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Lattice Boltzmann Method: Parallel Computing and Collision term effect

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***Abstract*— A Lattice Boltzmann solver is implemented using various techniques and the performance is discussed. Both Open Multi-Processing (OpenMP) and Message Passing Interface (MPI) parallelization techniques using the same numerical algorithm and employing different collision terms were executed. We compare the numerical solution of different programming paradigms to the well known cavity, Taylor-Green and Kida-vortex flows in order to achieve high performances in LBM simulation. The simulations include Lattice Boltzmann Method with single-relaxation-time (SRT) and Entropic model (ELBE). We explore the behavior and accuracy of the proposed models with different implementations. Our results clearly show that the entropic model remains effective in terms of accuracy and stability.**

***Keywords*— MPI, OpenMP, SRT, ELBE, Process time.**

I. INTRODUCTION

The lattice Boltzmann method, commonly called LBM, is a new alternative for the numerical simulation which sustains a rapid evolution in terms of physical models, computer implementations and engineering applications. Compared with classic computational fluid dynamics methods, the advantages of LBM include easy handling of complex geometries and boundary conditions [1] and efficient implementation for parallel computation [2]. Thus, several studies have been carried out in recent years to validate the approach for many heat transfer and reactive flow cases. The history of the LB method is well documented in the literature [3]. Its theoretical fundamentals are based upon the kinetic theory of gases which tries to understand the macroscopic behavior of fluids from the properties of their molecules. The evolutionary process and the formulation of LBM can be highlighted as the following: The Lattice Gas Cellular Automat (LGCA), the continuous Boltzmann-BGK then the Grad's Hermite-quadrature expansion. Beyond these formulations, the incompressible Navier-Stockes equations have been recovered. After the Chapman-Enskog analysis, the equilibrium distribution was written as finite expansions in the local velocity without formal link connecting the LBE to the Boltzmann equation. The first connection of the LBE to the Boltzmann equation has been established by He and Luo [4]. These formulations can construct models that recover incompressible Navier-Stokes equations. However, more studies are still needed to improve the stability of the mass, momentum and energy-conserving LB models.

The Bhatnagar-Gross-Krook (BGK) approximation [5] is the most popular lattice Boltzmann model. This approach derived from the Enskog equation. In this model the collision operator requires the same relaxation time to each physical quantity. Although it's simple implementation, the BGK-LBM suffers from numerical instability at high Reynolds (or Rayleigh number) number. To avoid this restriction, the direct way is to use a large number of grid points, however this will cost large computer resources and lower the computational efficiency. With the current trend in parallel computing, many studies used the single time BGK model with different programming paradigms [6]. However, the majority of published reults using parallel codes aimed to study physical phenomena [7], so little attention have been given to the performance and the efficiency of the implementation.

To remove numerical instability defects of LBM, some authors [8] used the multiple relaxation times model (MRT). The advantage of this model is that it has a maximum number of adjustable parameters. These parameters can be determined by optimizing the hydrodynamic properties of the model and linear stability analysis of the LBE evolution operator. To remedy the stability problem in LBM, some authors who refer to each other used entropic lattice Boltzmann schemes. The derivation of ELBE can be performed in many ways and the most popular one derived from the analog of the discrete Boltzmann H function of standard extensive statistical mechanics [9].

To stabilize numerical simulations of Lattice Boltzmann Method, some authors used Large Eddy Simulation models like other CFD methods [10]. In LES-LBM, different from the DNS-LBM, relaxation times are adjusted locally, according to the resolved strain tensor.

In order to compare between several LBM models, Luo et al. [11] used the lid-driven square cavity flow in two dimensions to perform a comparative study between several

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lattice Boltzmann (LB) models including the MRT-LB, TRT-LB, and LBGK D2Q9 models, and the entropic lattice Boltzmann equation (ELBE). They concluded that MRT-LB and TRT-LB schemes are superior over the ELBE and LBGK schemes in terms of accuracy, stability, and computational efficiency. Also they concluded that the ELBE model is the most inferior among the LB tested models. It must be mentioned that there is some controversy of results reported by the researchers in this topic. Thus, results reported by Luo et al. [11] are commented by I. V. Karlin and al. [12] and they demonstrated a considerable increase of stability with respect to conventional lattice Boltzmann schemes. The interested reader can refer to the mentioned papers to find out more details.

Another ways to improve the stability and the accuracy of the lattice Boltzmann method (LBM) is the choice of the boundary conditions. Ginzburg and D'Humières [13] used a unified approach of several boundary conditions in lattice Boltzmann models. They gave theoretical study of existing boundary conditions and their accuracy for general flows. They also obtained a third order accurate boundary condition for Couette and Poiseuille flows.

Based on the studies we found, there are several methods used to enhance LBM stability and accuracy. Using different collision models and high resolution with parallel implementation are of the most known strategies in this issue. We believe that some important points have to be discussed and analyzed, such as: The efficiency of parallel computing of LBM especially in a single machine and the effect of collision term in the accuracy of the results and the computing time. The main purpose of this study is then to compare between two implementation of LBM algorithm using OpenMP and MPI strategies and to evaluate some LB schemes with the most known collision models.

II. LATTICE BOLTZMANN METHOD (LBM)

The discrete evolution of the particle distribution function describing mass and momentum conservations for D3Q19 discrete velocity model is:

$$f_i(\boldsymbol{r}+\boldsymbol{c}_i\delta_t, t+\delta_t) - f_i(\boldsymbol{r},t) = \Omega(f_i) + F(\boldsymbol{r},t) \quad (1)$$

In the BGK collision model the operator $\Omega(\mathrm{f})$ is replaced by the well-known classical single time relaxation approach:

$$\Omega(f_i) = -\frac{1}{\tau}\left(f(\boldsymbol{r},t) - f^{\mathrm{eq}}(\boldsymbol{r},t)\right) \quad (2)$$

f^{eq} is the local equilibrium distribution function that has an appropriately prescribed functional dependence on the local hydrodynamic properties. $\boldsymbol{r}$ is the position vector, $f(\boldsymbol{r},\mathrm{t})$ is the 19-dimensional vectors for the distribution functions, $\Omega(f)$ is the collision term and F is the external force term. If $\boldsymbol{u}$ is the fluid velocity, the equilibrium distribution function can be expressed as:

$$f_i^{eq} = \omega_i\rho\left[1 + \left\{\frac{\boldsymbol{c_i}.\boldsymbol{u}}{c_s^2} + \frac{1}{2}\left(\left(\frac{\boldsymbol{c_i}.\boldsymbol{u}}{c_s^2}\right)^2 - \frac{\boldsymbol{u}.\boldsymbol{u}}{c_s^2}\right)\right\}\right] \quad (3)$$

c_s is the speed of sound. In the ELBE the collision term can be written as:

$$\Omega(f) = \alpha\beta\left(f^{\mathrm{eq}}(\boldsymbol{r},t) - f(\boldsymbol{r},t)\right) \quad (4)$$

f^{eq} is the local equilibrium that minimizes the entropy function $\mathrm{H} = \sum_{\mathrm{i}} f_i \ln(f_i/\omega_i)$. β matches the viscosity coefficient in the long-time large-scale dynamics of the kinetic scheme.

α is the maximal over-relaxation of the scheme, we note here that the crucial point of ELBE is the entropy condition.

$$H\left(f + \alpha(f - f^{\mathrm{eq}})\right) = H(f) \quad (5)$$

The parameter α is then obtained by solving the non-linear equation Eq.(5). In ELBE, the relaxation parameters are self-adjusted in order to preserve the positiveness of the density distribution function.

The formal solution of the minimization problem is of the Boltzmann type, i.e.:

$$f_i^{eq} = e^{(A + B_\theta C_{i\theta})} \quad (6)$$

where A and B_θ are the Lagrange multipliers. For D3Q19 model, the equilibrium function can be written as the product of three times the one-dimensional solution as follow:

$$f_i^{eq} = \omega_i\rho\prod_{j=1}^{3}\left(2 - \sqrt{1+3u_j^2}\right)\left(\frac{2u_j + \sqrt{1+3u_j^2}}{1-u_j}\right)^{c_{ij}} \quad (7)$$

where j denotes the dimensional index in 3D and $c_{ij}\epsilon\{-1,0,1\}$. The Newton-Raphson method is used to solve the non linear equation for α. In order to speed up the computational time, we use the following approximation of α if the deviation $\mathrm{D}_k = \left|\left(f_i^{eq} - f_i\right)/f_i^{eq}\right|$ is less than is between 10^{-6} and 10^{-2}.

$$\alpha = 2 - 4\frac{a_1}{a_2} + 16\left(\frac{a_2}{a_1}\right)^2 - \frac{8a_3}{a_1} + \frac{80a_2a_3}{a_1^2} - 80\left(\frac{a_2}{a_1}\right)^3 - 16\frac{a_4}{a_1}. \quad (8)$$

Where:

$$a_n = \frac{(-1)^{n-1}}{n(n+1)}\sum_{i=1}^{n_d}\frac{\left(f_i^{eq} - f_i\right)^{n+1}}{f_i^n}, \quad n \geq 1 \quad (9)$$

The starting point for the Newton-Raphson method is 2 for $t=0$ and α_{t-1} for t>0, where α_{t-1} is the computed value of α at time t-1. Finally, the ELBE with collision term given by Eq.(4) reduce a model equivalent to the SRT-LBE if we set α=2 during the simulation.

The computational procedure of the entropic Lattice Boltzmann algorithm is:

- ✓ Initialisation ρ and **u** and the particle distribution functions *{fi}*.
- ✓ Compute the equilibrium function $\{f_i^{eq}\}$ using Eq.(7) .
- ✓ Compute the maximal deviation $\mathrm{D_k}$.
- ✓ According to $\mathrm{D_k}$ →Use either the approximation given by Eq.(8) or Newton-Raphson method to compute the relaxation parameter α or simply set α=2 .

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- ✓ Compute the post-collision distributions using α and Eq.(5).
- ✓ Advection of $\{f_i\}$.
- ✓ Applying boundary conditions.
- ✓ Compute conserved quantities ρ and $\boldsymbol{u}$.

III. Parallelisation Strategies: OpenMP And MPI

The key steps describing the LBM algorithm are the streaming and collision processes. The collision step can be locally computed as follow:

$$f_i(\boldsymbol{r}, t^+) = f_i(\boldsymbol{r}, t) + \Omega(f) \qquad (10)$$

This step involves only the particles located in the same lattice. The majority of calculations is performed at this step. On the other hand, the symmetry of discrete speeds, explained and location make this stage a good candidate for parallel implementation.

The streaming step is not local in which each particle moves to the nearest node in the direction of its velocity following the equation:

$$f_i(\boldsymbol{r} + c_i, t + 1) = f_i(\boldsymbol{r}, t^+),\ i = 0,..18 \qquad (11)$$

The parallel implementation of the collision step using OpenMP technique can be easily performed by using the instruction "#pragma omp for". However, the number of threads must be mentioned before running the code.

The MPI implementation of the LBM with BGK collision model is shown in Fig. 1.

The densities are stored as double-precision floating point numbers. This requires extreme amounts of memory and CPU resources for a typical simulation. We use 3D decomposition for MPI parallel implementation in order to allow ideal data communications between subdomains.

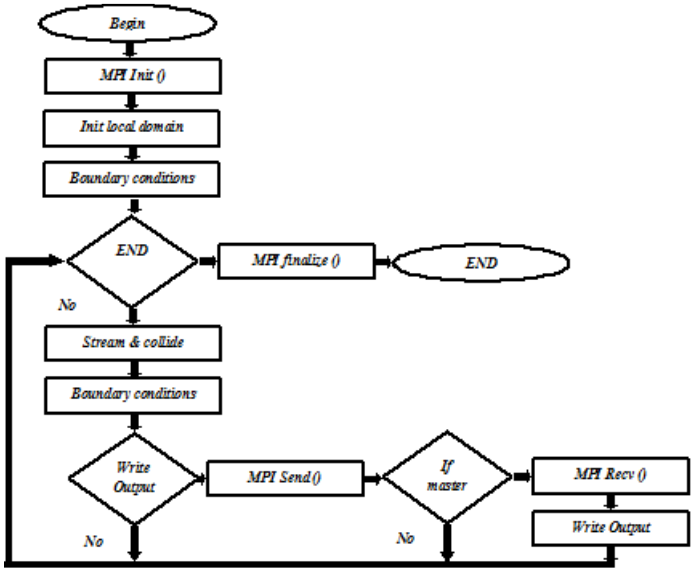

Fig. 1 MPI implementation with Master-Worker approach.

Since the CPU time will be considered, it is necessary to mention that the following calculations are performed using a single machine Intel Core i3-4160, 4th Generation (3M cache, 3.6GHz).

IV. Results And Discussions

A. Parallel computing

As a practical comparison of the described Lattice Boltzmann implementations, we consider the fully 3D flow in a cubic lid-driven cavity. This problem has been extensively employed as a standard benchmark for numerical methods and analyzed by a number of authors using a variety of solution procedures. The flow configuration and boundary conditions are as follows. The top wall moves with a uniform velocity U_0 while the other walls are fixed. As a compromise between accuracy and computational efficiency, the value of U_0 is fixed to 0.1. Hence the Reynolds number $Re = HU_0/\nu$ changed by different dimensionless kinematic viscosity. The incompressible Navier-Stokes equations are in the following form.

$$\nabla.\boldsymbol{u} = 0, \qquad (12)$$

$$\partial_t \boldsymbol{u} + (\boldsymbol{u}.\nabla)\boldsymbol{u} = -\nabla p + \frac{1}{Re}\nabla^2 \boldsymbol{u}. \qquad (13)$$

In the BGK, we use the standard "bounce-back" condition while in the entropic model we use the diffusive Maxwell boundary condition in order to reduce the noise in the distribution functions and therefore the macroscopic moments as follow [14]:

$$f_i(r, t + 1) = \gamma f_i^{eq}(u_w) \qquad (14)$$

At the top wall boundary γ is given by:

$$\gamma = \frac{f_9^c(r,t)+f_{10}^c(r,t)+f_{11}^c(r,t)+f_{12}^c(r,t)+f_{13}^c(r,t)}{f_9^{eq}(u_w)+f_{10}^{eq}(u_w)+f_{11}^{eq}(u_w)+f_{12}^{eq}(u_w)+f_{13}^{eq}(u_w)} \qquad (15)$$

Where f_i^c is the density distribution function after the collision process.

Using the BGK algorithm and different implementations namely openMP and MPI, simulations of lid driven cavity flow at low Reynolds number (Re=10) were carried. In the previous section we have described the approach followed to implement the D3Q19 LBM solver with OpenMP and MPI.

Fig. 3 describe the Processor time evolution and the number of Mega Lattice Site Updates per Second (MLUPS) for different threads numbers using openMP and MPI and grid sizes. The minimum calculation time tends to the number of threads (2 or 4) while remaining higher. The most basic observation here is that , we see that if the number of threads equal to the number of physical or logical threads (Intel Core i3), the calculation time is minimal and the number of Mega Lattice Site Updates per Second is maximal so the calculation is efficient. It is important to note that the original code must be widely modified by using MPI implementation in order to reach better performance.

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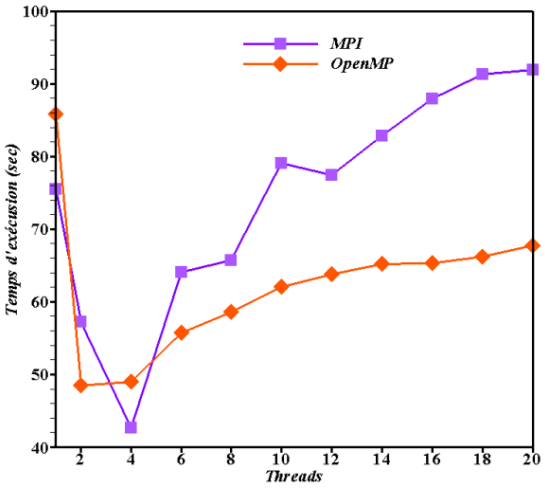

Fig. 2 Processor time evolution for different numbers of threads using openMP and MPI.

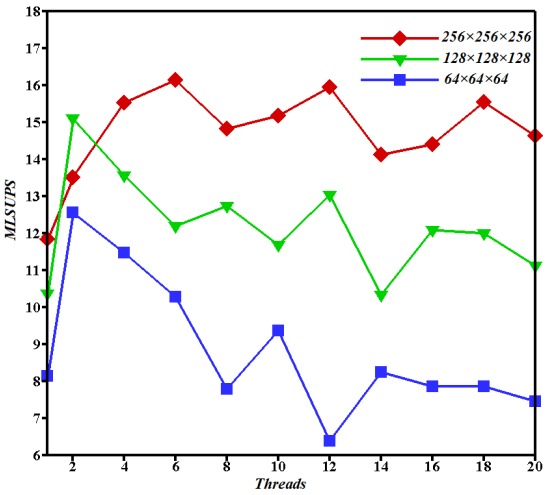

Fig. 1 Number of Mega Lattice Site Updates per Second (MLUPS) using different numbers of threads and grid sizes.

B. *Collision term effect*

In the following step, we perform numerical simulations in order to compare between the BGK and entropic models. Unsteady Taylor-Green vortex flow is considered which is described by the following initial conditions in periodic cubical domain:

$$\begin{cases} u_x = U_0 sin\left(\frac{x}{H}\right) cos\left(\frac{y}{H}\right) cos\left(\frac{z}{H}\right) \\ u_y = -U_0 cos\left(\frac{x}{H}\right) sin\left(\frac{y}{H}\right) sin\left(\frac{z}{H}\right) \\ u_z = 0 \end{cases} \quad (16)$$

Reynolds number is kept to 1600 while the velocity $U_0 = 0.0288$ in lattice unit. Computations were performed with D3Q27 model at two spatial resolutions: 64^3 and 128^3.

The aim of this study is not the discussion of the decayed turbulent flow since many studies based on valuable physical information are found in the literature and treated this issue in details. The reader can refer to [15] and references therein for more information. This standard benchmark is used to test the accuracy, stability and computational efficiency of the two described Lattice Boltzmann models.

The time evolution of kinetic energy provide a good indication of the manner in which the turbulent structures disappear. In Fig. 4, the energy evolution $E_k = \frac{1}{2V}\int_V \boldsymbol{u}^2 dV$ for both ELB and BGK simulations for Green-Taylor problem with the two successive grids are compared with the DNS [15]. ELB compares well with DNS results even with coarse grid size. It is important to mention that spectral method in the refernce [15] uses a grid size of 256^3. The results of the mesh 128^3 compares well those of the reference. However, the coarse mesh 64^3 is dissipative and gives values of the energy less than the reference especially in the range $4 \leq t \leq 12$.

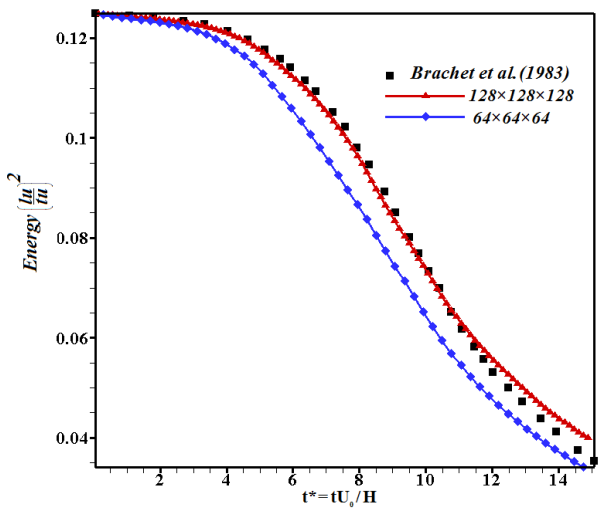

Fig. 4 Temporal evolution of the kinetic energy k(t) for Green-Taylor using ELB model.

Fig. 5 shows the iso-surfaces of vorticity magnitude at t*=0.141, t*=7.085 and t*=14.878, respectively using ELBE model. It is clear that the entropic model solve all the scales available in the computational domain. At first, the flow has a viscous behavior and the vortices begin to evolve and roll-up. Near t*=7 the smooth eddy structures begin to undergo changes in their structure and around t*=9 there is an appearance of the coherent structures. Beyond this time, the flow becomes completely turbulent and the structures degrade slowly. The structures become smaller in turbulent regime.

In table I we summarize the statistical data of the 10 nondimensional time steps t* obtained by BGK and ELB with the same grid size 128^3.

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TABLE I
STATISTICAL DATA COMPUTED BY USING BGK AND ELB MODELS.

Time t^*	Energy E_k		Enstrophy ξ	
	ELB	**BGK**	**ELB**	**BGK**
0.141	0.372798	0.372067	1.51659	4.3026
0.283	0.371066	0.370921	3.31556	3.74682
0.425	0.369516	0.369321	4.48078	5.11552
0.566	0.368003	0.367932	5.54661	5.51816
0.708	0.366298	0.366201	6.77422	6.66922
0.850	0.364119	0.363799	8.29798	8.1507
0.991	0.361475	0.360776	10.2754	9.79006
1.133	0.358232	0.35698	12.7717	11.6696
1.275	0.354341	0.35238	15.6113	13.6395

It is clear that the energy values obtained by two models are close at all computed times. However, only at the last stage ($t^* \geq 0.566$) the values of enstrophy $\xi = \frac{1}{2V}\int_V \boldsymbol{\Omega}^2 dV$ obtained by the two models are very close.

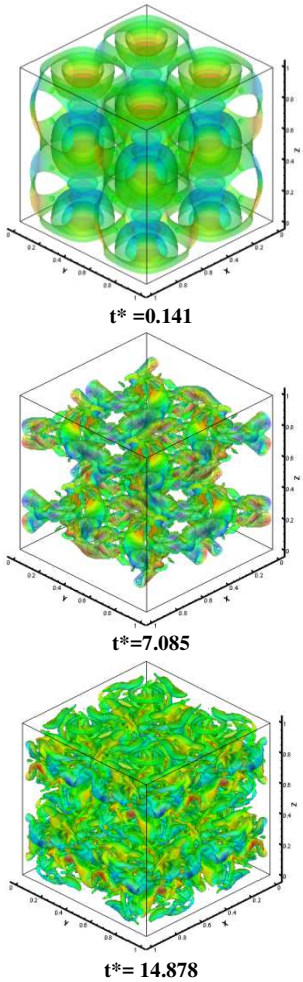


Fig. 5 Iso-surfaces of vorticity magnitude at $t^* = 0.141$, $t^* = 7.085$ and $t^* = 14.878$, respectively (ELB model).

Fig. 6 shows the temporal evolution of the kinetic energy k(t) for decaying isotropic turbulence (Kida-vortex) with initial Reynolds number Re=1000 using BGK and ELB models and different grid sizes. It can be observed that results of kinetic energy by using ELB method is truncated in the middle between those obtained by using BGK model with two different grid size 128^3 and 200^3. The entropic model not only stabilize the LBM simulation and enhance its stability, but also gives accurate results and remains stable with coarse grid more than the standard BGK model. This enhancement is performed by the numerical solution of entropy balance.

Fig. 7 shows the Q-criterion iso-surfaces and vorticity magnitude at $t^* = 0.141$, $t^* = 1.417$ and $t^* = 4.959$, respectively with ELB model. One can observe that ELB solve appropriately the finest structure of the flow and reproduces all the known features of the flow.

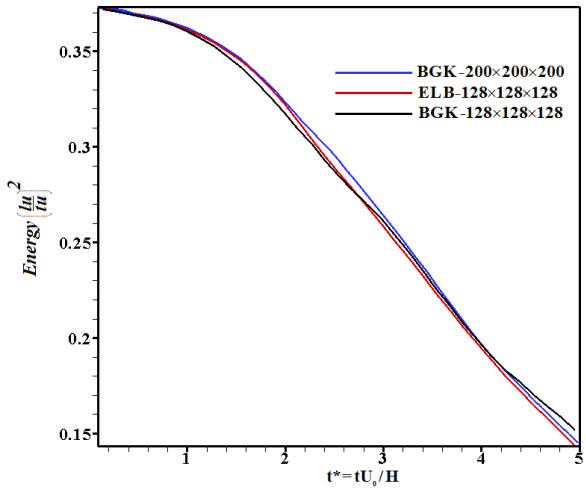
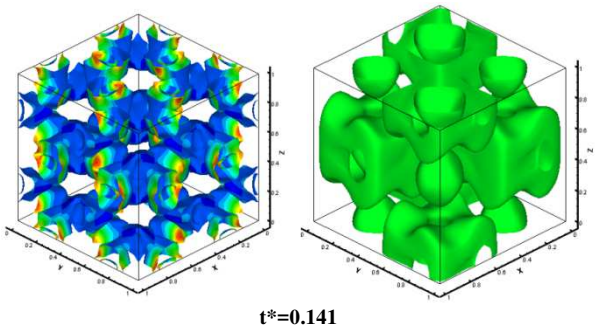


Fig. 6 Temporal evolution of the kinetic energy k(t) for Kida vortex using BGK and ELB models.



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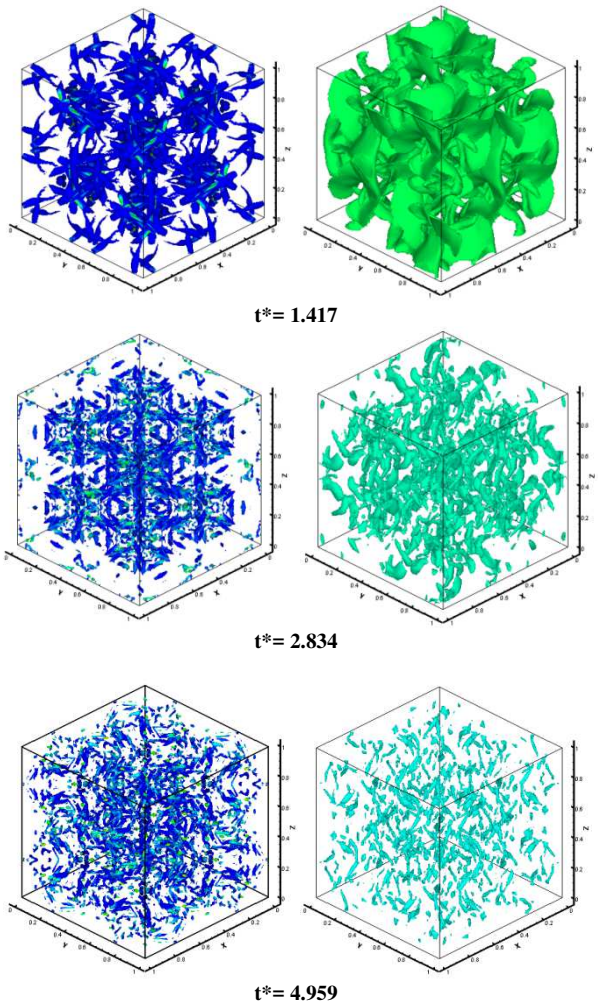

Fig. 7 Q-criterion iso-surfaces and vorticity magnitude at t* =0.141, t*=1.417 and t*=4.959, respectively (ELB model).

V. Conclusion

In this study, we have presented the general methodology for constructing and implementing LBM scheme on parallel architecture and with different collision term. To evaluate the capability and reliability computation of the entropic model, we use 3D decayed turbulence as a benchmark test. The ELBE remains unchallenged even with low resolutions. However, the calculation of the relaxation time in BGK model is less than computation effort in calculation of α parameter in ELBE. Moreover, thanks to the self adjustment of the relaxation parameter, our results highlight the subgrid feature of ELBE and that it has the correct limit of DNS when simulation is sufficiently resolved.

References

[1] A A Mohamad, *Applied Lattice Boltzmann Method for Transport Phenomena, Momentum, Heat and Mass Transfer*, Sure Printing, Calgary, 2007.

[2] J.C. Desplat , I. Pagonabarraga and P. Bladon, "Ludwig: A parallel Lattice-Boltzmann code for complex fluids", Computer Physics Communications, vol.134, pp. 273-290, 2001.

[3] S. Sauro , "*The Lattice Boltzmann Equation for Fluid Dynamics and Beyond (Numerical Mathematics and Scientific Computation)",* Clarendon press, Oxford, 2001.

[4] X. He and L.S. Luo, "Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation", Phys. Rev. E., vol. 56, pp. 6811-6817, 1997.

[5] P L Bhatnagar, E P Gross and M Krook, "A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems", Phys. Rev., vol.94, pp. 511-525, 1954.

[6] M. Ben Belgacem and B. Choparda, "A hybrid HPC/cloud distributed infrastructure: Coupling EC2 cloud resources with HPC clusters to run large tightly coupled multiscale applications", Future Generation Computer Systems., vol.42, pp. 1-16, 2015.

[7] L. P. Wang , P. C. Cheng , Z. Guo and Yu Zhaosheng, "Lattice Boltzmann simulation of particle-laden turbulent channel flow", Computers and Fluids., vol.124, pp. 226-236, 2016.

[8] D. D'Humieres, G. Irina, M. Krafczyk, P. Lallemand and L. S. Luo, "Multiple-Relaxation-Time Lattice Boltzmann Models in Three Dimensions", Philosophical Trans. Royal Soc. of London Series A-Math. Physical and Eng. Sciences, vol. 360, pp. 437-451, 2002.

[9] S. Ansumali and I.V. Karlin, "Entropy Function Approach to the Lattice Boltzmann Method", Journal of Statistical Physics., vol. 107, pp. 291-308, 2002.

[10] P. Sagaut, "Toward advanced subgrid models for Lattice-Boltzmann-based Large-eddy simulation: Theoretical formulations", Computers & Mathematics with Applications, vol. 59, pp. 2194-2199, 2010.

[11] L.S. Luo, W. Liao, X. Chen, ,Y. Peng and W. Zhang, "Numerics of the lattice Boltzmann method: Effects of collision models on the lattice Boltzmann simulations", Phys. Rev. E., vol. 83, pp. 1-24, 2011.

[12] IV Karlin, S Succi and S.S Chikatamarla, "Comment on "Numerics of the lattice Boltzmann method: effects of collision models on the lattice Boltzmann simulations", Phys Rev E Stat Nonlin Soft Matter Phys. 068701, pp. 1-4, 2011.

[13] I. Ginzburg and D. D'Humières, "Multireflection boundary conditions for lattice Boltzmann models", Phys. Rev. E., vol. 68, 066614, pp. 1-30, 2002.

[14] A.N. Gorban and Packwood D.J. "Enhancement of the stability of lattice Boltzmann methods by dissipation control", Physica A., vol. 414, pp. 285-299, 2014.

[15] M E. Brachet, I. Daniel , D. I. Meiron, A. Steven S. A. Orszag, B.G Nickel, R.H. Morf and U. Frisch, "Small-scale structure of the Taylor–Green vortex", Journal of Fluid Mechanics, vol. 130, pp. 411-452, 1983.

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