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The Lattice Boltzmann Equation on Irregular Lattices

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A general framework to extend the lattice Boltzmann equation to arbitrary lattice geometries is presented and numerically demonstrated for the case of a two-dimensional Poiseuille flow. The new scheme considerably extends the range of applicability of the Boltzmann method to problems requiring the use of nonuniform grids.

1. INTRODUCTION

Despite of its recent origin, the lattice Boltzmann equation (LBE) has already been successfully exploited in several fluid-dynamic applications, ranging from low-Reynolds flows in porous media to fully developed isotropic turbulence.[1] Yet, if compared with more conventional numerical techniques, LBE suffers from the limitation of being constrained to a special class of uniform and regular lattices ensuring rotational invariance. This limitation is particularly severe in many practical applications, where a selective distribution of the spatial nodes close to the critical regions of the flow is mandatory to fully capitalize on the computational resources. This motivates a considerable interest in extending the range of applicability of the LBE method to arbitrarily nonuniform meshes. This possibility has been recently pointed out by Higuera[2]; the idea is to use a coarse-grained distribution function which is defined at the center of macrocells, each of which can contain several nodes of the regular fine-grained grid where the original LBE dynamics takes place. This coarse-

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grained distribution function is then displaced in fractional amounts, whose value is fixed by the number of particles crossing the boundary of the macrocell per unit time. Before becoming practical, this idea has, however, to be quantitatively confronted with the important test of numerical diffusion, a problem apparently not addressed in the aforementioned work. In this paper we will exhibit a concrete example of a finite-volume LBE (FVLBE) largely free of numerical diffusion. This opens the way to the application of the LBE methodology to a number of important problems requiring the use of nonuniform grids.

2. FINITE-VOLUME FORMULATION OF LBE (FVLBE)

Our starting point is the usual LBE in a regular lattice[4]

$$f_i(\mathbf{x}+\mathbf{v}_i\tau, t+\tau) - f_i(\mathbf{x}, t) = \sum_j \Omega_{ij}(f_j - f_j^{\mathrm{eq},2}) \equiv \Omega_i \tag{1}$$

where $f_i \equiv f(\mathbf{x}, \mathbf{v}_i, t)$ is the particle population at node $\mathbf{x}$ in the direction $\mathbf{v}_i$ at time t. The velocity variable $\mathbf{v}_i$ is discretized on a suitable discrete lattice ensuring isotropy on a macroscopic level. In the sequel we shall refer to the 2D projection of the 4D FCHC lattice[3] defined by 4 nearest-neighbor links $\mathbf{v}_i = (1, 0)$, $(0, 1)$, $(-1, 0)$, and $(0, -1)$; four diagonal links $(1, 1)$, $(-1, 1)$, $(1, -1)$, and $(-1, -1)$; and a rest particle $(0, 0)$; for a total of 9 independent populations. The rhs of Eq. (1) represents the effect of the particle collisions, whose properties have been discussed in depth in previous publications.[1] This matrix is real and symmetric and fulfills the sum rules imposed by mass and momentum conservation. Finally, $f_i^{\mathrm{eq},2}$ represents the local equilibrium distribution function, expanded to second order in the local flow field $\mathbf{u}$ in order to retain advective effects:

$$f_j^{\mathrm{eq},2}(u) = Q_{j\alpha\beta}u_\alpha u_\beta; \qquad Q_{i\alpha\beta} = v_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}; \qquad \alpha, \beta = 1, 2 \tag{2}$$

It can be shown that in the continuum limit and provided that $\lambda \geqslant -2$, Eq. (1) converges to the Navier–Stokes equation for a continuum fluid, with a viscosity (in lattice units)

$$\nu_{\mathrm{LBE}} = -\frac{1}{6}\left(\frac{1}{\lambda} - \frac{1}{2}\right) \tag{3}$$

λ is the nonzero eigenvalue of Ω_{ij} associated with the set of eigenvectors $Q_{i\alpha\beta}$. This eigenvalue can be tuned to minimize the fluid viscosity, i.e., maximize the Reynolds number $Re = uL/\nu$. In principle, zero viscosity

could be achieved by choosing $\lambda = -2$, but in practice ν_{LBE} cannot be lowered below a threshold of the order of $1/N$, N being the number of grid points for dimension in the simulation, for, otherwise, unresolved scales would be excited in the flow. It should be stressed that in order for Eq. (1) to converge to the Navier–Stokes result in the continuum limit, it is essential that the velocity variable remain discretized in a suitable regular lattice in order to enforce the symmetry relations on the matrix Ω_{ij} which guarantee mass and momentum conservation as well as rotational invariance. This is the reason why the validity of LBE is limited to a uniform and regular grid. On the other hand, if we take the differential form of Eq. (1), there is no *a priori* reason why LBE should not be available to a coarse-graining procedure via a finite-volume (FV) technique. We feel that the FV method is particularly appropriate to this purpose because it represents the most natural continuation at a macroscopic level of those "first principles" (conservation laws) which form the common basis of the lattice gas and lattice Boltzmann method. Of course, one has to be careful that in the continuum limit, this FV formulation will still reproduce the Navier–Stokes equation. In this paper, we shall present a FV version of LBE with the desidered property (we shall hereafter refer to this property as to "hydrodynamic consistency," h-consistency for brevity).

As a first step, we introduce a two-dimensional macroscopic grid whose elementary cells are quadrilaterals of arbitrary shape (see Fig. 1).

A coarse-grained distribution F_P can then be defined via a cell-averaging operator $\hat{A}_P$ such that $F_P \equiv \hat{A}_P f = A^{-1} \int_{C_P} f \, dA$, where C_P is the cell centered around the point P. By acting with $\hat{A}_P$ on the differential form

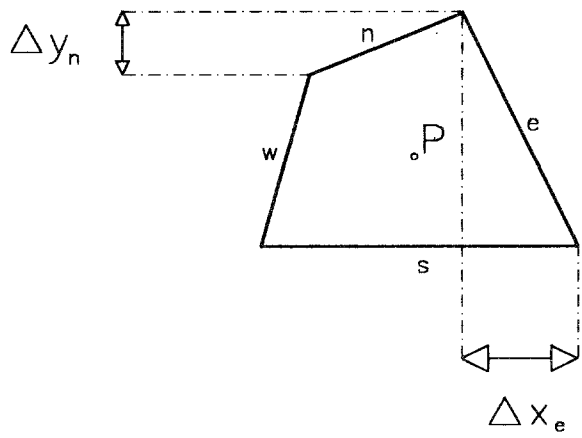

Fig. 1. A typical control cell for the finite-volume formulation of LBE.

of Eq. (1) and applying a first-order time-marching scheme, standard calculations lead to the following form of FVLBE:

$$\hat{F}_{iP} = F_{iP} - \Delta t \sum_{\sigma} g_{i\sigma} \sum_{\sigma'} R_{\sigma\sigma'} F_{iP_{\sigma'}}$$

$$+ \Delta t \sum_{j} \Omega_{ij} (F_{jP} - Q_{j\alpha\beta} U_{P\alpha} U_{P\beta} - Q_{j\alpha\beta} \langle u'_{P\alpha} u'_{P\beta} \rangle) \tag{4}$$

where a caret indicates the time $t + \Delta t$. The meaning of the symbols is as follows: $g_{i\sigma} = \mathbf{v}_i \cdot \hat{n}_\sigma) l_\sigma$ is the projection of the boundary edge l_σ, $\sigma = e, n, w, s$ standing for the "east," "north," "west," and "south" boundaries, along the direction $\mathbf{v}_i$; $R_{\sigma\sigma'}$ is the matrix representation of the reconstruction operator $\hat{R}$ expressing the boundary values $f_{i\sigma}$ in terms of the nodal values $F_{iP_{\sigma'}}$; $P_{\sigma'}$ describes a suitable neighborhood of P which depends on the order of the interpolation. This completes the streaming phase. As to the coarse-grain collision operator, $U_{P\alpha}$ represents the cell-averaged macroscopic flow ($U_{P\alpha} \equiv \hat{A}_P u_\alpha$), while u'_α is the fluctuating component of u_α (brackets denote cell-averaging). It is important to notice that these fluctuations are perfectly identified once a specific form of the reconstruction operator is chosen. For instance, by choosing a bilinear interpolator, it is clear that u'_α are also bilinear functions of space and can then be exactly computed in terms of gradients of the macroscopic field U. In this sense, the choice of the reconstruction operator is equivalent to a turbulence model. From Eq. (4), it is clear that both the streaming and the collision operators become "dressed" with a certain degree of non-locality which is explicitly fixed by the precise nature of the reconstruction operator.

The lowest order "h-consistent" FVLBE scheme is the one based on a piecewise constant ("pwc" hereafter) reconstruction operator and upwind spatial differencing. Lowest order means that no reconstruction at all is performed, so that in each macrocell the coarse-grained distribution function F takes just a single value. Upwind differencing means that the boundary values $f_{i\sigma}$ are set to the coarse-grain values corresponding to the macrocell from which "particles" are streaming in. As an example, for direction 1 (rightward streaming), we have $f_e = F_P$, $f_w = F_W$, where W indicates the "west" node. The pwc version of FVLBE is the closest one to the original LBE, in that it entails the minimal loss of locality. The price to pay for this simplicity is a significant increase of the numerical viscosity, that is, a significant reduction of the highest Reynolds number achievable in the simulation. A standard Fourier analysis of the pwc FVLBE scheme yields in fact the following value for numerical diffusion (in units of the fine lattice):

$$\nu_n = \frac{1}{2} \frac{(\Delta x - 1)}{\Delta t} \tag{5}$$

This expression tells us that, while in the fine lattice ($\Delta x = \Delta t = 1$) numerical diffusion is absent, for $\Delta x \gg 1$, ν_n scales like Δx, so that it rapidly overwhelmes the one pertaining to the uniform lattice, which cannot be lowered below a threshold of the order of 0.01 in present-day LBE simulations. The presence of numerical diffusion is clearly evidenced in Fig. 2, which refers to the flow speed u for a Poiseuille flow in a channel of width $H = 48$ lattice units for different values of the viscosity ν_{LBE}. The pressure gradient is adjusted in such a way as to yield a maximum speed $U_{\max} = 0.02$ in the absence of numerical diffusion. The simulation has been performed with 32 points, distributed as follows: 16 in the peripherical regions (spacing 1) and 16 in the central one (spacing 2), corresponding to a numerical viscosity $\nu_n = 0.5$.

A dramatic improvement is obtained by moving to the next order reconstruction operator, i.e., a piecewise linear representation of the distribution function ("pwl" hereafter). Leaving the details to a future and lengthier publication, we simply list the explicit form of this operator. For direction $i = 1$

$$f_e = \left[F_P + \left(\frac{F_P - F_W}{x_P - x_W} \right) x_e^* - x_P) \right] \tag{6}$$

and for direction $i = 2$

$$f_e = \left[F_P + \left(\frac{F_P - F_W}{x_P - x_W} \right) (x_e^* - x_P) \right] p + F_S(1-p); \qquad p = (1 - 0.5\Delta x^{-1}) \tag{7}$$

where W and S denote the centers of the "west" and "south" cells (similar expressions hold for the remaining directions) and x_e^* is a free parameter

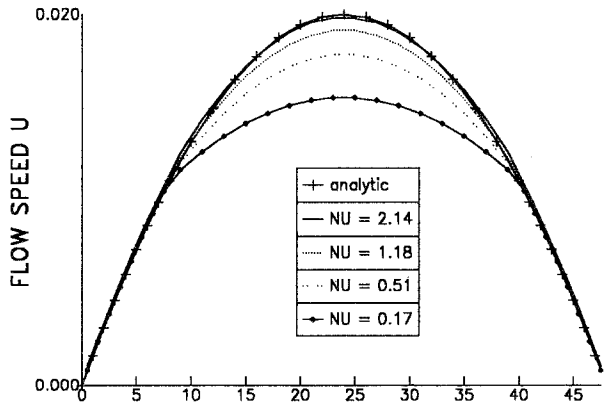

Fig. 2. Parabolic profiles obtained with the pwc FVLBE method for different values of the LBE viscosity (NU). Note that a reasonable agreement with the analytical result is attained only in the limit $\nu_{\mathrm{LBE}} \gg \nu_n$.

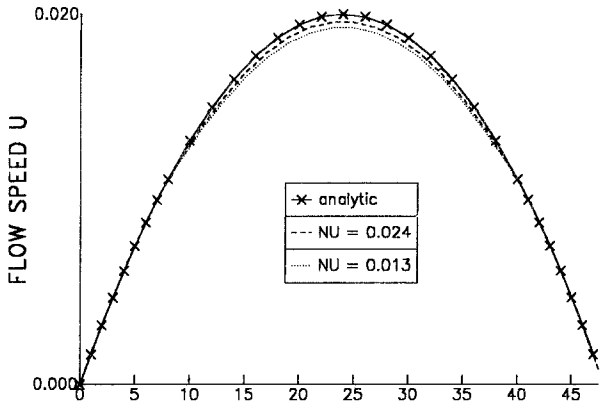

Fig. 3. Parabolic profiles obtained with the pwl FVLBE method for different values of the LBE viscosity (NU). Note the improvement of about two orders of magnitude with respect to the pwc method.

which is adjusted in such a way as to minimize numerical diffusion. Lengthy but straightforward algebra (most conveniently performed with the aid of an algebraic manipulator, SCRATCHPAD II in our case[6]) shows that in order to obtain $v_n = 0$ (in the case of a Cartesian lattice) one has to make the following position $x_e^* - x_p = 0.5(\Delta x - 1)$ for $i = 1$, and $x_e^* - x_p = 0.5(\Delta x - 1)/(1 - 0.5\Delta x^{-1})$ for $i = 2$. We note that for the case $i = 1$, x_e^* coincides with the location of the particles of the fine grid which cross the boundary of the macrocell C_p in a single time step. In the case $i = 2$ (streaming up-right), we have not been able to find an equivalently transparent geometrical interpretation. Finally, we point out the presence of the weight $(1 - p)$, which is associated with corner-transport-upwind[5] carrying the contribution from cell south to the flux on the east boundary. One can readily check that this term, while of higher order in $1/\Delta x$, is essential to the "h-consistency" of the pwl FVLBE scheme. This theoretical analysis is confirmed by numerical simulation, as shown in Fig. 3, which refers to the same numerical setup as Fig. 2, with the pwc scheme replaced by the pwl version. As one sees, the analytical results are perfectly reproduced up to very small values of v_{LBE} of the order of 10^{-2}, i.e., well compatible with those usually employed in uniform LBE simulations. The discrepancy for $v_{\mathrm{LBE}} < 0.02$ is due to the small error introduced there where Δx undergoes a discontinuous change (well visible in Fig. 3) and can certainly be alleviated by redestributing the grid points in a smoother way. Even in the present status, FVLBE has access basically to the same range of Reynolds numbers attainable by LBE at a minor cost in terms of computational nodes, and better geometrical flexibility. These advantages are

obtained at the expense of a (weak) loss of locality, which entails a corresponding increase of the computational work per node. Future research, to be performed on a case by case basis, will indicate the best compromise between the conflicting issues of geometrical flexibility and computational efficiency.

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