Automatic grid refinement criterion for lattice Boltzmann method

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Abstract

In all kinds of engineering problems, and in particular in methods for computational fluid dynamics based on regular grids, local grid refinement is of crucial importance.

To save on computational expense, many applications require to resolve a wide range of scales present in a numerical simulation by locally adding more mesh points. In general, the need for a higher (or a lower) resolution is not known a priori, and it is therefore difficult to locate areas for which local grid refinement is required. In this paper, we propose a novel algorithm for the lattice Boltzmann method, based on physical concepts, to automatically construct a pattern of local refinement. We apply the idea to the two-dimensional lid-driven cavity and show that the automatically refined grid can lead to results of equal quality with less grid points, thus sparing computational resources and time. The proposed automatic grid refinement strategy has been implemented in the parallel open-source library Palabos.

1 Introduction

The lattice Boltzmann method (LBM) is a numerical method which is widely used in the field of computational fluid dynamics. It has proven its importance with respect to other traditional numerical methods, as it has recently been used in many simulations of engineering interest (see [Aidun and Clausen 2010], [Parmigiani et al. 2011], [Malaspinas and Sagaut 2012] among others).
In order to overcome the limitations of the method which, in its most straightforward formulation, is restricted to uniform grids, the community has proposed several approaches to block-wise grid refinement (see Filippova and Hänel [1998], Dupuis and Chopard [2003], Chen et al. [2006]). The goal when using such methods is to increase the precision of the results through a local adaptation of the mesh resolution, with an acceptable computational effort.

In this paper we treat, independently of the underlying grid refinement algorithm, the question of how a grid refinement pattern is to be devised most efficiently. We must note that, while this point remains as of now open in the lattice Boltzmann community, this operation is of crucial importance, as all the potential gains of non–uniform grids are tightly coupled with their choice of arrangement in space.

In traditional numerical methods such as the finite differences, there exist frameworks for a posteriori error estimation. This allows to locally mark areas where the biggest local errors are found. The interested reader is invited to read Skeel [1986] for a list of error estimation techniques.

In the case of the LBM, this kind of error estimation has not been studied in depth. We can however cite Han et al. [2006] where the authors adapt the Richardson extrapolation method (commonly used in finite difference) to the LBM. They find that the error for two grids with different resolutions is proportional to the off–equilibrium part of the distribution function.

Another approach is proposed in Crouse et al. [2003]. The authors use the so–called sensors $\phi_s$ to provide local error estimates. In particular, in a grid with spatial discretization $\delta x$, they work with the divergence sensor defined as

$$\phi_s = \delta x^{3/2} |\nabla \cdot u|, \tag{1}$$

which is compared to an empirical value in order to generate a non–uniform grid for their simulation.

In this work, we propose a novel method to find zones that might require a local finer resolution, based on an anticipation of how the ratio between off–equilibrium and equilibrium parts of the velocity distribution functions converges towards the Knudsen number ($\text{Kn}$). In the convective rescaling, the Knudsen number is simply a constant, independent of the level of grid refinement. The novelties of our approach reside in the fact that we do not have to perform several simulations to estimate the local errors and that it also provides an estimation of the degree of refinement needed.

The structure of this document is as follows. We start by briefly introducing the LBM in order to define all the theoretical concepts and notations in Section 2. Then, in Section 3, we present the generic concepts of our criterion for automatic refinement. A numerical validation for the 2d lid-driven cavity is provided in Section 4 and Section 5 provides a conclusion and a discussion of future work.
2 The lattice Boltzmann method

The lattice Boltzmann method (LBM) is by now a well-known numerical method for computational fluid dynamics. In this section we have chosen to present only the basic concepts. For further details the reader is referred to Chopard and Droz [2005], Succi [2001], Wolf-Gladrow [2000].

We start by presenting the Boltzmann equation (BE). This equation describes the time evolution of large numbers of particles in a region of the space $x \in \mathbb{R}^3$ with a given velocity $\xi \in \mathbb{R}^3$, which are represented by the particle mass distribution function $f(x, \xi, t)$. The Boltzmann equation for a gas without external force with the BGK (for Bhatnagar, Gross, Krook, see Bhatnagar et al. [1954]) approximation with relaxation time $\tau$ is

\[
(\partial_t + \xi \cdot \nabla_x) f = -\frac{1}{\tau} (f(x, \xi, t) - f_{eq}(x, \xi, t)),
\]

where $f_{eq}$ is the equilibrium distribution function, given by the Maxwell–Boltzmann distribution.

Following the ideas presented in Shan et al. [2006], one can discretize the velocity space to a set of $q$ velocities. For example, in 2D, a well–known set of discrete velocities is given by the $D2Q9$ model (see Fig. 1)

\[
\{\xi_i\}_{i=0}^8 = \{(0,0),(-1,1),(-1,0),(-1,-1),(0,-1),
(1,-1),(1,0),(1,1),(0,1)\}.
\]

Figure 1: The D2Q9 lattice with the vectors representing the microscopic velocity set $\xi_i$. A rest velocity $\xi_0 = (0,0)$ is added to this set.

The BE after velocity discretization becomes

\[
(\partial_t + \xi_i \cdot \nabla_x) f_i(x, t) = -\frac{1}{\tau} (f_i(x, t) - f_{eq}(x, \xi_i, t)),
\]

where we have used the notation $f_i(x, t) \equiv f(x, \xi_i, t)$.

Next, this equation is integrated along characteristics with the trapezoidal rule. One obtains the following implicit equation

\[
f_i(x + \delta \xi_i, t + \delta t) - f_i(x, t) = -\frac{\delta t}{2\tau} \{f_i(x + \delta t \xi_i, t + \delta t) + f_i(x, t)
- f_{eq}(x + \delta t \xi_i, t + \delta t) - f_{eq}(x, t)\}.
\]
This equation can be converted in an explicit scheme by using the change of variable given by

$$\bar{f}_i = f_i + \frac{\delta t}{2\tau} (f_i - f_i^{eq})$$  \hspace{1cm} (6)$$

$$\bar{\tau} = \frac{2\tau + \delta t}{2\delta t}.$$  \hspace{1cm} (7)

Finally, we obtain the LBM BGK equation

$$\bar{f}_i(x + \delta t \xi_i, t + \delta t) - \bar{f}_i(x, t) = -\frac{1}{\bar{\tau}}[\bar{f}_i(x, t) - f_i^{eq}(x, t)].$$  \hspace{1cm} (8)

We note that Eq. (8) is the kinetic equation that we simulate in the LBM. From now on the bars are omitted for simplicity unless explicitly stated otherwise. Without loss of generality we also set $\delta t = 1$.

The discrete equilibrium distribution function is expressed by the truncated Maxwellian equilibrium

$$f_i^{eq} = w_i \rho \left( 1 + \frac{\xi_i \cdot u}{c_s^2} + \frac{1}{2c_s^4} Q_i : uu \right),$$  \hspace{1cm} (9)

where $\rho$ is the density, $u$ is the macroscopic velocity field, $Q_i = \xi_i \xi_i - c_s^2 I$, $c_s$ and $w_i$ the lattice speed of sound and the lattice weights respectively, which are given for the D2Q9 lattice by

$$c_s^2 = \frac{1}{3}, \quad w_0 = \frac{4}{9}, \quad w_{2,4,6,8} = \frac{1}{9}, \quad w_{1,3,5,7} = \frac{1}{36}.$$  \hspace{1cm} (10)

The density and the velocity fields are computed by the distribution function through the relations

$$\rho = \sum_{i=0}^{q-1} f_i = \sum_{i=0}^{q-1} f_i^{eq},$$  \hspace{1cm} (11)

$$\rho u = \sum_{i=0}^{q-1} \xi_i f_i = \sum_{i=0}^{q-1} \xi_i f_i^{eq}.$$  \hspace{1cm} (12)

For implementation purposes, a time-step is decomposed into two parts that are applied successively on the whole computational domain. The two-steps are called the “collide-and-stream” operation.

1. The collision, which modifies locally the value of the populations according to

$$f_i^{out}(x, t) = f_i(x, t) - \frac{1}{\bar{\tau}}[\bar{f}_i(x, t) - f_i^{eq}(x, t)].$$  \hspace{1cm} (13)

2. The streaming, which moves the populations to their neighbors according to their microscopic velocity

$$f_i(x + \xi_i, t + 1) = f_i^{out}(x, t).$$  \hspace{1cm} (14)
If we perform a multi-scale Chapman–Enskog (CE) expansion (see Chapman and Cowling [1960], Chopard and Droz [2005] for more details) one can show that the LBM BGK scheme is asymptotically equivalent to the weakly compressible Navier–Stokes equations

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\frac{1}{\rho} \nabla p + 2\nu \nabla \cdot (\mathbf{S}),
\end{align*}
\]

with \( p \) being the pressure, \( \mathbf{S} \) the strain tensor and \( \nu \) the kinematic viscosity defined by

\[
\begin{align*}
p &= c_s^2 \rho, \\
\mathbf{S} &= \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right), \\
\nu &= c_s^2 (\tau - 1/2).
\end{align*}
\]

The CE expansion is done under the assumption that \( f_i \) is given by a small perturbation of the equilibrium distribution

\[
f_i = f_i^{\text{eq}} + \varepsilon f_i^{(1)} + O(\varepsilon^2),
\]

where \( \varepsilon \ll 1 \) can be identified with the Knudsen number (see Huang [1987]). This can be seen by replacing the CE Ansatz (Eq. (20)) in Eq. (4), neglecting the time dependence of \( f_i \) and keeping only the lowest orders on both sides of the equation one remains with

\[
\begin{align*}
\xi_i \cdot \nabla f_i^{(0)} &\sim \frac{1}{\tau} f_i^{(1)}, \\
\frac{c_s}{L} f_i^{(0)} &\sim \frac{1}{\tau} f_i^{(1)}, \\
\frac{f_i^{(1)}}{f_i^{(0)}} &\sim \frac{\tau c_s}{L} = \frac{\lambda}{L} = \text{Kn},
\end{align*}
\]

with \( \text{Kn} \) the Knudsen number, \( \lambda = c_s \tau \) the mean free path and \( L \) the characteristic length of the system. In the second line we used the fact that the characteristic value of the microscopic velocity is given by the speed of sound, and that since we are interested only on the variation of macroscopic quantities, the gradient must scale like the characteristic size of the domain. The \( f_i \) can also be formally decomposed into

\[
f_i = f_i^{\text{eq}} + f_i^{\text{neq}},
\]

where \( f_i^{\text{neq}} \) is the off–equilibrium part of the particle distribution function. According to the assumptions of the CE expansion \( f_i^{\text{neq}} \) can be approximated to \( f^{(1)} \) when one neglects \( O(\varepsilon^2) \) terms

\[
f_i^{\text{neq}} \sim \varepsilon f^{(1)}.
\]
During the CE expansion, one finds that \( f_i^{(1)} \) is given by

\[
\varepsilon f_i^{(1)} = \frac{w_i}{2c_s^2} Q_i : \Pi^{(1)},
\]

where the tensor \( \Pi^{(1)} \equiv \sum_i \xi_i \varepsilon f_i^{(1)} \) is related to the strain rate tensor \( S \) through the relation

\[
\Pi^{(1)} = -2c_s^2 \rho \tau S.
\]

3 Grid refinement criterion algorithm

In this section we present the grid refinement criterion, independently of the actual algorithm used for the grid refinement. All relevant details about the grid refinement approach used in the validation section of this paper can be found in [Lagrava et al. 2012].

Our grid refinement criterion is based on the fact that the off-equilibrium and equilibrium parts of the distribution function are related by the Knudsen number through the relation

\[
f_{\text{neq}} \sim f_{\text{eq}} \text{Kn},
\]
as shown in Eq. (21).

Let us now consider a grid \( G_c \) with spatial spacing \( \delta x_c \). We also define a finer grid \( G_f \) with spatial step \( \delta x_f \), defined by the relationship \( \delta x_c = \delta x_f / n \), where \( n \) is a positive integer. Let’s assume that the same simulation is executed with both grids, and that the Reynolds number \( \text{Re} \) is the same in both cases. We recall that \( \text{Re} = \frac{u_{lb} N}{\nu_{lb}} \), where \( u_{lb}, \nu_{lb}, \) and \( N \) are respectively the characteristic velocity, viscosity and length scale of the system in lattice units. We also set \( u_{lb} \) to be constant in \( G_c \) and \( G_f \) (convective scaling), a fact which can be expressed through the relationship \( \delta t_c / \delta t_f = \delta x_c / \delta x_f \). This also implies that both simulations have the same Mach number

\[
\text{Ma} = \frac{u_{lb}}{c_s}.
\]

Finally, we note that the Knudsen number, which is defined as

\[
\text{Kn} = \frac{\lambda}{L_c} = \frac{c_s \tau}{L}
\]

\[
= \frac{u_{lb}}{c_s} \frac{c_s^2 \tau}{L u_{lb}} = \frac{u_{lb}}{c_s} \frac{\nu}{L u_{lb}} = \text{Ma}/\text{Re},
\]
is independent of the resolution. As a side remark, this statement would not hold in case of diffusive scaling, i.e. when the parameters between two grids scale like \( \delta t \sim \delta x^2 \).

The general idea of our refinement criterion is that the quality of our results are given by the measured Knudsen number (see Eq. (21)) when compared with the “theoretical” Knudsen number of Eq. (27). To formalize the automatic grid refinement process, we propose the following algorithm:
1. Choose a unique spatial resolution $\delta x$ for the computational domain $R$.

2. Divide the simulation domain $R$ in $m$–by–$n$ sub–domains $R_{i,j}$.

3. Perform the simulation over $R$.

4. Compute the Kn number from the relation $Kn = \frac{Ma}{Re}$.

5. For each sub–domain $R_{i,j}$ of $R$ compute the mean value of the quantity

$$C_{i,j} = \frac{1}{q|R_{i,j}|} \sum_{x \in R_{i,j}} \sum_{i=0}^{q-1} \left| \frac{f_{eq}^{i}}{f_{i}^{eq}} \right|,$$  

where $|R_{i,j}|$ is the number of grid points inside the $R_{i,j}$ region.

At this point one wants to determine if each region $R_{i,j}$ has a grid has a sufficient resolution. To do so we propose to compute the refinement factor $R_{i,j}^f$ defined as

$$R_{i,j}^f \equiv \text{round} \left( \log_2 \left( \frac{C_{i,j}}{Kn} \right) \right),$$

where round() denotes that the result of the logarithm is rounded to the closest integer. This quantity determines the ratio between $\delta x$ on our test grid $R$ and the target resolution on a subdomain $R_{i,j}$ one would like to obtain in order for its grid to be resolved enough. For example if $R_{i,j}^f = 0$ then no refinement is needed on the subdomain $R_{i,j}$, but if $R_{i,j}^f = 2$ then the grid in $R_{i,j}$ must be made four times finer.

4 Numerical results

We have chosen to test our algorithm for a steady state problem, as a dynamic, time-dependent adaptation of the grid is not the scope of this paper. The test case is the well known 2D lid-driven cavity, for which reference benchmark values are provided in Ghia et al. [1982].

The numerical setup and structure of the solution are depicted in Fig. 2. We work on a square bounded domain with no-slip walls, except for the top lid, which is subject to a constant right–directed velocity. In our particular case, the Reynolds number is fixed to $Re = 100$. The discrete time step of the simulation is pinned down by setting the velocity of the top lid in lattice units to $u_{lb} = 0.01$. In this numerical example, the Knudsen number is $Kn = u_{lb}/(c_s Re) = 0.00017$ (see Eqs. (26) and (27)).

We divide the domain in several regions $R_{i,j}$ (the example used here with five lines and five columns can be found in Fig. 3). We perform the measure of the quantity $C_{i,j}$ for a uniform resolution with $N = 15, 30, 60, 120, 240$. The values of $C_{i,j}/Kn$ for $N = 30$ are depicted in Fig. 4. The required refinement factor is then computed by taking the binary logarithm of $C_{i,j}/Kn$. 
Figure 2: Set-up for the cavity 2D example and norm of the non-dimensional velocity at steady state.

Figure 3: Division of the simulation domain in several regions.

Fig[3] compares the value of the $C_{i,j}$ coefficient to the Knudsen number at different levels of resolution. A white color means that the region $R_{i,j}$ must be refined ($C_{i,j} > Kn$), and gray means that the resolution is sufficient. It can be seen that at $N = 15$, the resolution is insufficient in the whole domain. At larger values of $N$, we observe that the white regions decrease until only the corners are left. It should be pointed out that the predictions of our algorithm seem reasonable, as the velocity gradients are obviously largest close to the top lid.
Figure 4: Fixing $N = 30$, $R_{i,j}^f$ for each region $R_{i,j}$.

Furthermore, it makes sense to require a higher grid resolution in the corners, in which the velocity imposed by the boundary condition is discontinuous.

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Figure 5: Areas in a 5–by–5 grid that require grid refinement, depending on the level of grid resolution $N$. White color means that further refinement is need (i.e. $C_{i,j} > Kn$), while gray stands for the fact that the resolution is sufficient.

Fig. 6 shows the grid dependence of the largest, the smallest, and the average value of the ratio between $C_{i,j}$ and $Kn$. It can be seen that this quantity obeys
a power law with exponent 1. In other words, one can take it for granted that $C_{i,j}$ is at most reduced by a factor two when the resolution is doubled.

![Figure 6: Convergence of several $C_{i,j}$ values divided by Kn.](image)

Using the results presented in Fig. 4, we generated a non-uniform mesh which is described in Fig. 7. The level zero is corresponding to $N_0 = 30$, level one to $N_1 = 60$, and the level two to $N_2 = 120$. In order to assess the quality of our automatic refinement technique, we generated a “naive” mesh (shown in Fig. 8). We also compared the results obtained with the two non-uniform grids with the results of a uniform grid with $N = 120$, and with reference results of Ghia et al. [1982]. In total, the number of points used in the “automatically” generated grid is 5436, while there are 6400 points in the naively generated one, and 14400 points in the uniform one. The economy in grid points of the naive mesh if of 44.4% as compared to the uniform case, and the economy of the automatic approach is of 15% as compared to the naive one.

![Figure 7: Level of refinement of each block on our non–uniform grid.](image)

We have computed the root mean square (RMS) for the centerline $x$-component of the velocity with the results of Ghia et al. [1982] at a Reynolds of Re = 100. The three results for the centerline velocity are depicted in Fig. 9. We have found
RMS values which are the same as the RMS value obtained with a uniform grid at \( N = 120 \), which is given by

\[
RMS_{120} = 0.00208, \quad RMS_{gr} = 0.00213, \quad RMS_{naive} = 0.00219, \quad (30)
\]

Here, \( RMS_{120} \), \( RMS_{gr} \), \( RMS_{naive} \) are the RMS values of the uniform grid, the automatic, and the naive grid refinement strategy respectively. We therefore conclude that our criterion for grid-refinement allows for results of good quality while requiring less computational power than the naive or uniform grids.

Figure 8: Three–level refinement, obtained by approximation, to achieve a good value of RMS as compared to Ghia et al. [1982].

Figure 9: Vertical centerline \( u_x \) velocity for reference solution, uniform and non–uniform grids.

Finally, the generation of the grid of Fig. 7 from Fig. 4 is not completely straightforward at first glance, since the resolution levels do not match between
the two figures. Nevertheless one must keep in mind that for our grid-refinement algorithm to be valid, on adjacent subdomains only a factor two is allowed for the ratio of resolutions. For example if \( R_{0,0}^f = N \) then \( R_{0,0}^f = N \pm 1 \) can actually be implemented. Therefore the inconsistency that seems to appear at first between Figs. 7 and 4 is rather due to this consistency constrain of resolution level ratio between different resolution regions.

5 Conclusions and future work

In this work we presented a novel algorithm, based on physical arguments, which allows a detection of regions where local grid refinement is needed for the lattice Boltzmann method. The detection is based on the evaluation of the local Knudsen number which is computed from the density distribution function. This method has the advantage on relying only on local information and is therefore very efficient in terms of parallelism. Our method is validated on the two dimensional lid driven cavity and shows that without any \textit{a priori} knowledge of the flow a good mesh is proposed and the results of the simulation are matching those of meshes (homogeneous and locally refined) with significantly more grid points. This technique is can be straightforwardly applied in three dimensions. Since no \textit{a priori} knowledge of the numerical setup it could also be used for adaptive grid refinement techniques in time dependent problems.

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