Journal of Physics: Conference Series

Stability investigation of implicit parametrical schemes for the systems of kinetic equations

IOP Conf. Series: Journal of Physics: Conf. Series **929** (2017) 012032 doi:10.1088/1742-6596/929/1/012032

Stability investigation of implicit parametrical schemes for the systems of kinetic equations

Elizaveta A Prokhorova, Gerasim V Krivovichev

Faculty of Applied Mathematics and Control Processes Saint Petersburg State University, 7/9 Universitetskaya nab., Saint Petersburg, 199034, Russian Federation

E-mail: proxliza@mail.ru, g.krivovichev@spbu.ru

Abstract. Systems of parametrical lattice Boltzmann equations (LBE's) are considered. The formulae for the apparent viscosity for the general representation of these systems is obtained by Chapman — Enskog asymptotic expansion on Knudsen number. Obtained expression represents viscosity as a function of the relaxation parameter and parameter of the LBE's. Necessary stability conditions in form of inequalities are derived from the non-negativity condition of the apparent viscosity. The validity of the stability conditions are demonstrated by the solution of lid-driven cavity flow problem.

1. Introduction

In last years lattice Boltzmann method (LBM) established itself as a powerful tool for the numerical solution of different problems of mechanics and physics of gases and fluids [1, 2, 3]. The main feature of the method is an application of *kinetic* equations, such as Boltzmann and Bhatnaghar – Gross – Krook (BGK) equations to the modelling of flows, instead of the equations of continuum mechanics (such as Navier – Stokes equations), as it is realized in traditional computational fluid mechanics. Great advantage of LBM consists with high parallelism of its computational algorithms (e.g. see [4, 5]).

One of the problems of the theory of LBM is a conditional stability of its main computational difference scheme named lattice Boltzmann equation (LBE), which has an explicit nature. This problem restrict the values of the relaxation parameter of the modelled system, so the range of the considered physical processes is restricted. The problem may be solved by the construction of implicit schemes.

Implicit schemes for LBM constructed by finite-difference and finite-element discretisation procedures are considered in [3, 6, 7, 8]. In [10] implicit scheme constructed by θ-method is applied to the solution of steady-flow problems. P. Asinari in [9] construct implicit schemes for multi-relaxation-time LBM with various orders of approximation. In [11] implicit LBE is constructed and applied to the solution of phase-change problem with Stefan condition. In [12] the second order LBE for multiphase systems is obtained. The equation is constructed by application of trapezoidal quadrature rule to the integral form of the system of kinetic equations.

In the presented paper the system of parametrical LBE's derived in [13] is investigated. The expression for the apparent viscosity is obtained by the method of Chapman – Enskog asymptotic expansion. Necessary stability conditions in form of inequalities on relaxation and scheme parameters are introduced. The validity of the proposed conditions is demonstrated by the numerical solution of lid-driven cavity flow problem.

The structure of the paper is follows. In section 2 the system of parametrical LBE's is presented. In section 3 the expression for the apparent viscosity is derived and stability conditions are formulated. In section 4 lid-driven cavity problem is considered. Some conclusion remarks are made in section 5.

2. Parametrical lattice Boltzmann equations

The system of BGK kinetic equations for the ensemble of particles with velocities $\mathbf{V}_i$ is written as:

$$\frac{\partial f_i}{\partial t} + \mathbf{V}_i \nabla f_i = -\frac{1}{\lambda}(f_i - f_i^{(eq)}), \tag{1}$$

where $f_i = f_i(t, \mathbf{r})$ are the distribution functions of particles with velocities $\mathbf{V}_i = V\mathbf{e}_i$, where $V = l/\delta t$, l is a mean free path, δt is a mean free time, $\mathbf{e}_i$ are the dimensionless vectors, t is a time, $\mathbf{r}$ is a vector of space variables, λ is a relaxation time, $f_i^{(eq)}$ are the equilibrium distribution functions. In two-dimensional case the following set of vectors named $D2Q9$ pattern may be used [1]: $\mathbf{e}_1 = (0, 0)$, $\mathbf{e}_2 = (1, 0)$, $\mathbf{e}_3 = (0, 1)$, $\mathbf{e}_4 = (-1, 0)$, $\mathbf{e}_5 = (0, -1)$, $\mathbf{e}_6 = (1, 1)$, $\mathbf{e}_7 = (-1, 1)$, $\mathbf{e}_8 = (-1, -1)$, $\mathbf{e}_9 = (1, -1)$.

System (1) may be rewritten in integral form on the time interval $[t, t + \delta t]$ [14]:

$$f_i(t + \delta t, \mathbf{r} + \mathbf{V}_i \delta t) - f_i(t, \mathbf{r}) = -\frac{1}{\lambda}\int_0^{\delta t} (f_i(t + \xi, \mathbf{r} + \mathbf{V}_i \xi) - f_i^{(eq)}(t + \xi, \mathbf{r} + \mathbf{V}_i \xi))d\xi. \tag{2}$$

System of integral equations (2) in [13] is rewritten in equivalent form with parametrical coefficients:

$$f_i(t + \delta t, \mathbf{r} + \mathbf{V}_i \delta t) - f_i(t, \mathbf{r}) = -\frac{1-\sigma}{\lambda}\int_0^{\delta t} (f_i(t + \xi, \mathbf{r} + \mathbf{V}_i \xi) - f_i^{(eq)}(t + \xi, \mathbf{r} + \mathbf{V}_i \xi))d\xi -$$

$$-\frac{\sigma}{\lambda}\int_0^{\delta t} (f_i(t + \xi, \mathbf{r} + \mathbf{V}_i \xi) - f_i^{(eq)}(t + \xi, \mathbf{r} + \mathbf{V}_i \xi))d\xi, \tag{3}$$

where $\sigma \in [0, 1]$ is a dimensionless parameter.

Parametrical LBE's may be obtained from system (3) by discretization of (3) on the time and space grids and by application of quadrature formulas to the computation of integrals in right part of (3). In [13] six systems of parametrical LBE's are obtained by application of simple quadrature formulas of low algebraic accuracy. These difference equations may be presented in following form:

$$f_i(t_j + \delta t, \mathbf{r}_{kl} + \mathbf{V}_i \delta t) - f_i(t_j, \mathbf{r}_{kl}) = A(f_i(t_j, \mathbf{r}_{kl}) - f_i^{(eq)}(t_j, \mathbf{r}_{kl})) +$$

$$+B(f_i(t_j + \delta t, \mathbf{r}_{kl} + \mathbf{V}_i \delta t) - f_i^{(eq)}(t_j + \delta t, \mathbf{r}_{kl} + \mathbf{V}_i \delta t)), \tag{4}$$

where $A = A(\sigma, \tau)$, $B = B(\sigma, \tau)$, $\tau = \lambda/\delta t$ is a dimensionless relaxation time, t_j is a node of time grid constructed with step δt, $\mathbf{r}_{kl}$ is a node of space grid constructed with step l. System (4) represent systems of implicit difference equations which are defined by following dependencies of A and B on σ:

1) system 1: $A = -(1 - \sigma)/\tau$, $\quad B = -\sigma/\tau$.

2) system 2: $A = -\sigma/\tau$, $\quad B = -(1 - \sigma)/\tau$.

3) system 3: $A = -(1-\sigma)/2\tau, \quad B = -(1+\sigma)/2\tau$.
4) system 4: $A = -(1+\sigma)/2\tau, \quad B = -(1-\sigma)/2\tau$.
5) system 5: $A = -\sigma/2\tau, \quad B = (\sigma-2)/2\tau$.
6) system 6: $A = (\sigma-2)/2\tau, \quad B = -\sigma/2\tau$.

3. Apparent viscosity of parametrical LBE's

The expression for apparent viscosity plays an important role in practical computations as a tool for the stability analysis and as a value of kinematic viscosity, used in computations of real flows, different from the real value of the viscosity, which in case of $D2Q9$ pattern is presented as [15]:

$$\nu = \frac{\lambda V^2}{3}. \tag{5}$$

The formulae for the apparent viscosity may be derived from differential approximation of (4) by the method of Chapman — Enskog asymptotic expansion [15].

Differential approximation of (4) is obtained by application of Taylor formulae:

$$f_i(t+\delta t, \mathbf{r}+\mathbf{V}_i\delta t) = f_i(t,\mathbf{r}) + \frac{\partial f_i(t,\mathbf{r})}{\partial t}\delta t + \frac{\partial f_i(t,\mathbf{r})}{\partial x_\alpha}V_{i\alpha}\delta t + \frac{(\delta t)^2}{2}\frac{\partial^2 f_i(t,\mathbf{r})}{\partial t^2} +$$

$$+\frac{(\delta t)^2}{2}\frac{\partial^2 f_i(t,\mathbf{r})}{\partial x_\alpha \partial x_\beta}V_{i\alpha}V_{i\beta} + (\delta t)^2\frac{\partial^2 f_i(t,\mathbf{r})}{\partial t \partial x_\alpha}V_{i\alpha} + o(\delta t^2). \tag{6}$$

where the Einstein summation rule on Greek indices α and β is realised and $x_1 = x$, $x_2 = y$, $V_{i1} = V_{ix}$, $V_{i2} = V_{iy}$.

The method of Chapman — Enskog expansion is based on the following expression on Knudsen parameter $\varepsilon = l/L$, where L is a typical length of the flow domain:

$$f_i \approx f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)}, \tag{7}$$

where $f_i^{(0)} = f_i^{(eq)}$, $f_i^{(1)}$ and $f_i^{(2)}$ satisfy the following properties:

$$\sum_{i=1}^{n} f_i^{(1)} = \sum_{i=1}^{n} f_i^{(2)} = 0, \quad \sum_{i=1}^{n} f_i^{(1)}\mathbf{V}_i = \sum_{i=1}^{n} f_i^{(2)}\mathbf{V}_i = \mathbf{0}. \tag{8}$$

Derivatives on independent variables are represented by following multiscale expansions [15, 16]:

$$\frac{\partial}{\partial t} = \varepsilon\frac{\partial}{\partial t_1} + \varepsilon^2\frac{\partial}{\partial t_2}, \quad \frac{\partial}{\partial x_\alpha} = \varepsilon\frac{\partial}{\partial x_{1\alpha}}, \tag{9}$$

where t_1, t_2, x_{11}, x_{12} are the new variables.

Macrovariables, such as density $\rho(t,\mathbf{r})$ and velocity $\mathbf{u}(t,\mathbf{r})$ are represented by following formulas [16]:

$$\rho(t,\mathbf{r}) = \sum_{i=1}^{n} f_i(t,\mathbf{r}), \quad \rho(t,\mathbf{r})\mathbf{u}(t,\mathbf{r}) = \sum_{i=1}^{n}\mathbf{V}_i f_i(t,\mathbf{r}). \tag{10}$$

By substitution of (6),(7),(9) into (4) and by application of (8) and (10) the following equations for macrovariables are obtained:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha}(\rho u_\alpha) = 0, \tag{11}$$

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \nu \frac{\partial}{\partial x_\beta}\left(\rho\left(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta}\right)\right), \tag{12}$$

where ν is an apparent viscosity represented in case of $D2Q9$ pattern by following formulae:

$$\nu = \left(1 + \frac{A - B}{2}\right)\frac{\tau}{3}\frac{l^2}{\delta t}. \tag{13}$$

System (11)–(12) may be characterized as *quasihydrodynamical* system for modelling of semi-compressible flows. In case of incompressible regime $\rho = const$ and system (11)–(12) is rewritten in form of Navier — Stokes system:

$$\frac{\partial u_\alpha}{\partial x_\alpha} = 0, \quad \frac{\partial u_\alpha}{\partial t} + u_\beta \frac{\partial u_\alpha}{\partial x_\beta} = -\frac{1}{\rho}\frac{\partial p}{\partial x_\alpha} + \nu \Delta u_\alpha.$$

As it can be seen, expression (13) is different from the expression for real viscosity (5) due to the presence in (13) of the fictitiuos term $\tau l^2(A - B)/(6\delta t)$, which is named numerical viscosity. This fact must be considered in computations of real flows.

Necessary stability conditions may be obtained from the condition $\nu \geq 0$ and are presented by following theorem:

Theorem. Let system (4) is stable on initial conditions. So the following conditions on coefficients σ and τ are realized:

1) For system 1:

$$\sigma \geq \frac{1}{2} - \tau,$$

is valid $\forall \sigma \in [1/2, 1]$, $\forall \tau > 0$.

2) For system 2:

$$\sigma \leq \tau + \frac{1}{2},$$

is valid $\forall \sigma \in [0, 1/2]$, $\forall \tau > 0$.

3) For system 3:

$$\sigma \geq -2\tau,$$

is valid $\forall \sigma \in [0, 1]$, $\forall \tau > 0$.

4) For system 4:

$$\sigma \leq 2\tau,$$

is valid $\forall \sigma \in [0, 1]$ when $\tau > 1/2$ $\forall \sigma \in [0, 2\tau]$ when $\tau < 1/2$.

5) For system 5:

$$\sigma \leq 1 + 2\tau,$$

is valid $\forall \sigma \in [0, 1]$ when $\forall \tau > 0$.

6) For system 6:

$$\sigma \geq 1 - 2\tau,$$

is valid $\forall \sigma \in [0, 1]$ when $\tau > 1/2$ and $\forall \sigma \in [1 - 2\tau, 1]$ when $0 < \tau < 1/2$, when $\sigma = 1$ is valid $\forall \tau > 0$.

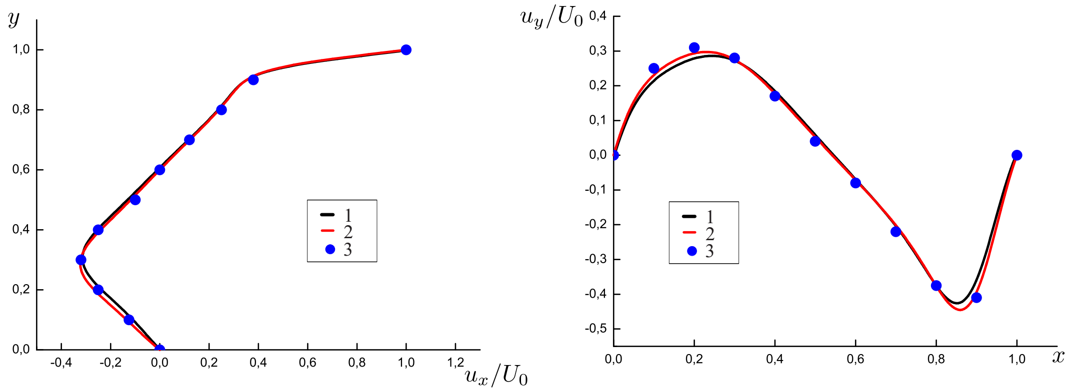

Figure 1. The results of computation at $Re = 400$. Black line — the case of $\sigma = 1$, red line — case of $\sigma = 1/2$, results from [17] are represented by blue dots

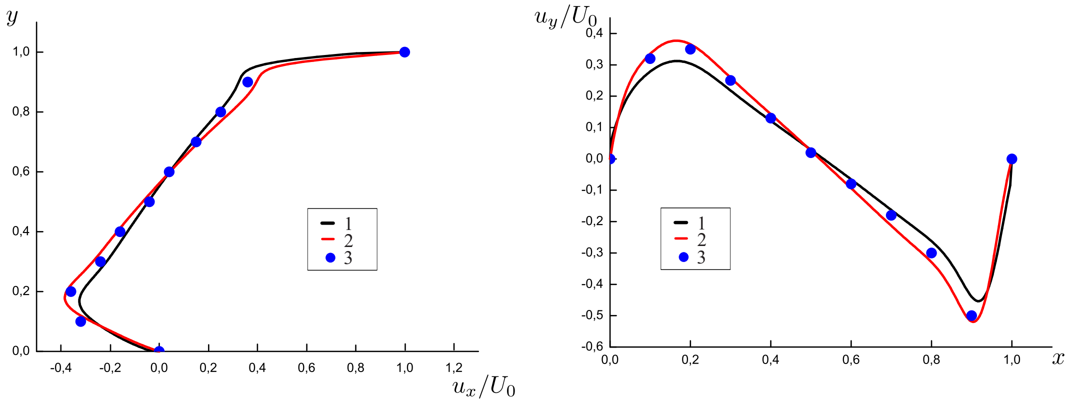

Figure 2. The results of computation at $Re = 1000$. Black line — the case of $\sigma = 1$, red line — case of $\sigma = 1/2$, results from [17] are represented by blue dots

4. Numerical solution of lid-driven cavity flow problem

The problem is stated in rectangular domain $\{(x, y)|x \in [0, P], y \in [0, P], P > 0\}$. Boundary conditions are written as [17]:

$$u_x(t, x, 0) = u_y(t, x, 0) = 0, \quad u_x(t, x, P) = U_0, \quad u_y(t, x, P) = 0, \quad x \in [0, P],$$

$$u_x(t, 0, y) = u_y(t, 0, y) = u_x(t, P, y) = u_y(t, P, y) = 0, \quad y \in [0, P),$$

where $U_0 = const \neq 0$. Boundary conditions for distribution functions f_i reproduced presented boundary conditions on velocity are realized by the approach described in [18].

Results of computations on the space grid of 100×100 nodes are compared with the results from [17] at cases of different values of Reynolds number Re. The scheme based on system 1 is applied at cases of $\sigma = 1$ (first order) and $\sigma = 1/2$ (second order). This results are presented at fig. 1–2. The systems of nonlinear equations at every grid node are solved by Newton method. Two schemes obtained from system 1 at cases of $\sigma = 1$ and $1/2$ are considered. At fig. 1 case of Reynolds number $Re = 400$ is considered at case of 6000 time nodes, when at $\sigma = 1$ $\tau = 0.1126$ and at $\sigma = 1/2$ $\tau = 0.6126$, at fig. 2 — the case of $Re = 1000$ with 1000 time nodes, when at $\sigma = 1$ $\tau = 0.2354$ and at $\sigma = 1/2$ $\tau = 0.7354$. The plots of u_x/U_0 are presented at the line

$\{x = 0.5P, y \in [0, P]\}$, plots of u_y/U_0 — at the points of line $\{x \in [0, P], y = 0.5P\}$. As it can be seen, the obtained results are demonstrated the validity of presented stability conditions. At table 1 the values of the norm of the vector of mean square errors for u_x and u_y are presented. As it can be seen, the results obtained by scheme of second order are closest to the null at all values of Re and may be considered as a numerical solution obtained with higher order of accuracy.

Table 1. The values of the norm of the vector of mean square errors of the velocity vector components at different values of Re.

σ	$Re = 50$	$Re = 100$	$Re = 400$	$Re = 1000$
1	$5.0514 \cdot 10^{-4}$	$1.1237 \cdot 10^{-4}$	$5.1427 \cdot 10^{-4}$	$2.3744 \cdot 10^{-3}$
1/2	$5.8641 \cdot 10^{-5}$	$3.0376 \cdot 10^{-5}$	$3.4718 \cdot 10^{-5}$	$2.2343 \cdot 10^{-4}$

5. Conclusion

In the presented paper parametrical LBE's are considered. The formulae for the apparent viscosity is obtained by Chapman — Enskog asymptotic expansion. Obtained expression represents viscosity as a function of the relaxation parameter and parameter of the LBE's. Necessary stability conditions in form of inequalities are derived from the non-negativity condition of the apparent viscosity. The validity of the stability conditions are demonstrated by the solution of lid-driven cavity flow problem.

The proposed idea may be realized in analytical investigation of parametrical LBE's with many time steps, obtained by application of quadrature formulas of different algebraic orders.

Acknowledgements

The reported study was funded by Russian Foundation of Basic Research according to research project No. 16-31-00021 mol_a.

References

[1] Chen S and Doolen J D 1998 *Ann. Rev. Fluid Mech.* **30** 329
[2] Krivovichev G V and Panchenko M S 2016 *Appl. Math. Sci.* **10** 947
[3] Krivovichev G V 2014 *Appl. Math. Sci.* **8** 1605
[4] Hong P-Y, Huang L-M, Lin L-S and Lin C A 2015 *Computers and Fluids* **110** 1
[5] Ye Y, Li K, Wang Y and Deng T 2015 *Computers and Fluids* **110** 114
[6] Cao N, Chen S, Jin S and Martinez D 1997 *Phys. Rev. E* **55(1)** 55R21
[7] Li Y, LeBoeuf E J and Basu P K 2004 *Phys. Rev. E* **69** 065701
[8] Seta S and Takahashi R 2002 *J. Stat. Phys.* **7** 557
[9] Asinari P 2006 *Phys. Rev. E* **73** 056705
[10] Bernaschi M, Succi S and Chen H 2001 *J. Sci. Comp.* **16** 135
[11] Eshlaghi M and Felicelli S D 2012 *Int J Heat Mass Transf.* **55** 2420
[12] Sankaranarayanan B, Shan X, Kevrekidis I G and Sundaresan S 2002 *J. Fluid Mech.* **452** 61
[13] Krivovichev G V 2014 *Appl. Math. Sci.* **8** 5003
[14] He X and Luo L-S 1997 *Phys. Rev. E* **55(6)** R6333
[15] Sofonea V 2003 *J. Comp. Phys.* **184**, 422
[16] Wolf-Gladrow D A 2000 *Lattice-Gas Cellular Automata and Lattice Boltzmann Models* (Berlin: Springer)
[17] Ghia U, Ghia K N and Shin C T 1982 *J. Comp. Phys.* **48** 387
[18] Le Coupanec E and Verschaeve J C G 2011 *Math. Comp. Simul* **81** 2632.