Using Lattice Boltzmann scheme for anisotropic diffusion problems

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12 March 2008 *

Abstract

The lattice Boltzmann method is briefly introduced using moments. We use this method to model diffusion problems. We have adapted a general methodology for equivalent equations to the explicit determination of discrete gradient and fluxes for this problem. We validate this new approach with a detailed comparison with finite differences. We show some results for an anisotropic test case.

Keywords : Lattice Boltzmann Equation, Anisotropic diffusion problems.

1 Lattice Boltzmann scheme

The lattice Boltzmann equation (LBE) is a numerical method based on kinetic theory to simulate various hydrodynamic systems. It uses a small number of velocities; the Lattice Boltzmann Equation (LBE) was derived by Higuera and Jiménez [HJ89] from lattice gas automata of Frisch et *al.* [FHP86]. The LBE is a mesoscopic method and deals with a small number of functions $\{f_i\}$ that can be interpreted as populations of fictitious "particles". The dynamics of these "particles" is such that time, space and momentum are

* Presented at the Fifth FVCA Conference, Aussois, 8-13 June 2008. To appear in *Hermes Science Publications.*

discretized. The “particles" evolve in a succession of collision and propagation steps on the nodes of a regular lattice $\mathcal{L}$ parametrized by a spatial scale Δx. This lattice is composed by a set $\mathcal{L}^0 \equiv \{x_j \in (\Delta x \mathbb{Z})^d\}$ of nodes or vertices where d is the dimension of space. We define Δt as the time step of the evolution of LBE and let the celerity $\lambda \equiv \frac{\Delta x}{\Delta t}$. We choose the velocities $v_i, i \in (0 \ldots q)$ such that $v_i \equiv c_i \frac{\Delta x}{\Delta t} = c_i \lambda$, where c_i are vectors connecting neighbouring nodes of $\mathcal{L}$.
For the sake of simplicity we consider the particular D2Q9 [dH92] model (*i.e.* $d = 2$ two-dimensional LBE model with nine velocities $q = 8$). In this model, we choose the velocities $c_i, i \in (0 \ldots 8)$ defined by: $c = (0,0)$, $(1,0)$, $(0,1)$, $(-1,0)$, $(0,-1)$, $(1,1)$, $(-1,1)$, $(-1,-1)$, $(1,-1)$.

The populations f_i evolve according to the LBE scheme which can be written as follows [Du07]:

$$(1) \quad f_i(x_j, t + \Delta t) = f_i^*(x_j - v_i \Delta t, t), \quad 0 \le i \le 8,$$

where the superscript $*$ denotes post-collision quantities. Therefore during each time increment Δt there are two fundamental steps: collision and advection.
• In the advection step the “particles" move from a lattice node x_j to either itself (with the velocity $\mathbf{v}_0 = 0$), one of the four nearest neighbors (with the velocity $\mathbf{v}_i$, $1 \le i \le 4$), or one of the four next-nearest neighbors (with the velocity $\mathbf{v}_i$, $5 \le i \le 8$).
• The collision step consists in the redistribution of the populations $\{f_i\}$ at each node x_j. It is modeled by the operator subscript $*$ in (1) and is best described in the space of moments m_k [dH92]. They are obtained by a linear transformation of vectors f_j:

$$m_k = \sum_j M_{k\,j} f_j .$$

Explicit formula for $M_{k\,j}$ coefficient is given in [dH92]. Note that matrix M is invertible. The moments have an explicit physical significance (*e.g.* [LL00]): $m_0 \equiv T$ is the temperature (density), m_1 and m_2 are x-momentum, y-momentum, m_3 is the energy, m_4 is related to energy square, m_5 and m_6

are x-energy flux and y-energy flux and m_7, m_8 are diagonal stress and off-diagonal stress.
To simulate diffusion problems, we conserve only the first moment m_0 in the collision step and obtain one macroscopic scalar equation. For the other quantities (non-conserved moments), we assume that they relax towards equilibrium values m_k^{eq} that are nonlinear functions of the conserved quantities and set:

$$(2) \quad m_k^* = (1 - s_k)\, m_k + s_k m_k^{eq}, \quad 1 \le k \le 8,$$

where $s_k \equiv \frac{\Delta t}{\tau_k}$ is a relaxation rate ($0 < s_k < 2$ for stability). The relaxation rates s_k are not necessarily identical as in the so called BGK case [QHL92]. The equilibrium values m_k^{eq} of the non-conserved moments in equation (2) determine the macroscopic behaviour of the scheme (*i. e.* of equation (1)). Indeed with the following choice of equilibrium values: $m_3^{eq} = \alpha T$, $m_4^{eq} = \beta T$, $q_x^{eq} = 0$, $q_y^{eq} = 0$, $p_{xx}^{eq} = a_{xx} T$ and $p_{xy}^{eq} = a_{xy} T$ and using Taylor expansion [Du07] or Chapman-Enskog procedure [FHH87] we find the diffusion equation up to order three in Δt:

$$\frac{\partial T}{\partial t} - \mathrm{div}(\mathrm{K}\nabla T) = \mathrm{O}(\Delta t^3),$$

where $\mathrm{K} = (k_{i,j})_{1 \le i,j \le 2}$ is the diffusion tensor with $k_{11} = \frac{\lambda^2 \Delta t}{6}(\frac{1}{s_1} - \frac{1}{2})(4 + \alpha + 3a_{xx})$, $k_{12} = k_{21} = \frac{\lambda^2 \Delta t}{2}(\frac{1}{s_1} + \frac{1}{s_2} - 1) a_{xy}$ and $k_{22} = \frac{\lambda^2 \Delta t}{6}(\frac{1}{s_2} - \frac{1}{2})(4 + \alpha - 3a_{xx})$. These equations reduce to the standard isotropic diffusion equation for $a_{xx} = a_{xy} = 0$ and $s_1 = s_2 = s$, with the diffusion coefficient

$$\kappa = \frac{\lambda^2}{6} \Delta t\, (4 + \alpha)(\frac{1}{s} - \frac{1}{2}).$$

With a given velocity field (v_x, v_y), if we take $m_1^{eq} = \lambda v_x T$ and $m_2^{eq} = \lambda v_y T$ the LBE scheme describes the following advection-diffusion [GdH07] equation: $\frac{\partial T}{\partial t} + v.\nabla T - \mathrm{K}\Delta T = \mathrm{O}(\Delta t^2)$.

In this section we deal with boundary conditions for lattice Boltzmann method. We explain in detail how to reconstruct classical bounce-back or anti-bounce back boundary conditions using a general Taylor expansion proposed in [Du07]. Let $\partial\Omega$ a boundary surface cutting the link between fluid node

x_b and an outside one $x_e \equiv x_b - \Delta x$ (see Figure 1).

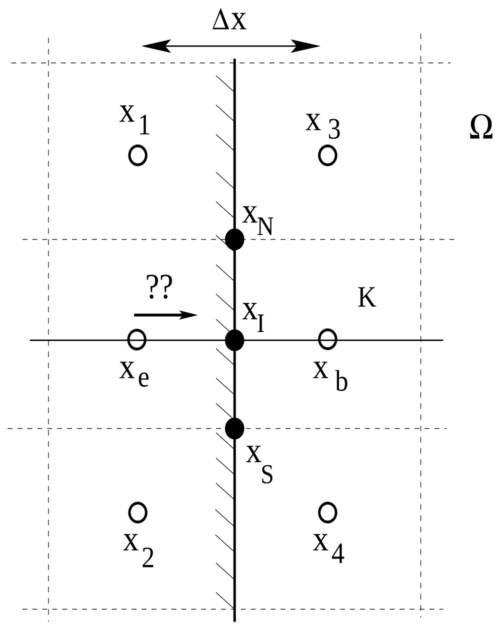

Figure 1. *A boundary surface cutting the link between node x_b (a fluid node) and $x_e \equiv x_b - \Delta x$ (a fictitious outside node).*

Let $f_i(x_b, t), i \in (0 \ldots 8)$ be the population at node x_b and at time t. After the collision step distribution $f_3^*(x_b, t)$ has left the fluid and goes to the fictitious node x_e. At time $t + \Delta t$ we have to define the unknown population $f_1(x_b, t + \Delta t)$ which comes from node x_e and is equal to $f_1^*(x_e, t)$. So the choice of this population will determine the boundary conditions. Here we consider the case of Dirichlet boundary conditions at $\partial\Omega$ which intersects the link between x_e and x_b at $x_e + \frac{\Delta x}{2}$.

• To have $T(x_e + \frac{\Delta x}{2})$ on $\partial\Omega$ in the configuration of Figure 1 up to order 1 in Δt we do the following scheme:

$f_1(x_b, t + \Delta t) = -f_3(x_e, t + \Delta t) + \frac{1}{36}(4 - \alpha - 2\beta + 9a_{xx})\, T(x_e + \frac{\Delta x}{2}),$

$f_5(x_b, t + \Delta t) = -f_7(x_2, t + \Delta t) + \frac{1}{36}(4 + 2\alpha + \beta + 9a_{xy})\, T(x_S),$

$f_8(x_b, t + \Delta t) = -f_6(x_1, t + \Delta t) + \frac{1}{36}(4 + 2\alpha + \beta - 9a_{xy})\, T(x_N).$

By using moments and relation (1) we have:

$$f_1(x_b, t+\Delta t) = f_1^*(x_e, t) = \frac{1}{36}(4m_0 + \frac{6m_1^*}{\lambda} - m_3^* - 2m_4^* - 6m_5^* + 9m_7^*)(x_e, t),$$
$$f_3(x_e, t+\Delta t) = f_3^*(x_b, t) = \frac{1}{36}(4m_0 - \frac{6m_1^*}{\lambda} - m_3^* - 2m_4^* + 6m_5^* + 9m_7^*)(x_b, t).$$

We have the following development of non-equilibrium moments at second order on Δt (as described in [Du08]):

$$(3) \quad m_k^* = m_k^{eq} + \Delta t \left(\frac{1}{2} - \sigma_k\right) \theta_k + \mathrm{O}(\Delta t^2), \quad k \geq 2,$$

where $\sigma_k \equiv \left(\frac{1}{s_k} - \frac{1}{2}\right)$ and θ_k is the defect of conservation defined by:

$$\theta_k \equiv \partial_t m_k^{eq} + \sum_{j,\alpha} M_{k\,j} M_{\alpha\,j} \partial_\alpha f_j^{eq}.$$

The detailed expansion of these coefficients is given in [Du08] and is used below. Now we consider the quantities $f_1(x_b, t+\Delta t) + f_3(x_e, t+\Delta t)$, and we use the above identity and the different expressions of the θ_k, we get:

$$\begin{aligned}
&f_1(x_b, t+\Delta t) + f_3(x_e, t+\Delta t) = \\
&= \tfrac{1}{72}(4 - \alpha - 2\beta + 9a_{xx})\left(T(x_e) + T(x_b)\right) + \mathrm{O}(\Delta t) \\
&= \tfrac{1}{36}(4 - \alpha - 2\beta + 9a_{xx}) T(x_e + \tfrac{\Delta x}{2}) + \mathrm{O}(\Delta t).
\end{aligned}$$

To obtain the other identities we perform similar operations on the quantities f_5, f_6, f_7 and f_8. We note here that if we have homogeneous boundary conditions (*i.e.* $T(x_e + \frac{\Delta x}{2}) = 0$) we obtain classical boundary condition called "anti-bounce back". Note that Ginzburg [Gi05] proposes more elaborate boundary conditions of higher order by using the Chapman-Enskog method.

• Gradient and Flux

Compared to classical numerical methods, the lattice Boltzmann method uses more parameters and variables. It turns out that in steady state situations some of these variables can be used to determine the first and second space derivatives $\frac{\partial T}{\partial x_\alpha}$ and $\frac{\partial^2 T}{\partial x_\alpha x_\beta}$ in all nodes $x \in \mathcal{L}^0$, and the flux along the interface

of the control volume K.
• The gradient of the solution on the node x_i at time t can be evaluated as follows. By using Taylor expansions we get a general second order expression of non-conservative moments:

$$(4)\quad m_k = m_k^{eq} - \Delta t(\frac{1}{2}+\sigma_k)\left[\theta_k - \Delta t(\sigma_k\partial_t\theta_k + \sigma_l\Lambda^{\ell}_{k\alpha}\partial_\alpha\theta_\ell)\right] + \mathrm{O}(\Delta t^3),\ k \geq 1,$$

where $\Lambda^{\ell}_{kp} = \sum_j M_{k\,j}\, M_{p\,j}\, M^{-1}_{j,\ell}$.

To determine first order space derivatives of T for the present diffusion problem, we use equation (4) for moments m_1 and m_2:

$$\begin{aligned} m_1 &= -\lambda^2\Delta t\left(\frac{1}{2}+\sigma_1\right)\left[\frac{(4+\alpha+3a_{xx})}{6}\frac{\partial T}{\partial x} + a_{xy}\frac{\partial T}{\partial y}\right] + \mathrm{O}(\Delta t^3), \\ m_2 &= -\lambda^2\Delta t\left(\frac{1}{2}+\sigma_2\right)\left[a_{xy}\frac{\partial T}{\partial x} + \frac{(4+\alpha-3a_{xx})}{6}\frac{\partial T}{\partial y}\right] + \mathrm{O}(\Delta t^3). \end{aligned}$$

Similarly the determination of second order space derivatives of T is obtained using equation (4) for moments m_3, m_7 and m_8:

$$\begin{aligned} m_3 =& \alpha T + \Delta t^2\left(\frac{1}{2}+\sigma_3\right)\lambda^2\left[\left(\sigma_1\frac{4+\alpha+3a_{xx}}{6} + \sigma_5\frac{\alpha+\beta-3a_{xx}}{3}\right)\frac{\partial^2 T}{\partial x^2} + \right. \\ & \left. + (\sigma_2\frac{4+\alpha+3a_{xx}}{6} + \sigma_6\frac{\alpha+\beta+3a_{xx}}{3})\frac{\partial^2 T}{\partial y^2} + (\sigma_1+\sigma_2+\sigma_5+\sigma_6)\,a_{xy}\frac{\partial^2 T}{\partial x\partial y}\right], \\ m_7 =& a_{xx}T + \Delta t^2\left(\frac{1}{2}+\sigma_7\right)\frac{\lambda^2}{3}\left[\left(\sigma_1\frac{4+\alpha+3a_{xx}}{6} - \sigma_5\frac{\alpha+\beta-3a_{xx}}{3}\right)\frac{\partial^2 T}{\partial x^2} + \right. \\ & \left. + (\sigma_6\frac{\alpha+\beta+3a_{xx}}{3} - \sigma_2\frac{4+\alpha-3a_{xx}}{6})\frac{\partial^2 T}{\partial y^2} + (\sigma_1-\sigma_2+\sigma_6-\sigma_5)\,a_{xy}\frac{\partial^2 T}{\partial x\partial y}\right], \end{aligned}$$

$$\begin{aligned} m_8 = a_{xy}T + \Delta t^2\left(\frac{1}{2}+\sigma_8\right)\frac{\lambda^2}{3}&\left[(2\sigma_2+\sigma_6)a_{xy}\frac{\partial^2 T}{\partial x^2} + (2\sigma_1+\sigma_5)a_{xy}\frac{\partial^2 T}{\partial y^2} + \right. \\ & + \left(\sigma_1\frac{4+\alpha+3a_{xx}}{3} + \sigma_2\frac{4+\alpha-3a_{xx}}{3} + \right. \\ & \left.\left. + \sigma_5\frac{\alpha+\beta-3a_{xx}}{3} + \sigma_6\frac{\alpha+\beta+3a_{xx}}{3}\right)\frac{\partial^2 T}{\partial x\partial y}\right]. \end{aligned}$$

We note that we could have used the combination m_5 and m_6 for ∇T and m_4, m_7 and m_8 for second order space derivatives. Note that applying the new methodology with Taylor expansion instead of Chapman-Enskog one [dH92] is original in this framework of diffusion problems.
We show now that the lattice Boltzmann method for purely diffusive problems relates to classical Fourier law. The mass flux j is generally defined as the amount of particles that cross an interface at a given time instance. The flux can be defined at the interface $(x_S, x_N) \equiv (SN)$ between two lattice nodes x_e and $x_b \equiv x_e + \Delta x$ as (see Figure 1):

$$\begin{aligned} j_{SN}(x_e + \frac{\Delta x}{2}, t+\Delta t) &= \lambda\left(f_1(x_b, t+\Delta t) - f_3(x_e, t+\Delta t)\right) + \\ &+\lambda\Psi_1\left(f_5(x_b, t+\Delta t) - f_7(x_2, t+\Delta t) + f_5(x_3, t+\Delta t) - f_7(x_b, t+\Delta t)\right) + \\ &+\lambda\Psi_2\left(f_8(x_b, t+\Delta t) - f_6(x_1, t+\Delta t) + f_8(x_4, t+\Delta t) - f_6(x_b, t+\Delta t)\right), \end{aligned}$$

where Ψ_1 and Ψ_2 are two scalars determined by:

$$\begin{aligned} \frac{1}{\Delta x}\int_{SN} \mathrm{div}(\mathrm{K}.\nabla T).n_{SN}dy &= K_{11}\frac{\partial T}{\partial x}(x_I, t) + K_{12}\frac{\partial T}{\partial y}(x_I, t) + \mathrm{O}(\Delta x) = \\ &= -j_{SN}(x_I, t+\Delta t) + \mathrm{O}(\Delta x), \end{aligned}$$

where $x_I = x_e + \frac{\Delta x}{2}$ (see Figure 1). If we suppose that $\frac{\partial T}{\partial x}$ is constant along SN and with the help of Taylor expansion we obtain the first equality of the above calculus. To find Ψ_1 and Ψ_2, we develop the quantity j_{SN} by using (3), then we choose Ψ_1 and Ψ_2 such that this quantity is equal to the normal flux. In the case of isotropic problems (*i.e.* $a_{xx} = a_{xy} = 0$), we find $\Psi_1 = \Psi_2 = \frac{1}{2}$.

2 Numerical results

First we have tested our scheme for the following 1D problem: $-\mathrm{K}u''(x) = c$ in $]0, 1[$, $u(0) = u(1) = 0$. We take periodic condition on y, anti-bounce back condition on x to have homogeneous Dirichlet boundary conditions and the following parameters: $\alpha = -2$, $\beta = 1$, $a_{xx} = a_{xy} = 0$, $s_1 = s_2 = 1.2$, $s_3 = 1.8$, $s_4 = 1.2$, $s_5 = s_6 = 1.5$ and $s_7 = s_8 = 1.3$. The results concerning the ℓ^2 relative errors between the exact affine solution $u(x) = x(1-x)c/(2\mathrm{K})$ and the solution calculated with the D2Q9 LBE scheme shows second order accuracy.

Second we have tested our scheme for the following 2D isotrope diffusion problem with Dirichlet and Neumann bounday conditions: $-\mathrm{K}\Delta u = f$ in $\Omega =]0,1[^2$, $u = \overline{u}$ on Γ_D, $\partial_n u = g$ on Γ_N, where K is a scalar, $f = -2\mathrm{K}$, $\Gamma_D \equiv \{0\} \times (0,1) \cup \{1\} \times (0,1)$, $\overline{u} = 0$ on $\{0\} \times (0,1)$, $1-3y$ on $\{1\} \times (0,1)$ and $g = -3x$ on $\Gamma_N \equiv (0,1) \times \{0\} \cup (0,1) \times \{1\}$. The analytical solution of this problem is: $u(x,y) = x^2 - 3xy$. We take anti-bounce back condition on x to have Dirichlet boundary condition, bounce back condition on y to have Neumann boundary and the following parameters: $\alpha = -2$, $\beta = 1$, $a_{xx} = a_{xy} = 0$, $s_1 = s_2 = 1.2$, $s_3 = 1.1$, $s_4 = 1.4$, $s_5 = s_6 = 1.5$ and $s_7 = s_8 = 1.5$. The Figure 2 shows ℓ^2 relative errors between the exact solution and the solution calculated with the D2Q9 LBE, which is second order accuracy.

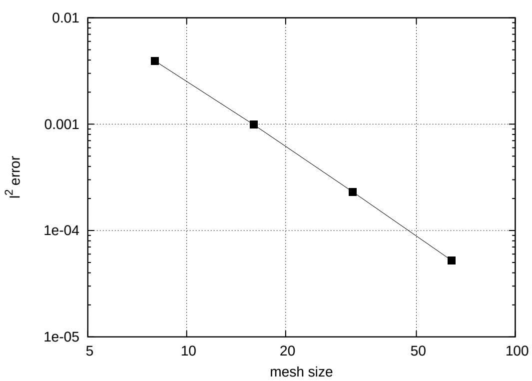

Figure 2. *The* ℓ^2 *error between analytical solution and approximate one vs mesh size.*

We have also used our algorithm to solve the following anisotropic diffusion problem so called "oblique flow":

$$-\mathrm{div}(\mathrm{K}\nabla u) = 0 \quad \text{in} \quad \Omega =]0,1[^2, \qquad u = \overline{u} \quad \text{on} \quad \partial\Omega.$$

where $\mathrm{K} = R_\theta \, \mathrm{diag}(1, 10^{-3}) \, R_\theta^{-1}$, R_θ is the rotation of angle $\theta = 40$ degrees, and $\overline{u} = 1$ on $(0, 0.2) \times \{0\} \cup \{0\} \times (0, 0.2)$, 0 on $(0.8, 1) \times \{1\} \cup \{1\} \times (0.8, 1)$, $\frac{1}{2}$ on $(0.3, 1) \times \{0\} \cup \{0\} \times (0.3, 1)$, $\frac{1}{2}$ on $(0, 0.7) \times \{1\} \cup \{1\} \times (0, 0.7)$. The Figure 3 shows the approximate solution on regular mesh (151×151), calculated by D2Q9 scheme after convergence (*i.e.* 5.10^5 iterations) with $s_1 = 1.3$, $s_2 = 1.8$ and $\beta = 1$ (other parameter are fixed to have K as diffusion tensor). The value of the maximum of the approximate solution in the same mesh is $T_{max} = 0.9984$ and the minimum one $T_{min} = 0.0015$. In Figure 4 (a) and

(b) we compare ∇T calculated by centred finite difference method and by using moments m_1 and m_2 (figure (a)) or by using m_5 and m_6 (figure (b)). In Figure 5 we compare $\frac{\partial^2 T}{\partial x_\alpha x_\beta}$ calculated by finite differences and by using non-equilibrium moments (m_3, m_7 and m_8). Note that there are 9×151^2 unknowns in this problem but no matrix inversion is necessary with this entirely explicit scheme.

Figure 3. *Approximate solution on regular rectangular mesh (*151×151 *nodes). The gray scale of the figure corresponds to a linear variation from* 0 *(black) to* 1 *(white).*

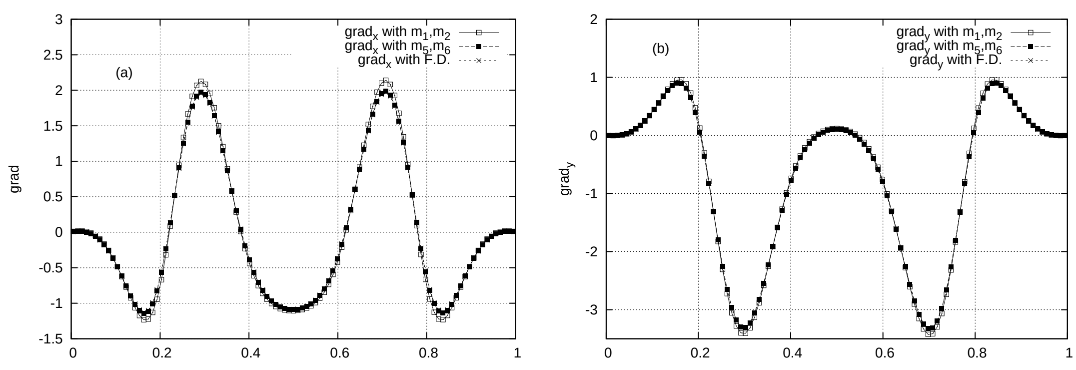

Figure 4. (a) *Left figure:* $\frac{\partial T}{\partial x}$ *vs* x*, right figure* (b) $\frac{\partial T}{\partial y}$ *vs* x *at* $y = 1/2$*.*

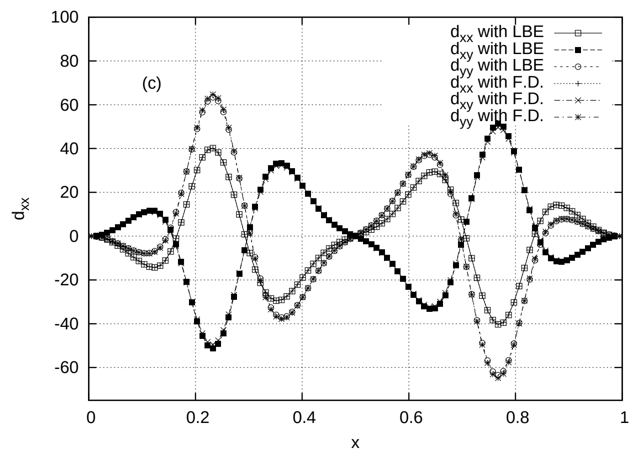

Figure 5. *Second order spatial derivatives of temperature vs x at $y = 1/2$.*

3 Conclusion

Lattice Boltzmann scheme is a very simple second order accurate method for fluid mechanics, thermal and acoustic problems. We have obtained interesting results for a not trivial test case. However, as it is a really unstationary methodology, it is not extremely efficient to simulate elliptic diffusion problems as it takes many time steps to reach a steady state. We have performed similar work in three space dimensions based on lattice Boltzmann models to simulate anisotropic diffusion equation. Similar work has been done by I. Ginzburg [Gi07].

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