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Article *in* International Journal of Modern Physics B · January 2003

DOI: 10.1142/S0217979203017059

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International Journal of Modern Physics B
Vol. 17, Nos. 1 & 2 (2003) 33–39

LARGE-EDDY SIMULATIONS WITH A MULTIPLE-RELAXATION-TIME LBE MODEL

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Received 9 August 2002

We include Smagorinsky's algebraic eddy viscosity approach into the multiple-relaxation-time (MRT) lattice Boltzmann equation (LBE) for large-eddy simulations (LES) of turbulent flows. The main advantage of the MRT-LBE model over the popular lattice BGK model is a significant improvement of numerical stability which leads to a substantial reduction of oscillations in the pressure field, especially for turbulent flow simulations near the numerical stability limit. The MRT-LBE model for LES is validated with a benchmark case of a surface mounted cube in a channel at Re = 40 000. Our preliminary results agree well with experimental data.

1. Introduction

The reliable prediction of internal turbulent flows in complex geometries still remains a challenge even for state-of-the-art computational fluid dynamics (CFD) tools with sophisticated numerical discretizations and turbulence models. In the last decade algebraic closure models have shown some encouraging results and seem to be able to simulate a variety of turbulent flows relevant in engineering.[1]

Lattice-Boltzmann models have been proven to be efficient simulation tools for a variety of complex flow problems. However, turbulence modeling within the framework of the lattice Boltzmann equation remains an unsolved issue. Although it has been realized[2] that the eddy viscosity model of Smagorinsky[3] can be easily implemented in the lattice Boltzmann equation (LBE) with the single relaxation time approximation due to Bhatnagar, Gross, and Krook[4] (BGK approximation),[5,6] there are very few substantiated LES validations utilizing the lattice Boltzmann

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method. Only very recently good results[7] are obtained for simulations of a well documented benchmark test case — a surface mounted cube in a channel,[8,9] at Re = 40 000 by using the lattice BGK (LBGK) model with the Smagorinsky model.[2] It is well understood that the numerical stability of LBGK models is substantially inferior to the corresponding multiple relaxation time (MRT) LBE models.[10] The significant improvement in numerical stability by using the MRT-LBE models can directly result in a drastic gain in computational efficiency. Thus it is only natural to incorporate MRT-LBE models with the Smagorinsky eddy viscosity model[3] to improve the capability of LBE-LES simulations of turbulent flows.

The remaining part of this paper is organized as follows. Section 2 concisely describes the MRT-LBE with the Smagorinsky eddy viscosity model. Section 3 provides a summary of the LES simulation results of the flow over a cube mounted on one wall of a channel at Re = 40 000 by using the three-dimensional MRT LBE model with fifteen velocities (D3Q15). Finally Section 4 concludes the paper.

2. MRT-LBE Model with Eddy Viscosity of Smagorinsky Model

In the formulation of the linear Boltzmann equation with multiple relaxation time approximation, the lattice Boltzmann evolution equation is written as:[10,11,12]

$$|f(\boldsymbol{r}_i + \boldsymbol{e}_\alpha \delta t,\, t + \delta t)\rangle - |f(\boldsymbol{r}_i,\, t)\rangle = -\mathsf{M}^{-1}\widehat{\mathsf{S}}\left[\, |m(\boldsymbol{r}_i,\, t)\rangle - |m^{(\mathrm{eq})}(\boldsymbol{r}_i,\, t)\rangle \,\right], \qquad (1)$$

where M is the transformation matrix mapping a vector $|f\rangle$ in the discrete velocity space $\mathbb{V} = \mathbb{R}^b$ to a vector $|m\rangle$ in the moment space $\mathbb{V} = \mathbb{R}^b$,

$$|m\rangle = \mathsf{M}|f\rangle, \qquad |f\rangle = \mathsf{M}^{-1}|m\rangle. \qquad (2)$$

In particular, for the fifteen velocity model in three dimensions (D3Q15),

$$\mathsf{M} = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-2 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
16 & -4 & -4 & -4 & -4 & -4 & -4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
0 & -4 & 4 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & 0 & -4 & 4 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
0 & 0 & 0 & 0 & 0 & -4 & 4 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
0 & 2 & 2 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1
\end{pmatrix}. \qquad (3)$$

In Eq. (1), $|\cdot\rangle$ denotes a b-dimensional vector in $\mathbb{R}^b$ ($b = (N+1)$ is the total number of discrete velocities and N is the number of non-zero velocities):

$$|f(\boldsymbol{r}_i,\, t)\rangle \equiv (f_0(\boldsymbol{r}_i,\, t),\, f_1(\boldsymbol{r}_i,\, t),\, \ldots,\, f_N(\boldsymbol{r}_i,\, t))^{\mathsf{T}},$$
$$|f(\boldsymbol{r}_i + \boldsymbol{e}_\alpha \delta t,\, t+\delta t)\rangle \equiv (f_0(\boldsymbol{r}_i,\, t+\delta t),\, \ldots,\, f_N(\boldsymbol{r}_i + \boldsymbol{e}_N \delta t,\, t+\delta t))^{\mathsf{T}},$$
$$|m(\boldsymbol{r}_i,\, t)\rangle \equiv (m_0(\boldsymbol{r}_i,\, t),\, m_1(\boldsymbol{r}_i,\, t),\, \ldots,\, m_N(\boldsymbol{r}_i,\, t))^{\mathsf{T}}, \quad \text{and}$$
$$|m^{(\text{eq})}(\boldsymbol{r}_i,\, t)\rangle \equiv (m_0^{(\text{eq})}(\boldsymbol{r}_i,\, t),\, m_1^{(\text{eq})}(\boldsymbol{r}_i,\, t),\, \ldots,\, m_N^{(\text{eq})}(\boldsymbol{r}_i,\, t))^{\mathsf{T}},$$

where T is the transpose operator, and $m_\alpha^{(\text{eq})}$ is the equilibrium value of the moment m_α. The collision matrix $\widehat{\mathsf{S}} = \mathsf{M} \cdot \mathsf{S} \cdot \mathsf{M}^{-1}$ is diagonal in the moment space $\mathbb{M} = \mathbb{R}^b$: $\widehat{\mathsf{S}} \equiv \mathrm{diag}(s_0,\, s_1,\, \ldots,\, s_N)$ where $s_\alpha \geq 0$. The fifteen moments for the fifteen velocity model in three dimensions (D3Q15) are

$$|m\rangle = (\rho,\, e,\, \epsilon,\, j_x,\, q_x,\, j_y,\, q_y,\, j_z, q_z,\, 3p_{xx},\, p_{ww},\, p_{xy},\, p_{yz},\, p_{zx},\, m_{xyz})^{\mathsf{T}},$$

where ρ is the mass density, e the energy, ϵ the energy square, $\boldsymbol{j} = (j_x,\, j_y,\, j_z)$ the momentum, $\boldsymbol{q} = (q_x,\, q_y,\, q_z)$ the heat flux, $(p_{xx},\, p_{ww},\, p_{xy},\, p_{yz},\, p_{zx})$ stresses, and m_{xyz} a third order moment. If we use the incompressible LBE model[13] with speed of sound $c_s^2 = 1/3$, the equilibria for D3Q15 model are given by:[12]

$$e^{(\text{eq})} = -\rho + \frac{1}{\rho_0}\boldsymbol{j}\cdot\boldsymbol{j}, \qquad \epsilon^{(\text{eq})} = -\rho, \qquad m_{xyz}^{(\text{eq})} = 0, \tag{5}$$

$$q_x^{(\text{eq})} = -\frac{7}{3}j_x, \qquad q_y^{(\text{eq})} = -\frac{7}{3}j_y, \qquad q_z^{(\text{eq})} = -\frac{7}{3}j_z, \tag{6}$$

$$p_{xx}^{(\text{eq})} = \frac{1}{3\rho_0}\left[2j_x^2 - (j_y^2 + j_z^2)\right], \qquad p_{ww}^{(\text{eq})} = \frac{1}{\rho_0}\left[j_y^2 - j_z^2\right], \tag{7}$$

$$p_{xy}^{(\text{eq})} = \frac{1}{\rho_0}j_x j_y, \qquad p_{yz}^{(\text{eq})} = \frac{1}{\rho_0}j_y j_z, \qquad p_{xz}^{(\text{eq})} = \frac{1}{\rho_0}j_x j_z. \tag{8}$$

In the Smagorinsky model,[3] the turbulent viscosity ν_t is related to the strain rate $\mathsf{S}_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ and a filter length scale Δ_x as follows:

$$\nu_t = (C_S \Delta_x)^2 \overline{S}, \qquad \overline{S} = \sqrt{\textstyle\sum_{i,j} \mathsf{S}_{ij} \cdot \mathsf{S}_{ij}}, \tag{9}$$

where C_S is the Smagorinsky constant.

We note that the second-order moments of the distribution function

$$\mathsf{P}_{ij} = \sum_\alpha e_{\alpha i} e_{\alpha j} f_\alpha = c_s^2 \rho \delta_{ij} + \rho u_i u_j - \frac{1}{s_{xx}} 2c_s^2 \rho \mathsf{S}_{ij}, \tag{10}$$

where $e_{\alpha i}$ denotes the i-th Cartesian component of a discrete velocity $\boldsymbol{e}_\alpha$, are in fact related to the second-order moments $3p_{xx}$, p_{ww}, p_{xy}, p_{yz}, and p_{zx}. In above formula, s_{xx} is the relaxation rate for these second-order moments and c_s is the sound speed. (In the setting of LBGK equation, $s_{xx} = 1/\tau$.) Therefore,

$$\mathsf{S}_{ij} = \frac{s_{xx}}{2c_s^2 \rho}[c_s^2 \rho\, \delta_{ij} + \rho u_i u_j - \mathsf{P}_{ij}] = \frac{s_{xx}}{2c_s^2 \rho} \mathsf{Q}_{ij}. \tag{11}$$

The second-order monomials $\{e_{\alpha i}e_{\alpha j}|i,\, j \in \{x,\, y,\, z\}\}$ can be projected to the orthogonal basis vectors $\{|\phi_\beta\rangle|\beta = 0,\, 1,\, \ldots,\, N\}$ dual to the eigen-vectors of M:[12]

$$e^2_{\alpha x} = \frac{1}{3}\left(2|\phi_0\rangle_\alpha + |\phi_1\rangle_\alpha + |\phi_9\rangle_\alpha\right), \tag{12}$$

$$e^2_{\alpha y} = \frac{1}{6}\left(4|\phi_0\rangle_\alpha + 2|\phi_1\rangle_\alpha - |\phi_9\rangle_\alpha + 3|\phi_{10}\rangle_\alpha\right), \tag{13}$$

$$e^2_{\alpha z} = \frac{1}{6}\left(4|\phi_0\rangle_\alpha + 2|\phi_1\rangle_\alpha - |\phi_9\rangle_\alpha - 3|\phi_{10}\rangle_\alpha\right) = e^2_{\alpha y} - |\phi_{10}\rangle_\alpha, \tag{14}$$

$$e_{\alpha x}e_{\alpha y} = |\phi_{11}\rangle_\alpha, \quad e_{\alpha y}e_{\alpha z} = |\phi_{12}\rangle_\alpha, \quad e_{\alpha z}e_{\alpha x} = |\phi_{13}\rangle_\alpha, \tag{15}$$

thus the components of tensor Q can be explicitly given in terms of the moments:

$$\mathsf{Q}_{mn} \equiv \frac{1}{3}\delta\rho\,\delta_{mn} + j_m j_n - \mathsf{P}_{mn}, \qquad m,\, n \in \{x,\, y,\, z\}, \tag{16}$$

$$\mathsf{P}_{xx} = \frac{1}{3}\left[(e + 2\delta\rho) + 3p_{xx}\right], \tag{17}$$

$$\mathsf{P}_{yy} = \frac{1}{3}\left[(e + 2\delta\rho) + \frac{1}{2}(3p_{ww} - 3p_{xx})\right] = \mathsf{P}_{xx} + \frac{1}{2}(p_{ww} - 3p_{xx}), \tag{18}$$

$$\mathsf{P}_{zz} = \mathsf{P}_{yy} - p_{ww}, \tag{19}$$

$$\mathsf{P}_{xy} = p_{xy}, \quad \mathsf{P}_{yz} = p_{yz}, \quad \mathsf{P}_{zx} = p_{zx}, \tag{20}$$

where $\delta\rho$ is the density fluctuation.[12,13] With the above formulas and assuming $\rho_0 = 1$, the turbulent viscosity ν_t can be readily computed:

$$\nu_t = 3(C_S\Delta_x)^2\overline{S} = \frac{3}{2}s_{xx}(C_S\Delta_x)^2\overline{Q}, \qquad \Delta_x = 1. \tag{21}$$

It should be noted that Eq. (10) may imply that the relaxation rate s_{xx} is the one used in the previous time step, *i.e.*, before the advection takes place.[14] If we require that ν_t depends on the value of S_{ij} at the current time,[2] then we have

$$\tau_t = 3\nu_t = \frac{1}{2}\left(\sqrt{\tau_0^2 + 18C_s^2\Delta_x^2\overline{Q}} - \tau_0\right), \qquad \overline{Q} = \sqrt{\textstyle\sum_{i,j}\mathsf{Q}_{ij}\cdot\mathsf{Q}_{ij}}, \tag{22}$$

$$\tau_0 = 3\frac{UL}{\mathrm{Re}} + \frac{1}{2}, \qquad s_{xx} = \frac{1}{\tau_0 + \tau_t}, \tag{23}$$

where U, L, and Re are characteristic flow velocity, the length, and the Reynolds number, respectively. The above formulas for ν_t and s_{xx} are used in our simulations.

3. Numerical Results

We conduct numerical simulations of the flow over a cube mounted on one wall of a channel at a Reynolds number of 40 000 using the D3Q15 LES-MRT-LBE model with $C_S = 0.16$. This flow has been studied in detail both experimentally[9] and numerically,[8] thus it can be used as testing case for the LES-LBE model. Fig. 1 depicts the complex structures of the mean flow, as observed in experiments.[9]

We apply a logarithmic inflow velocity profile and $\boldsymbol{\nabla}\rho = \mathbf{0}$ in streamwise direction with a reference pressure at the exit, and no-slip (bounce back) boundary

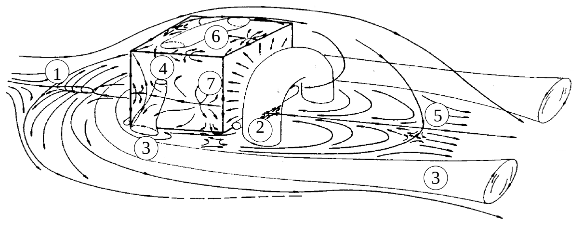

Fig. 1. Flow over a cube mounted on one wall of a channel. Mean flow structures of the flow observed in experiment[9] and captured by the LBE-LES simulations.

conditions for all walls except the two lateral ones where free-slip boundary conditions are applied. A uniform grid of size $301 \times 61 \times 211$ is used (the size of the cube is $H^3 = 30^3$). After an initial run of $50T_0$ (T_0 is the turn-over time $H/U_{\max}$, and $U_{\max} = 0.044$ is the maximum inlet velocity), the flow velocity is averaged over time for another $150T_0$. This averaged velocity field is compared to existing data.[8,9]

Table 1. Attachment/separation length. X_{F1}, X_T, X_{R1}, and X_{R2} are positions of the upstream stagnation point to the cube, the reattachment length at top, the primary and secondary downstream stagnation points from the cube.

Method	X_{F1} ①	X_T ⑥	X_{R1} ⑤	X_{R2}
LBE-LES	1.04	—	1.94	0.07
Exp.[9]	1.040	—	1.612	?
NS-LES[8]	0.8085 – 1.287	0.814 – 0.837	1.432 – 1.722	0.134 – 0.265
RANS[8]	0.650 – 0.950	0.432 (k-ϵ)	2.182 – 2.731	0.020 – 0.252

All significant flow features are captured by the simulation. Table 1 only provides a summary of our results. (A detailed description of the simulations by using the LBGK equation can be found elsewhere.[7]) Other important flow features, namely, the horse shoe vortex ②, the trumpet vortex ③, the vortices ④ and the horizontal stagnation lines ⑦ at each side are reproduced in the simulations. The top vortex ⑥ does not reattach, confirming the experimental observation.[9] Fig. 3 shows the experimental[9] and numerical results for the streamlines on the vertical center plane.

4. Conclusions

We present an LES extension for a MRT-LBE model. The MRT model is more stable than its LBGK counterpart and greatly reduces the spurious oscillations in the pressure field. We also report preliminary results of simulations for the flow over a cube mounted on one wall of a channel at Re = 40 000 by using the LES-LBE model. Our results agree reasonably well with experimental data. A further analysis of stabilities of various MRT-LBE models (D3Q15 and D3Q19) and numerical investigations of turbulent flows by using LBE-LES models are currently underway.

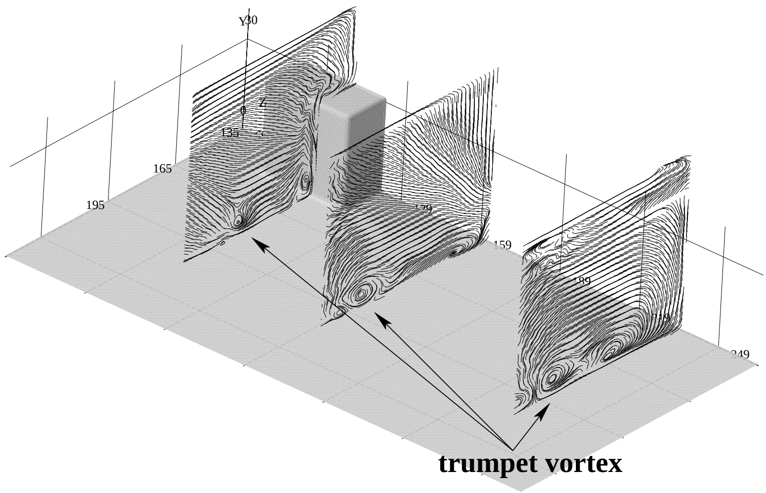

Fig. 2. Trumpet vortex observed in LES-LBE simulation (cf. Fig. 1).

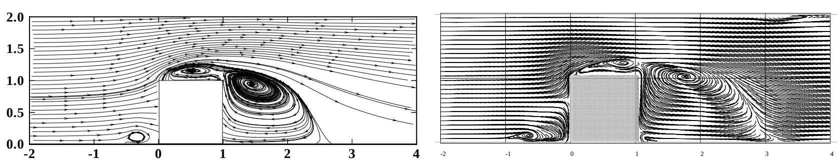

Fig. 3. Vertical mid plane streamlines: experiment[8] (left) *vs.* LBE-LES simulation (right).

Acknowledgments

MK and JT would like to thank the Deutsche Forschungsgemeinschaft (DFG) for financial support. LSL would like to thank D. d'Humières for valuable discussions. His work is partially supported by the United States Air Force Office for Scientific Research under Grant No. F49620-01-1-0142 (technical monitor: Dr. J. Tishkoff).

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