Appl. Math. Inf. Sci. **9**, No. 4, 1687-1692 (2015)

Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.12785/amis/090404

Numerical Stability Analysis of Lattice Boltzmann Equations for Linear Diffusion

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Received: 5 Oct. 2014, Revised: 5 Jan. 2015, Accepted: 6 Jan. 2015
Published online: 1 Jul. 2015

Abstract: The lattice Boltzmann equations for the linear diffusion modeling in cases of D2Q5, D2Q7 and D2Q9 lattices are considered. Families of the numerical schemes with the dependence on scalar parameter are introduced. The stability analysis of schemes is performed in parameter space. The stability is studied numerically by von Neumann method. Optimal parameter values for the presented families are defined.

Keywords: lattice Boltzmann method, linear diffusion, stability, von Neumann method

1 Introduction

Nowadays the lattice Boltzmann method (LBM) has established itself as a powerful tool for the numerical solution of a wide range of physical problems. In the LBM the values of functions describing physical process on macrolevel (such as density, temperature, energy etc) are calculated from the values of distribution functions of fictitious particles, introduced at each node of the lattice in physical space. The evolution of the distribution functions is governed by the system of discrete kinetic equations called lattice Boltzmann equations (LBE) [1,2].

One of the main applications of LBM is the computational fluid dynamics (CFD), where it has proven successful to solve problems for weakly compressible viscous flows [1,2,3] and much more complex situations as multiphase and multicomponent flows [4,5], flows in porous media [6,7] and free surface flows [8]. The popularity of the LBM is based on its straightforward parallelism, due to the explicit nature of LBE with intensive local computation. The method is successfully adopted for computations on single and multiple graphical processing units (GPU) using Compute Unified Device Architecture (CUDA) technology [9,10,11].

Recently, the LBM shows potentials to solution of linear and nonlinear partial differential equations (PDE's) such as Laplace equation [12], Korteweg – de Vries equation [13,14], Korteweg – de Vries – Burgers equation [14,15], Burgers – Huxley equation [14], Lorenz system [16] and nonlinear hyperbolic systems [17]. In this type of numerical schemes the solution of PDE is obtained as a sum of distribution functions which are the solutions of LBE's. The formulas for equilibrium distribution functions and parameters of LBE's are defined so that the Chapman – Enskog expansion method led to the initial PDE.

The motivation of the research work is caused by the necessity of the investigation of LBE's for linear diffusion equation (LDE) presented in other papers. The investigation of such LBE's were performed only by comparison of numerical solutions of test problems. In this paper the comparison of the schemes is performed due to its stability properties.

The main objective of the paper is investigation and comparison of LBE's for LDE in parameter space due to its stability properties. Another objective is to find the parameter values, which are optimal for stabilization of the numerical schemes.

In this study the single relaxation time (SRT) LBE-based numerical schemes for the solution of LDE are considered. The investigation of these schemes is restricted to two-dimensional problems in the absence of internal sources. The schemes introduced in [18,19,20,21,22,23,24,25,26,27,28,29,30] are investigated. For D2Q5, D2Q7 and D2Q9 lattices the families of LBE-based schemes with the dependence on external

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scalar parameters are introduced. The optimal values of the parameters for all families are obtained using the von Neumann method. It must be noted, that in the paper we restrict the analysis to the case of SRT LBEs. The multiple-relaxation-time (MRT) LBEs and its stability properties are considered in [37,38,39].

The paper is organized as follows. In Section 2 LBE's for the solution of LDE are considered. In Section 3 the problem for the stability investigation is considered. In Section 4, the results of the stability analysis are discussed. A summary is given in Section 5.

2 Lattice Boltzmann Equations for Linear Diffusion

The system of LBE's with SRT Bhatnaghar – Gross – Krook collision term has the following form:

$$f_i(t+\delta t,\mathbf{r}+\mathbf{V}_i\delta t)=f_i(t,\mathbf{r})-\frac{1}{\tau}\big(f_i(t,\mathbf{r})-\\ -f_i^{(eq)}(c(t,\mathbf{r}))\big), \tag{1}$$

where t is the time, δt — time step, $\mathbf{r}=(x,y)$ — node of the lattice (grid in physical space) with lattice spacing l, $f_i, i=1,\dots,n, n\in\mathbf{N}$ — distribution functions of fictitious particles with velocities $\mathbf{V}_i$, which can move without interactions between neighbouring lattice nodes during one time step, τ is the dimensionless relaxation time ($\tau=\lambda/\delta t$, where λ is the relaxation time), $f_i^{(eq)}$ — equilibrium distribution functions, $c(t,\mathbf{r})$ is the solution of LDE (concentration).

It must be noted, that in LBE's for CFD problems equilibrium distribution functions $f_i^{(eq)}$ are chosen in a way for approximation of Maxwell's distribution functions at small values of Mach number [1,2,3]. But for the applications of LBM to the solution of LDE, which has the following form:

$$\frac{\partial c}{\partial t}=D\Delta c, \tag{2}$$

where D is the diffusion coefficient, the expressions for $f_i^{(eq)}$ has to obey the following constraint [18,24,25]:

$$c(t,\mathbf{r})=\sum_{i=1}^{n}f_i(t,\mathbf{r})=\sum_{i=1}^{n}f_i^{(eq)}(t,\mathbf{r}). \tag{3}$$

For the validity of the formula (3) the expressions for $f_i^{(eq)}$ can be chosen in the following form:

$$f_i^{(eq)}=W_i c(t,\mathbf{r}), \tag{4}$$

where $W_i\geq 0$ are weights, which satisfy the following condition: $\sum\limits_{i=1}^{n}W_i=1$. The LDE (2) can be obtained from (1) by the Chapman – Enskog expansion method with the usage of (3) and (4) [18].

In the case of the advection-diffusion equation:

$$\frac{\partial c}{\partial t}+\mathbf{U}\nabla c=D\Delta c, \tag{5}$$

where $\mathbf{U}$ is the velocity of the fluid, the expressions for $f_i^{(eq)}$ have more complex forms than (4), due to the dependence on hydrodynamical macrovariables $\mathbf{U}(t,\mathbf{r})$ and density $\rho(t,\mathbf{r})$ [30]. It must be noted, that LBE for the simulation of (5) can be used for the simulation of (2) in the case of zero velocity $\mathbf{U}=\mathbf{0}$ [25,26,27,28,29].

The velocities $\mathbf{V}_i$ are introduced in the following form: $\mathbf{V}_i=V\mathbf{v}_i, i=1,\dots,n$, where $V=l/\delta t$ and $\mathbf{v}_i$ are the lattice vectors. In the paper the following lattices are considered:

1) D2Q5 lattice:

$$\mathbf{v}_1=(0,0),\mathbf{v}_2=(1,0),\mathbf{v}_3=(0,1),\mathbf{v}_4=(-1,0),\mathbf{v}_5=(0,-1).$$

2) D2Q7 lattice:

$$\mathbf{v}_1=(0,0),\mathbf{v}_2=(1/2,\sqrt{3}/2),\mathbf{v}_3=(-1/2,\sqrt{3}/2),\\ \mathbf{v}_4=(-1,0),\mathbf{v}_5=(-1/2,-\sqrt{3}/2),\\ \mathbf{v}_6=(1/2,-\sqrt{3}/2),\mathbf{v}_7=(1,0).$$

3) D2Q9 lattice:

$$\mathbf{v}_1=(0,0),\mathbf{v}_2=(1,0),\mathbf{v}_3=(0,1),\mathbf{v}_4=(-1,0),\mathbf{v}_5=(0,-1),\\ \mathbf{v}_6=(1,1),\mathbf{v}_7=(-1,1),\mathbf{v}_8=(-1,-1),\mathbf{v}_9=(1,-1).$$

It must be noted, that one of the main applications of the LBE-based numerical schemes for LDE is the simulation of of Laplace and Poisson equations [22,26,27,28,31] by LDE simulation in the stationary regime.

The expression for the coefficient D depending on lattice parameters l, δt and LBE parameter τ can be obtained by the Chapman — Enskog method application to (1). The expression for D has the following form:

$$D=\left(\tau-\frac{1}{2}\right)\frac{\gamma l^2}{\delta t},$$

where γ is the dimensionless parameter, whose values can differ for every type of LBE.

2.1. The case of D2Q5 lattice. In the paper of D. A. Wolf-Gladrow [18] the LBE with the following parameters values is introduced: $W_1=0$, $W_{2,3,4,5}=1/4$, $\gamma=1/2$. It must be noted that the case of $W_1=0$ corresponds to the D2Q4 lattice.

In the papers of C. Huber et al [20,21] the following parameter values were proposed: $W_1=1/3$, $W_{2,3,4,5}=1/6$, $\gamma=1/3$. In the paper of S. Chen et al [19] for the simulation of the equation for one component of the vorticity vector, which has the form (5), the LBE with $W_i=1/5$, $i=1,\dots,5$, $\gamma=2/5$ is introduced.

2.2. The case of D2Q7 lattice. In the paper of C. Ponce-Dawson et al [23] the following parameter values are introduced: $W_i=1/7$, $i=1,\dots,7$, $\gamma=3/7$. R. Blaak and P. M. A. Sloot in [24] presented a LBE with the following parameters: $W_1 = 1/2$, $W_{2,\ldots,7} = 1/12$, $\gamma = 1/4$.

2.3. The case of D2Q9 lattice. In [24] the following set of parameters values is introduced: $W_1 = 4/9$, $W_{2,3,4,5} = 1/9$, $W_{6,7,8,9} = 1/36$, $\gamma = 1/3$. It must be noted, that these values are used in LBM application to the simulation of incompressible viscous Newtonian fluid [1, 2, 3, 4]. X. He et al [30] construct LBE for heat-convection problems by the discretization method proposed in [32, 33]. The following parameter values $W_1 = 0$, $W_{2,3,4,5} = 1/6$, $W_{6,7,8,9} = 1/12$, $\gamma = 2/3$ are obtained. In [26, 27, 28] the proposed LBE's are used for the simulation of the Poisson — Boltzmann equation and in [25, 29] for the simulation of the heat equation.

2.4. Parametrical families of LBE's. As it is known (for example, see [34]) the existence of the scalar numerical parameter in the family of finite-difference schemes provide the opportunity to control some important properties such as stability, dispersion, dissipation etc. In most cases scalar dimensionless numerical parameter $\sigma \in [0,1]$ is introduced by addition and subtraction of the product of the term of scheme on the parameter. In [24] two parametrical families of LBE's are proposed — for the cases of D2Q7 and D2Q9 lattices.

The weights W_i of the equilibrium distributions are not fixed by the constraint of Eq. (3) and the Chapman — Enskog expansion of Eq. (1). One can put more of less weights on the rest particles (weight W_1 for lattice velocity $\mathbf{v}_1 = \mathbf{0}$). By varying of σ ($0 < \sigma < 1$) one can define a whole family of models with $W_1 = \sigma$ and $W_{2,\ldots,7} = (1-\sigma/6)$ for the model D2Q7. The LBE's discussed in [23] and [24] belong to this family with σ values of $1/7$ and $1/2$, respectively.

The LBE family for D2Q9 lattice is introduced by $W_1 = \sigma$, $W_{2,3,4,5} = (1-\sigma)/5$, $W_{6,7,8,9} = (1-\sigma)/20$ and $\gamma = 3(1-\sigma)/5$. The LBE's from [24] corresponds to $\sigma = 4/9$. As it can be seen, there is no way to obtain LBE's from [30] from this family.

In this paper, a new parametrical family for the case of D2Q5 lattice is proposed. This family is determined by the following weights: $W_1 = \sigma$, $W_{2,3,4,5} = (1-\sigma)/4$. Such representation of W_i dependence on σ can be justified by the fact that such expressions for W_i satisfy the conditions

$$W_i \geq 0, \quad \sum_{i=1}^{n} W_i = 1,$$

which are imposed on W_i due to the (3) and (4). By the method of Chapman — Enskog expansion the following expression for γ can be obtained: $\gamma = (1-\sigma)/2$. The case of $\sigma = 0$ correspond to the LBEs from [18], case of $\sigma = 1/5$ to LBEs from [19] and case of $\sigma = 1/3$ — to LBEs from [20, 21].

One of the main problems in the investigation of numerical schemes is the determination of optimal values of σ. In this paper the problem is solved by the stability analysis of the LBEs in space of the parameters τ and σ. In this paper optimal values correspond to the minimal values of the maximums of absolute values of eigenvalues of the transition matrix of finite-difference scheme. The obtained LBEs with optimal values are compared with LBEs presented in other papers.

3 Von Neumann Stability Analysis

The system (1) in dimensionless form can be written as:

$$f_i'(t'+1, \mathbf{r}'+\mathbf{v}_i) = f_i'(t', \mathbf{r}') - \frac{1}{\tau}\big(f_i'(t', \mathbf{r}') - \\ - f_i^{(eq)}(c'(t', \mathbf{r}'))\big), \tag{6}$$

where t', $\mathbf{r}'$, c', f_i' are dimensionless variables.

The dimensionless system (6) is a system of linear difference equations with constant coefficients. For its stability investigation the von Neumann method can be used [35]. Let $\overline{f}_i$ are the equilibrium solutions of (6) which correspond to the constant solution of the dimensionless LDE $c' = 1$: $\overline{f}_i = f_i^{(eq)}(1) = C_i = const$.

The solutions of Eq. (6) can be presented in the following form:

$$f_i'(t', \mathbf{r}') = \overline{f}_i + \delta f_i'(t', \mathbf{r}'), \tag{7}$$

where $\delta f_i'$ are the deviations of f_i' from the constant equilibrium solutions $\overline{f}_i$.

After substitution of (7) in (6) and with the usage of (3) and (4), the system for $\delta f_i'$ can be obtained:

$$\delta f_i'(t'+1, \mathbf{r}'+\mathbf{v}_i) = \delta f_i'(t', \mathbf{r}') - \frac{1}{\tau}\big(\delta f_i'(t', \mathbf{r}') - \\ - W_i \sum_{p=1}^{n} \delta f_p'(t', \mathbf{r}')\big). \tag{8}$$

According to the von Neumann method, the solutions of (8) can be presented in following form:

$$\delta f_i'(t', \mathbf{r}') = F_i(t') \exp(\mathbf{i}\mathbf{S}\mathbf{r}'^T), \tag{9}$$

where $\mathbf{i}^2 = -1$, $\mathbf{S} = (\theta_x, \theta_y)^T$, $\theta_x, \theta_y \in [-\pi, \pi]$. After the substitution of (9) in (8), the system for $F_i(t')$ can be obtained:

$$F_i(t'+1) = \sum_{p=1}^{n} G_{ip} F_p(t'), \tag{10}$$

where G_{ip} are the components of transition matrix $\mathbf{G}$:

$$G_{ip} = \begin{cases} \exp(-\mathbf{i}\mathbf{S}\mathbf{v}_i^T)\left(1 - \frac{1}{\tau} + \frac{W_i}{\tau}\right), & i = p, \\ \exp(-\mathbf{i}\mathbf{S}\mathbf{v}_i^T)\frac{W_i}{\tau}, & i \neq p. \end{cases}$$

The problem for the stability investigation of the equilibrium solution of (6) is reduced to the stability investigation of the null solution of system (10). According to the spectral criterion [35], the solution will be stable, if the absolute values of all eigenvalues of $\mathbf{G}$ are less than unity. The eigenvalue problems for $\mathbf{G}$ were solved numerically by applying the QR-algorithm using FORTRAN90 EISPACK routines [36].

The stability investigation is performed in two-dimensional space of the parameters (τ, σ) with the interval from $1/2$ to 100 for τ values. In the domain of parameter values $[1/2, 100] \times [0, 1]$ the uniform grid with 500×500 nodes was constructed, in the two-dimensional space (θ_x, θ_y) uniform grid with 200×200 nodes was considered. For every node (τ, σ) the value of function $\Lambda(\tau, \sigma)$

$$\Lambda(\tau, \sigma) = \max_{(\theta_x, \theta_y)} \left(\max_i |\lambda_i(\tau, \sigma, \theta_x, \theta_y)| \right), \qquad (11)$$

was calculated, where λ_i are the eigenvalues of matrix $\mathbf{G}$.

For the definition of optimal values of σ the minimal values of Λ are obtained by simple search on the constructed grid in parameter space.

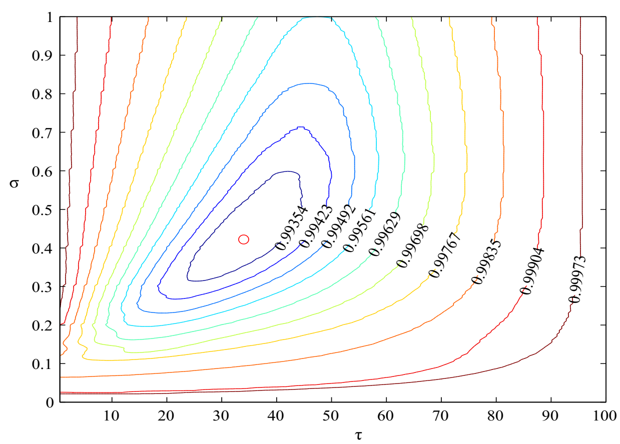

Fig. 1. Isolines of Λ for the case of D2Q5 lattice.

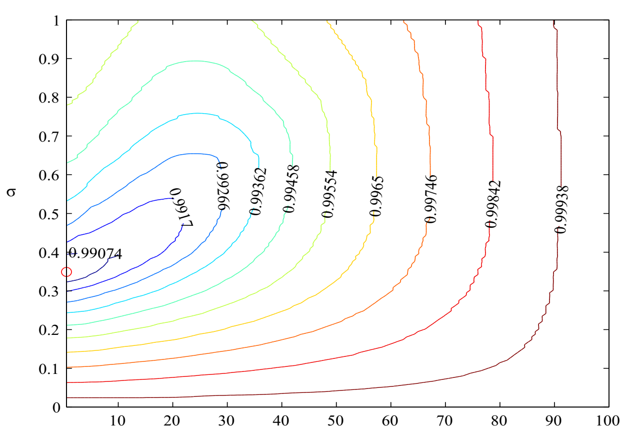

Fig. 2. Isolines of Λ for the case of D2Q7 lattice.

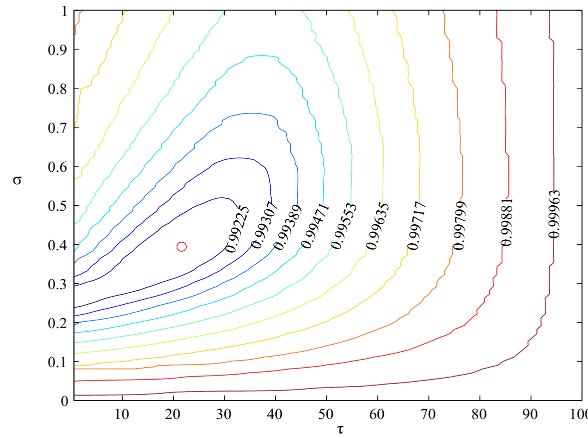

Fig. 3. Isolines of Λ for the case of D2Q9 lattice.

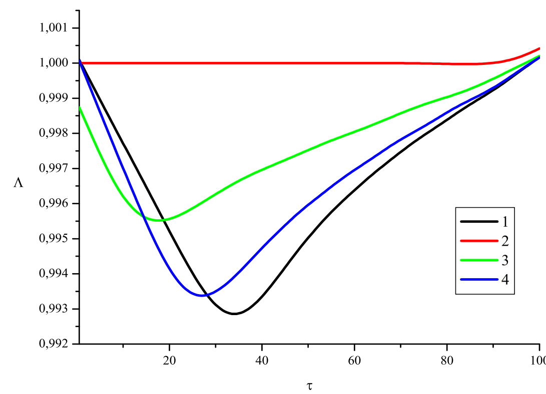

Fig. 4. Plots of Λ for the case of D2Q5 lattice at fixed values of σ. 1 — $\sigma = \overline{\sigma} = 0.4221$; 2 — $\sigma = 0$; 3 — $\sigma = 1/5$; 4 — $\sigma = 1/3$.

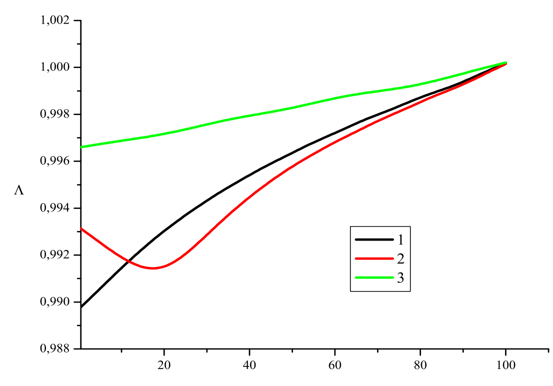

Fig. 5. Plots of Λ for the case of D2Q7 lattice at fixed values of σ. 1 — $\sigma = \overline{\sigma} = 0.3489$; 2 — $\sigma = 1/2$; 3 — $\sigma = 1/7$.

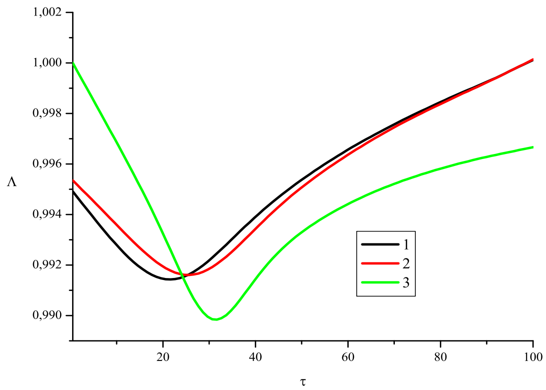

Fig. 6. Plots of Λ for the case of D2Q9 lattice at fixed values of σ. 1 — $\sigma = \overline{\sigma} = 0.3939$; 2 — $\sigma = 4/9$; 3 — scheme from [30].

4 Numerical Results

The plots of the isolines of Λ are presented at Fig. 1–3 for D2Q5, D2Q7 and D2Q9 lattices. The minimum points are marked by the red circles. Due to the lack of the analytical representation of function $\Lambda(\tau,\sigma)$ all the propositions on minimum points of all schemes for the cases of all lattices must be considered as a results of numerical calculations.

4.1. D2Q5. For the case of the D2Q5 lattice the minimal value of Λ is equal to 0.9929 and corresponds to $\sigma = \overline{\sigma} = 0.4221$, $\tau = 34.28$. For the fixed value of $\sigma = \overline{\sigma}$ the values of Λ that are greater than unity occur near the boundary values $\tau = 1/2$ and $\tau = 100$.

For the case of $\sigma = 0$ (Wolf-Gladrow's scheme [18]), Λ is equal to unity in the range $0.5 < \tau < 84.02$ and $\Lambda > 1$ when $\tau > 84.02$.

In the case of $\sigma = 1/3$ (LBEs from [20,21]) the minimal value of Λ is equal to 0.9934 and correspond to $\tau = 27.04$. As for the case of $\sigma = \overline{\sigma}$, the values of Λ greater than unity occurs near the boundaries of the τ range (Fig. 4).

For the case of $\sigma = 1/5$ [19] the minimal value of Λ is equal to 0.9955 and is realized at $\tau = 16.14$, the values of Λ greater than unity are realized near the boundary $\tau = 100$.

The plots of Λ with fixed values of σ, corresponds to LBEs discussed above, are presented in Fig. 4. As it can be seen, the scheme based on LBEs from [20,21] is "closer" (with respect to stability properties in terms of stability criterion Λ) than other presented schemes to the scheme with optimal parameter $\overline{\sigma}$. It must be noted that for the values of τ closer to $1/2$ (correspond to the case of small values of D) the scheme of S. Chen et al [19] has good stability properties.

4.2. D2Q7. The results of calculations (see Fig. 5) demonstrate, that for all presented LBEs the values of Λ are less than unity when τ is closer to $1/2$ and greater than unity when τ is closer to 100 (Fig. 5). The minimal value of Λ is equal to 0.9898 and it occurs when $\sigma = \overline{\sigma} = 0.3489$, $\tau = 1/2$, meaning that the minimum is realized on the lower boundary of the τ domain. It must be noted, that $\tau = 1/2$ corresponds to the case of $D = 0$, meaning that LBEs with optimal parameter $\overline{\sigma}$ can be applied to the linear diffusion modelling for small values of D.

The minimal value for the case of $\sigma = 1/7$ [23] is equal to 0.9965 and realized at $\tau = 1/2$, as for the case of the scheme with $\overline{\sigma}$.

For the case of $\sigma = 1/2$ (Blaak and Sloot LBEs [24]) the minimal value is realized at $\tau = 17.19$ and it is equal to 0.9914.

After the analysis of the results of numerical calculations it can be noted, that due to the stability criterion Λ the system of LBE's from [24] has a good stability properties for the case of moderate values of τ, than other considered schemes. For the case of small values of D scheme with optimal value $\overline{\sigma}$ can be recommended for practical computations.

4.3. D2Q9. The LBEs with optimal parameters corresponds to the following values: $\sigma = \overline{\sigma} = 0.3939$, $\tau = 21.60$ and the minimal value of Λ is equal to 0.9914. For the LBEs with $\sigma = 4/9$ [24] the minimal value is equal to 0.9916 at $\tau = 25.62$. As it can be seen from Fig. 6, plots for the presented LBEs are close to each other.

The plot for the analog of Λ (which depend only on τ) for the LBEs from [30] is presented at Fig. 6. Plot analysis demonstrates that the minimal value for this LBEs is less than the minimal values for the schemes presented above. The minimal value for this scheme is equal to 0.9899 and realized at $\tau = 31.65$. It means that this LBE-based scheme is a more preferable for simulations due to its stability properties according to the criterion $\Lambda(\tau,\sigma)$, than LBEs from the parametrical family presented in [24].

There is no scheme in presented parametrical family for this type of lattice which can be considered as optimal for the case of small values of D.

5 Conclusion

The paper is dedicated to the stability analysis of LBEs in 2D. Parametrical families of numerical schemes are presented for the cases of D2Q5, D2Q7 and D2Q9 lattices. Stability analysis is performed based on the von Neumann method. The optimal values of parameter σ correspond to the minimal values of function $\Lambda(\tau,\sigma)$, which is chosen as stability criteria in this paper, are obtained.

As the result of the numerical computations, LBEs for the D2Q5 and D2Q7 lattices with good stability properties are obtained. For D2Q5 lattice family the scheme from [19] can be considered as optimal for small values of diffusion coefficient D. For moderate values of D the optimal value of parameter is presented in the article. In the case of D2Q7 family optimal scheme for the case of small values of D is obtained. For moderate values of D scheme from [24] can be recommended. For the case of the D2Q9 lattice it is shown, that the scheme based on LBEs from [30] is more preferable for simulations due to its stability properties for the cases of moderate values of D. There is no optimal scheme for D2Q9 lattice for the case of small values of D for the stability criterion used in this paper.

It must be noted, that all propositions and recommendations are made only for the case of stability criterion $\Lambda(\tau,\sigma)$ which can also be considered as a criterion for the comparison of LBEs based numerical schemes. For other criteria another optimal values of the scheme parameters can be obtained.

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