Predictor-Corrector Finite-Difference Lattice Boltzmann Schemes

G. V. Krivovichev and E. V. Voskoboinikova

Department of Applied Mathematics and Processes of Control
Saint-Petersburg State University, Saint-Petersburg, Russian Federation

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Abstract

Predictor-corrector finite-difference lattice Boltzmann schemes are proposed. An approach with separate approximation of spatial derivatives in the advective term of kinetic equations and an approach when this term is replaced by a single finite difference are considered. Explicit finite-difference schemes are used at both the stages of the computation process. The lid-driven cavity flow problem and the Taylor — Green problem are solved numerically in a wide range of the Reynolds number. It is shown that the proposed schemes allow a larger time step compared to well-known upwind schemes.

Mathematics Subject Classification: 76-04; 76M10; 65N30

Keywords: lattice Boltzmann method, finite-difference schemes, predictor-corrector method

1 Introduction

The lattice Boltzmann method (LBM) has become a powerful approach for simulation of fluids in various regimes. Instead of solving of hydrodynamical equations, in LBM-based approach a system of kinetic equations is used [3],[13]. Simple implementation of boundary conditions together with inherent grid generation makes the method geometrically versatile, and it is thus convenient for simulation of complex systems such as multiphase flows [6],[7].
The computational rules of LBM are successfully adopted for realization of computations on single and multiple graphical processing units (GPUs) [2], [8].

In this study predictor–corrector finite–difference lattice Boltzmann schemes (FDLBSs) are considered. Every scheme is based on two stages — predictor and corrector steps. First step is realized to obtain predictive approximation of the numerical solution, and second one is realized for correction of approximation. Explicit schemes are used on both stages. Two types of schemes are compared: with separate approximations of derivatives in advective terms of kinetic equations and schemes with unified approximation of this terms [9],[11].

The paper is organized as follows. In Section 2 FDLBSs are considered. In Section 3 two test problems are solved and numerical results are compared. Concluding remarks are made in Section 4.

2 Predictor–corrector finite–difference lattice Boltzmann schemes

The main idea of LBM is that the fluid is considered as an ensemble of mesoscopic particles. Particles could move without collisions between the nodes of spatial lattice and undergo collisions at lattice nodes. Each particle can move between the nodes per time step \( \delta t \).

In this study 2D spatial lattice constructed with step \( l \) is considered. In this case so-called D2Q9 lattice could be used, that is defined by following set of vectors: \( \mathbf{V}_i = V \mathbf{v}_i, \ i = 1, \ldots, n \), where \( V = l/\delta t \) is a typical velocity and dimensionless vectors \( \mathbf{v}_i \) are presented as: \( \mathbf{v}_1 = (0,0), \mathbf{v}_2 = (1,0), \mathbf{v}_3 = (0,1), \mathbf{v}_4 = (-1,0), \mathbf{v}_5 = (0,-1), \mathbf{v}_6 = (1,1), \mathbf{v}_7 = (-1,1), \mathbf{v}_8 = (-1,-1), \mathbf{v}_9 = (1,-1) \).

The dynamics of the particles is described by the following system of equations in dimensionless variables:

\[
\frac{\partial f_i}{\partial t} + \mathbf{v}_i \nabla f_i = -\frac{1}{\tau}(f_i - f_i^{(eq)}), \tag{1}
\]

where \( f_i = f_i(t, \mathbf{r}) \) are dimensionless distribution functions of particles with velocities \( \mathbf{v}_i \), \( t \) is a dimensionless time, \( \mathbf{r} = (x,y) \) is a dimensionless vector of spatial variables, \( f_i^{(eq)} \) are dimensionless equilibrium distributions, \( \tau \) is a dimensionless relaxation parameter. System (1) is obtained from kinetic Boltzmann equation with Bhatnagar–Gross–Krook collision operator [1].

At first, the construction of predictor–corrector FDLBS with separate approximations of derivatives on spatial variables will be considered. Let us rewrite (1) in vector form:

\[
\frac{\partial \mathbf{f}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{f})}{\partial x} + \frac{\partial \mathbf{G}(\mathbf{f})}{\partial y} = \mathbf{S}(\mathbf{f}), \tag{2}
\]
where \( \mathbf{f} = (f_1, \ldots, f_9)^T; \mathbf{F}, \mathbf{G} \) are linear vector-functions of \( \mathbf{f} \): \( F_i = v_{ix}f_i, \ G_i = v_{iy}f_i; \mathbf{S} \) are nonlinear vector-functions of \( \mathbf{f} \) (due to the nonlinear dependence of \( f_i^{(eq)} \) on \( \mathbf{f} \) [3]).

Time grid with step \( \Delta t \) is considered. Spatial step is equal to \( h \). For the construction of the scheme, realized on predictor step, all derivatives from (2) are approximated at node \((t_n, \mathbf{r}_{jk})\) (where \( \mathbf{r}_{jk} = (x_j, y_k) \)), with upward finite differences:

\[
\frac{\partial f}{\partial t}(t_n, \mathbf{r}_{jk}) \approx \frac{f_{jk}^{n+1} - f_{jk}^n}{\Delta t}, \quad \frac{\partial \mathbf{F}}{\partial x}(t_n, \mathbf{r}_{jk}) \approx \frac{\mathbf{F}^{n+1}_{jk} - \mathbf{F}^n_{jk}}{h},
\]

\[
\frac{\partial \mathbf{G}}{\partial y}(t_n, \mathbf{r}_{jk}) \approx \frac{\mathbf{G}^{n+1}_{jk} - \mathbf{G}^n_{jk}}{h}.
\]

So the formulae for the scheme may be written as:

\[
f_{jk}^{n+1} = f_{jk}^n - \frac{\Delta t}{h}(\mathbf{F}^{n+1}_{jk} - \mathbf{F}^n_{jk}) - \frac{\Delta t}{h}(\mathbf{G}^{n+1}_{jk} - \mathbf{G}^n_{jk}) + \Delta t \mathbf{S}(f_{jk}^n). \tag{3}
\]

Numerical solution, obtained by (3) will be denoted as \( \mathbf{f}^n_{jk} \).

For the construction of the scheme for corrector step all derivatives are approximated at node \((t_{n+1/2}, \mathbf{r}_{jk})\). Time derivative is approximated with half step \( \Delta t/2 \):

\[
\frac{\partial f}{\partial t}(t_{n+1/2}, \mathbf{r}_{jk}) \approx \frac{f_{jk}^{n+1/2} - f_{jk}^{n+1/2}}{\Delta t/2}.
\]

Derivatives on \( x \) and \( y \) are approximated by backward differences:

\[
\frac{\partial \mathbf{F}}{\partial x}(t_{n+1/2}, \mathbf{r}_{jk}) \approx \frac{\mathbf{F}^{n+1/2}_{jk} - \mathbf{F}^{n+1/2}_{jk-1}}{h}, \quad \frac{\partial \mathbf{G}}{\partial y}(t_{n+1/2}, \mathbf{r}_{jk}) \approx \frac{\mathbf{G}^{n+1/2}_{jk} - \mathbf{G}^{n+1/2}_{jk-1}}{h}.
\]

The following scheme is obtained:

\[
f_{jk}^{n+1/2} = f_{jk}^{n+1/2} - \frac{\Delta t}{2h}(\mathbf{F}^{n+1/2}_{jk} - \mathbf{F}^{n+1/2}_{jk-1}) - \frac{\Delta t}{2h}(\mathbf{G}^{n+1/2}_{jk} - \mathbf{G}^{n+1/2}_{jk-1}) + \frac{\Delta t}{2} \mathbf{S}(f_{jk}^{n+1/2}). \tag{4}
\]

Let us approximate the solution in node \((t_{n+1/2}, \mathbf{r}_{jk})\) by following rule:

\[
f_{jk}^{n+1/2} \approx \frac{1}{2}(f_{jk}^n + f_{jk}^{n+1}). \tag{5}
\]

It is assumed, that the following approximations may be considered:

\[
\mathbf{F}_{jk}^{n+1/2} \approx \mathbf{F}_{jk}^{n+1}, \quad \mathbf{G}_{jk}^{n+1/2} \approx \mathbf{G}_{jk}^{n+1}, \quad \mathbf{S}_{jk}^{n+1/2} \approx \mathbf{S}_{jk}^{n+1}. \tag{6}
\]

After the substitution of (5) and (6) into (4), the implicit scheme without the values at node \((t_{n+1/2}, \mathbf{r}_{jk})\) is obtained. To construct the explicit scheme,
the solution obtained by (3) must be substitute into the right part of the implicit scheme.

As a result, the scheme realized on corrector step is obtained:

$$f_{jk}^{n+1} = \frac{1}{2}(f_{jk}^n + \tilde{f}_{jk}^n) - \frac{\Delta t}{2h}(\tilde{F}_{jk}^{n+1} - \tilde{F}_{j-1,k}^{n+1}) - \frac{\Delta t}{2h}(\tilde{G}_{jk}^{n+1} - \tilde{G}_{j-1,k}^{n+1}) + \frac{\Delta t}{2}\tilde{S}_{jk}^{n+1},$$  

(7)

where $\tilde{F} = F(\tilde{f})$, $\tilde{G} = G(\tilde{f})$, $\tilde{S} = S(\tilde{f})$.

Let us rewrite constructed scheme (3)–(7) for application to solution of system (1) with predictor step:

$$\tilde{f}_i(t_{n+1}, r_{jk}) = f_i(t_n, r_{jk}) - \frac{\Delta t}{h}v_{ix}(f_i(t_n, r_{j+1,k}) - f_i(t_n, r_{jk})) - \frac{\Delta t}{h}v_{iy}(f_i(t_n, r_{jk+1}) - f_i(t_n, r_{jk})) - \frac{\Delta t}{\tau}(f_i(t_n, r_{jk}) - f_i^{(eq)}(f(t_n, r_{jk}))),$$  

(8)

and corrector step:

$$f_i(t_{n+1}, r_{jk}) = \frac{1}{2}(f_i(t_n, r_{jk}) + \tilde{f}_i(t_{n+1}, r_{jk})) - \frac{\Delta t}{2h}v_{ix}(\tilde{f}_i(t_{n+1}, r_{jk}) - \tilde{f}_i(t_{n+1}, r_{j-1,k})) - \frac{\Delta t}{2h}v_{iy}(\tilde{f}_i(t_{n+1}, r_{jk}) - \tilde{f}_i(t_{n+1}, r_{jk-1})) - \frac{\Delta t}{2\tau}(\tilde{f}_i(t_{n+1}, r_{jk}) - f_i^{(eq)}(\tilde{f}(t_{n+1}, r_{jk}))).$$  

(9)

In this study the obtained scheme (8)–(9) will be called PC1.

In [5],[9],[11] FDLBSs based on unified approximation of advective terms $v_i\nabla f_i$ are considered. In this study the scheme of such type is considered. On the predictor step the scheme with following approximation is considered:

$$v_i\nabla f_i(t_n, r_{jk}) \approx \frac{1}{h}(f_i(t_n, r_{jk}) + v_i h) - f_i(t_n, r_{jk}),$$

on the corrector step the scheme with following approximation is used:

$$v_i\nabla f_i(t_n, r_{jk}) \approx \frac{1}{h}(f_i(t_n, r_{jk}) - f_i(t_n, r_{jk} - v_i h)).$$

All other operations for the construction of the scheme are the same as for the scheme PC1. The following scheme is obtained:

$$\tilde{f}_i(t_{n+1}, r_{jk}) = f_i(t_n, r_{jk}) - \frac{\Delta t}{h}(f_i(t_n, r_{jk}) + v_i h) - f_i(t_n, r_{jk}) - \frac{\Delta t}{\tau}(f_i(t_n, r_{jk}) - f_i^{(eq)}(f(t_n, r_{jk}))).$$  

(10)
Predictor–corrector finite–difference lattice Boltzmann schemes

\[
\begin{align*}
  f_i(t_{n+1}, r_{jk}) &= \frac{1}{2} (f_i(t_n, r_{jk}) + \tilde{f}_i(t_{n+1}, r_{jk})) - \frac{\Delta t}{2h} (\tilde{f}_i(t_{n+1}, r_{jk}) - \tilde{f}_i(t_{n+1}, r_{jk} - v_i h)) - \\
  &- \frac{\Delta t}{2\tau} (\tilde{f}_i(t_{n+1}, r_{jk}) - f_i^{(eq)}(\tilde{f}(t_{n+1}, r_{jk}))).
\end{align*}
\]

(11)

The scheme (10)–(11) will be called PC2.

It is easy to obtain that schemes PC1 and PC2 approximate (1) with second order on \(\Delta t\) and \(h\). By the method of Chapman — Enskog expansion [11] the expression for kinematic viscosity \(\nu\) could be obtained:

\[
\nu = \frac{\tau l^2}{3\delta t}.
\]

This expression is equal to the expression for \(\nu\) for system (1).

The abilities of the application of the schemes PC1 and PC2 to the solution of practical problems is demonstrated by the solution of two test hydrodynamical problems — problem of 2D lid-driven cavity flow and problem of 2D Taylor — Green vortices.

3 Solution of the test problems

The main aim of the computations is to compare schemes PC1 and PC2 between each other and with upwind schemes of first and second orders introduced in [10]. In this study this schemes will be called as UW1 and UW2.

Boundary conditions for \(f_i\) are realized by Zou and He approach [14]. The comparison of the schemes are realized by evaluation of the values of Courant number \(\gamma = V \Delta t / h\), where \(V = 1\) is a dimensionless mean speed. The maximal value of \(\gamma\), that defines the upper boundary of stability domain is obtained in computation process by variation of \(\gamma\) values. This value will be denoted as \(\tilde{\gamma}\).

3.1 Solution of 2D lid-driven cavity flow problem

Spatial domain \(\{(x, y)|x \in [0, 1], y \in [0, 1]\}\) is considered. Boundary conditions on components of \(u\) has the following form:

\[
\begin{align*}
  u_x(t, x, 0) &= u_y(t, x, 0) = 0, & u_x(t, x, 1) &= U_0, & u_y(t, x, 1) &= 0, & x \in [0, 1], \\
  u_x(t, 0, y) &= u_y(t, 0, y) = u_x(t, 1, y) &= u_y(t, 1, y) &= 0, & y \in [0, 1),
\end{align*}
\]

where \(U_0 = 1\) is the velocity of the top lid.

At the initial moment \(t = 0\) vector \(u\) is considered as zero vector. Numerical solution, obtained by FDLBSs is compared with solution obtained in [4]. Uniform grid with 200 \(\times\) 200 nodes is considered.

At fig. 1–2 plots of \(u_x\) and \(u_y\) are demonstrated. Values of \(\tilde{\gamma}\) are considered in table 1. As it can be seen, for the cases of schemes PC1 and PC2 values of
$	ilde{\gamma}$ are greater than for well-known schemes. The values of $	ilde{\gamma}$ for scheme PC2 are greater than for scheme PC2.

![Fig. 1. Plots of the components of velocity vector $u$ at $Re = 100$: 1 — results obtained by scheme PC2; 2 — results obtained in [4]](image)

![Fig. 2. Plots of the components of velocity vector $u$ at $Re = 400$: 1 — results obtained by scheme PC2; 2 — results obtained in [4]](image)

Table 1. Value of $	ilde{\gamma}$ at different values of $Re$ for 2D lid-driven cavity flow problem.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>PC2</th>
<th>PC1</th>
<th>UW1</th>
<th>UW2</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.514</td>
<td>0.442</td>
<td>0.398</td>
<td>0.221</td>
</tr>
<tr>
<td>100</td>
<td>0.423</td>
<td>0.415</td>
<td>0.352</td>
<td>0.204</td>
</tr>
<tr>
<td>200</td>
<td>0.312</td>
<td>0.306</td>
<td>0.269</td>
<td>0.177</td>
</tr>
<tr>
<td>300</td>
<td>0.249</td>
<td>0.241</td>
<td>0.221</td>
<td>0.153</td>
</tr>
<tr>
<td>400</td>
<td>0.206</td>
<td>0.204</td>
<td>0.187</td>
<td>0.135</td>
</tr>
</tbody>
</table>
3.2 Solution of Taylor — Green problem

Spatial domain \( \{(x, y) | x \in [0, 2\pi], y \in [0, 2\pi]\} \) is considered. Boundary conditions are written as:

\[
\begin{align*}
u_x(0, y, t) &= -U_0 e^{-2t/Re} \sin(y), & u_x(2\pi, y, t) &= -U_0 e^{-2t/Re} \sin(y), \\
\quad u_y(x, 0, t) &= U_0 e^{-2t/Re} \sin(x), & u_y(x, 2\pi, t) &= U_0 e^{-2t/Re} \sin(x), \\
\quad u_x(x, 0, t) &= u_x(x, 2\pi, t) = u_y(0, y, t) = u_y(2\pi, y, t) = 0.
\end{align*}
\]

At the initial moment following conditions are used:

\[
\begin{align*}
u_x(x, y, 0) &= -U_0 \cos(x) \sin(y), & \quad u_y(x, y, 0) &= U_0 \sin(x) \cos(y).
\end{align*}
\]

Analytical solution is obtained in [12] and has the following form:

\[
\begin{align*}
u_x(x, y, t) &= -U_0 e^{-2t/Re} \cos(x) \sin(y), & \quad u_y(x, y, t) &= U_0 e^{-2t/Re} \sin(x) \cos(y).
\end{align*}
\]

The computations were performed at \( U_0 = 1 \) on the grid with \( 200 \times 200 \) nodes. On fig. 3 numerical solution is compared with analytical solution presented above. Plots are presented at moment \( t = 2 \). Values of \( \tilde{\gamma} \) are presented at table 2.

![Fig. 3. Plots of the components of velocity vector \( \mathbf{u} \) at \( Re = 100 \): 1 — results obtained by scheme PC2; 2 — analytical solution](image)

<table>
<thead>
<tr>
<th>( Re )</th>
<th>PC2</th>
<th>PC1</th>
<th>UW1</th>
<th>UW2</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.418</td>
<td>0.411</td>
<td>0.354</td>
<td>0.198</td>
</tr>
<tr>
<td>100</td>
<td>0.312</td>
<td>0.306</td>
<td>0.265</td>
<td>0.158</td>
</tr>
<tr>
<td>200</td>
<td>0.209</td>
<td>0.205</td>
<td>0.187</td>
<td>0.132</td>
</tr>
<tr>
<td>300</td>
<td>0.153</td>
<td>0.149</td>
<td>0.141</td>
<td>0.109</td>
</tr>
<tr>
<td>400</td>
<td>0.122</td>
<td>0.119</td>
<td>0.115</td>
<td>0.093</td>
</tr>
</tbody>
</table>

All notions on schemes PC1 and PC2 for this problem are the same as for 2D lid-driven cavity flow problem.
4 Summary

In this study predictor–corrector finite–difference lattice Boltzmann schemes are considered. Schemes are constructed for the solution of the system of quasi-linear kinetic equations. Schemes with separate and unified approximations of advective terms are constructed and compared. The ability of computation with larger time step in comparison with well-known upwind schemes is demonstrated.

Stability of the schemes obtained may be investigated by von Neumann method [9].

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