\varepsilon}S^2\right) \quad (11)$$

$$\eta_i(\mathbf{x}+\mathbf{c}_i, t+1)-\eta_i(\mathbf{x}, t)=\mu(\eta_i-\eta_i^{eq})-C_1 kS^2-C_2\frac{\varepsilon^2}{k} \quad (12)$$

where λ and μ are adjusted in such a way as to match the eddy viscosities $\alpha_k \nu_t$ and $\alpha_\varepsilon \nu_t$, respectively. Projection upon $1_i=(1, 1,..., 1)$ and $\mathbf{c}_i$, respectively, yields (recall that $\sum_i \mathbf{c}_i=0$)

$$\begin{aligned}\partial_t k+\nabla\cdot\mathbf{J}_k&=\lambda(k-k^{eq})-\varepsilon+\frac{k^2}{\varepsilon}S^2-2kS\\ \partial_t\mathbf{J}_k+\nabla\cdot\vec{\Pi}_k&=\mu(\mathbf{J}_k-\mathbf{J}_k^{eq})\end{aligned} \quad (13)$$

where

$$\begin{aligned}\mathbf{J}_k&=\sum_i \mathbf{c}_i\chi_i\\ \vec{\Pi}_k&=\sum_i \mathbf{c}_i\mathbf{c}_i\chi_i\end{aligned} \quad (14)$$

We have assumed the following form for the equilibrium distribution:

$$\chi_i^{eq}=\frac{k}{2d}\left(1+\frac{\mathbf{c}_i\cdot\mathbf{u}}{c_s^2}\right) \quad (15)$$

where the constant $c_s=c/D^{1/2}$ represents the sound speed. This yields

$$k^{eq}=k, \qquad \mathbf{J}_k^{eq}=k\mathbf{u} \quad (16)$$

and

$$\vec{\Pi}_k^{eq}=kc_s^2\mathbf{I} \quad (17)$$

where $\mathbf{I}$ is the unit tensor. By adiabatic relaxation of $\mathbf{J}_k$, from Eq. (13) we obtain

$$\mathbf{J}_k\approx k\mathbf{u}+\frac{1}{\mu}\nabla\cdot(kc_s^2\mathbf{I}) \quad (18)$$

By plugging Eq. (18) into Eq. (13), we obtain

$$\partial_t k+\nabla\cdot\left(k\mathbf{u}+\frac{k}{\mu}c_s^2\right)=-\varepsilon+\frac{2k}{d}S-\frac{k^2}{\varepsilon}S^2 \quad (19)$$

which is precisely the equation for k with the identification

$$\nu_t = -\frac{c_s^2}{\mu}, \qquad \text{i.e.} \quad \mu \simeq -\varepsilon \frac{c_s^2}{k^2}$$

A similar argument in Eq. (11) leads to the equation for the mean dissipation ε. This theoretical result shows that in principle the k–ε turbulence model can be naturally embodied within the LBE formulation provided μ is made a suitable function of k, ε.

Work is in progress to assess the efficiency of the scheme for flows of engineering interest.

5. CONCLUSION

Two major developments of LB theory, the capability of dealing with complex geometries and to incorporate some of the most common turbulence models, have been briefly discussed. It was shown that the basic structure of LBE is flexible enough to accommodate both the aforementioned extensions. In particular, a new class of flow simulations, namely three-dimensional turbulent flow channel, is made accessible to an appropriate generalization of the finite-volume technique. The actual efficiency of the corresponding numerical scheme as compared to the standard CFD method can only be found by direct experimentation. However, there is no reason to believe that the most appealing features of LBE, i.e., easy handling of complex boundary conditions and amenability to parallel computing, cannot be carried over into these generalized schemes.

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