

## Entropic lattice Boltzmann scheme: accuracy and optimization strategies

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In the recent years, the interest in numerical methods for fluid dynamics has increased significantly. Historically computational fluid dynamics deals with the numerical solution of the Navier-Stokes equations of continuum mechanics. In this work we approach the problem using the lattice Boltzmann method (LBM), that attracted significant attention as an alternative technique to solve complex fluid flow. Basically the LBM solve the macroscopic dynamics of fluid flows via a mesoscopic technique based on a reduced version of the Boltzmann kinetic equation that preserve all the details strictly needed to recover hydrodynamic behaviour (mass, momentum and energy conservation). This simulation strategy is realized via a mesoscopic dynamic of fictitious particles and through an elegant and simple equation (Lattice Boltzmann Equation - LBE). The time evolution of the discrete population of particles  $\mathbf{f} \in \mathbb{R}^9$  is obtained by the single-time relaxation collision operator introduced by Bhatnagar-Gross-Krook (BGK) (cfr. 9, 6, 13, 3)

$$(0.1) \quad f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) = f_i(\mathbf{x}, t) + \theta (f_i^{eq} - f_i), \quad i = 0, \dots, 8$$

where  $f_i(\mathbf{x}, t)$  is the probability of finding a particle at lattice site  $\mathbf{x}$  at time  $t$ , moving along the lattice direction defined by the discrete speed  $\mathbf{c}_i$ . The left-hand side of this equation represents the molecular free-streaming, whereas the right-hand side represents molecular collisions via a single-time relaxation towards local equilibrium  $f_i^{eq}$  on a typical single timescale  $\tau$ , called relaxation parameter, and  $\theta = (2\delta t)/(2\tau + \delta t)$  is the relaxation rate. This local equilibrium is taken in the form of a quadratic expansion of a (local) Maxwellian. LBM has proved to be an accurate and efficient tool for simulating a variety of non-trivial fluid dynamics problems, such as incompressible (cfr. 14, 9) and turbulent flows (cfr. 7). However, as recognized by many authors (cfr. 1, 4, 12), the application of the BGK collision operator suffers of numerical instability problems, especially in conjunction with high-Reynolds number flows. Therefore, improvements of the stability properties of lattice kinetic schemes are developing rapidly. A technique, that showed an higher stability (cfr. 1, 4), can be obtained if the LBM is based on an analogue of

the Boltzmann  $H$ -theorem (cfr. 1, 2, 4, 11, 15), by constructing the collision integral on the basis of the entropy function and by stabilizing the updates on the basis of the discrete-time  $H$ -theorem (see 9), known as entropic lattice Boltzmann method (ELBM). The updating rule of ELBM is basically the same of the LBM, except in the computation of the relaxation parameter  $\theta$ , obtained in order to satisfy the monotonicity of the  $H$ -function, through a two-step geometric procedure: in the first step, populations are changed in the direction of the bare collision,  $\Delta = \mathbf{f}^{eq} - \mathbf{f} \in \mathbb{R}^b$ , and a parameter  $\alpha$  is computed to maintain the  $H$  function constant at each time step (cfr. 2); in the second step, the magnitude of the  $H$ -function decreases and dissipation is introduced, through a parameter  $\beta$ , related to the viscosity  $\nu = c_s^2(1/\beta - 1)/2$ . This delivers the *effective* relaxation frequency  $\theta = \alpha\beta$ . The purpose of our work is to address the accuracy and the performance of the ELBM with respect to the lattice LBGK scheme. For this reason we apply the ELB technique to the lid-driven cavity flow, which has become a standard benchmark (cfr. 10) in which the non-linear component of the Navier-Stokes equation plays a major role. The cavity is a steady, incompressible flow that sets up in a square box where one of the walls (here the top wall) moves at a constant velocity. Despite its simple geometry, a complex flow takes place into the cavity, with multiple counter-rotating recirculating regions. Three main vortices of different dimensions are usually observed: a pair of small vortices (left and right secondary vortices) is located in the lower corners and a big vortex occupies the upper portion of the cavity (primary vortex). Fixing the viscosity and the cavity shape, the complexity of the flow depends only on the Reynolds number. The top boundary moves from left to right with a constant and uniform velocity  $\mathbf{u} = (0.1, 0)$ , in lattice units. The domain is discretized with  $100 \times 100$  nodes. At the beginning of the simulation a uniform initial density  $\rho = 2.7$  is set and the fluid velocity is zero everywhere, except at the top-side nodes. The numerical results obtained by using ELB shows a good agreement with literature data, as summarized in Table 0.1, where the location of the vortices centers are a good indicator of accuracy. Figure 0.1 shows the stream function obtained with  $Re = 2000$  using LBM and ELBM, while Figure 0.2 shows the trasverse profile of the longitudinal and transverse velocity at the centerline, for Reynolds ranging between 400 and 2000.

**Conclusion:** The comparison with literature data and with standard LBM shows that ELBM offers higher stability at a moderate price in terms of computational overhead, due to several strategies we studied to reduce this cost. It is therefore expected that these optimization techniques may result in even higher savings for other types of complex fluid flows.

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Table 0.1: Vortex centers coordinates at various Reynolds numbers. Present work (a); BGK simulations (b); Literature data (c) (cfr. 10) and (d) (cfr. 5).

$Re$		Primary vortex		Lower left vortex		Lower right vortex	
		$x$	$y$	$x$	$y$	$x$	$y$
400	a	0.5500	0.6000	0.0500	0.0500	0.8850	0.1250
	b	0.5500	0.6070	0.0450	0.0600	0.8950	0.1400
	c	0.5608	0.6078	0.0549	0.0510	0.8902	0.1255
1000	a	0.5260	0.5620	0.0900	0.0770	0.8550	0.1150
	b	0.5230	0.5550	0.0900	0.0800	0.8400	0.1000
	c	0.5333	0.5647	0.0902	0.0784	0.8667	0.1137
	d	0.5308	0.5652	0.0833	0.0781	0.8640	0.1118
2000	a	0.5200	0.5500	0.0890	0.1000	0.8300	0.1000
	b	0.5200	0.5540	0.0900	0.1100	0.8350	0.1000
	c	0.5255	0.5490	0.0902	0.1059	0.8471	0.0980
5000	a	0.5150	0.5400	0.0780	0.1350	0.8050	0.0750
	c	0.5176	0.5373	0.0784	0.1373	0.8078	0.0745

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Figure 0.1: Stream function: left side ELB, right side BGK. Top velocity  $\mathbf{U} = (0.1, 0)$ .  $100 \times 100$  grid. Reynolds number 2000 from top to bottom.

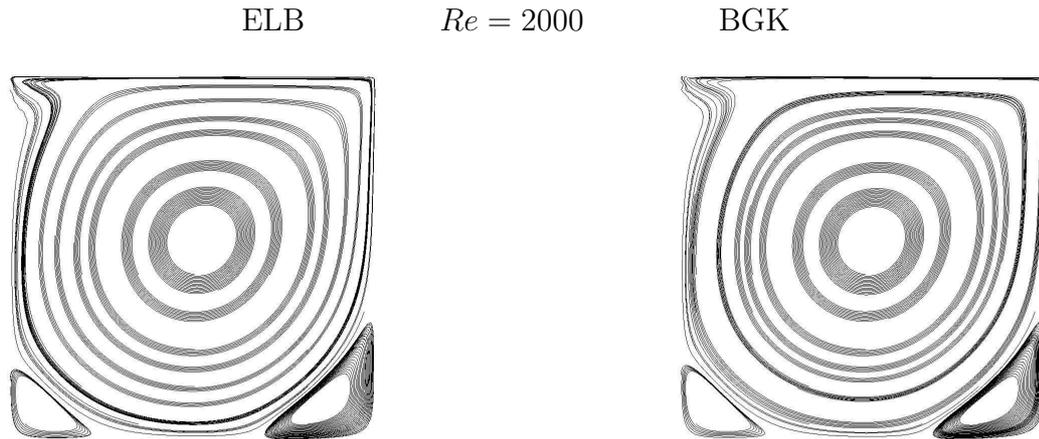


Figure 0.2: Profile of the longitudinal and transverse velocities  $u, v$  at the centreline  $x = L/2$  - Comparison with literature data, cfr. 8 (scatter points).

