Vol 17 No 1, January 2008
1674-1056/2008/17(01)/0238-11
Chinese Physics B
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Lattice Boltzmann method with the cell-population equilibrium*

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(Received 5 June 2006; revised manuscript received 24 May 2007)

The central problem of the lattice Boltzmann method (LBM) is to construct a discrete equilibrium. In this paper, a multi-speed 1D cell-model of Boltzmann equation is proposed, in which the cell-population equilibrium, a direct non-negative approximation to the continuous Maxwellian distribution, plays an important part. By applying the explicit one-order Chapman–Enskog distribution, the model reduces the transportation and collision, two basic evolution steps in LBM, to the transportation of the non-equilibrium distribution. Furthermore, 1D dam-break problem is performed and the numerical results agree well with the analytic solutions.

Keywords: lattice Boltzmann method, non-negative equilibrium, cell approximation scheme, dam-break

PACC: 4700, 0270, 0520D

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has emerged as a powerful tools for modelling complex fluid dynamic problems.[1−5] Originally, the LBM was developed as a modification of the lattice gas model.[6] Later derivations[7,8] revealed that the method was a special discretization of the continuous Boltzmann equation. The derivation of the LBM[7] from the Boltzmann equation is essentially based on Grad's moment method.[9] On the other hand, many kinetic schemes for the compressible Euler system based on the original Maxwellian distribution were developed. For the compressible Navier–Stokes system, kinetic schemes were developed by Chou and Baganoff [10] and in the Deshpande group.[11,12] A slightly different approach was taken by Xu and Prendergast.[13] Some authors noted the closeness of the LBM to the kinetic schemes,[14,15] both methods exploit the fact that the Boltzmann evolution is essentially equivalent to Euler or Navier–Stokes evolution if the state is in or close to local thermodynamic equilibrium. While most of the kinetic schemes were developed and routinely used for the solution of compressible equations, the LBM operates in the incompressible limit.[16−18] However, the two methods even coincide for a particular parameter constellation. This implies that the observations which are valid for kinetic schemes also have a direct consequence on LBM.[19]

The central issue of the LBGK (Lattice–Bathnagar–Gross–Krook) method is the local equilibrium. The discretization of the continuous local equilibrium is necessary for LBM or kinetic schemes in view of computation.[20,21] However, most of discrete schemes cannot provide a non-negative local equilibrium or evolutionary distribution. A general approach to construct positive equilibrium distributions has been presented by Junk[22] and Perthame[23] who used the entropy principle. In these direct velocity models, variational approaches construct local equilibrium which amount to a maximization of a strictly concave function (entropy function) and subject to certain constraints. However, Lagrange multipliers included in the solution cannot usually be explicitly expressed.

A cell-population equilibrium is proposed in this paper. This equilibrium is a direct approximation to the Maxwellian distribution. And then a simple LBGK scheme follows an obvious physical manner. The particles with different velocities cross from one cell to another in a computational cycle. As conse-

*Project supported by the National Natural Science Foundation of China (Grant Nos 70271069 and 60773195).
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quence, the changes of the population present a natural discretization of Maxwellian distribution. Furthermore, the scheme can easily develop a helpful multi-speed LBM algorithm to increase the ability of capturing shock wave.

This paper is organized as follows. Section 2.1 describes how to construct the cell-population equilibrium. Section 2.2 presents the multi-speed evolution formula of LBM. The standard test example, the 1D dam-break problem, is taken to examine our scheme in Section 2.3. Some concluding remarks are drawn in Section 3. A final appendix discusses the equivalency between the Boltzmann evolution and 1D shallow water equation with diffusion term by means of Chapman–Enskog expansion.

2. A discrete velocity model induced by the cell approximation of Maxwell distribution

2.1. Cell approximation scheme

Within the lattice Boltzmann scheme, the evolution of the density distribution function in fluid systems obeys the Boltzmann equation. By using the well-known single time relaxation BGK model for the collision operator, the continuous Boltzmann equation can be written as

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = \frac{1}{\lambda}(q - f). \tag{1}$$

Here $f(x, c, t)$ is the single-particle distribution function, c is the microscopic particle velocity and $q(x, c, t)$ is the equilibrium distribution. The relaxation time λ controls the rate of approaching equilibrium. The hydrodynamic quantities, such as the water level $h(x, t)$, the macro-velocity $u(x, t)$, and the energy can be given in terms of the distribution functions as follows:

$$\begin{aligned} h(x,t) &= \int_R f(x,c,t)\mathrm{d}c, \\ h(x,t)u(x,t) &= \int_R cf(x,c,t)\mathrm{d}c, \end{aligned} \tag{2}$$

$$h(x,t)u(x,t)^2 + 0.5gh(x,t) = \int_R c^2 q(x,c,t)\mathrm{d}c, \tag{3}$$

where g is the gravity acceleration.

The simplification leads to restrict the particle velocity c, previously a continuous variable, to take values in a discrete set $\{c_0, c_1, \ldots, c_N\}$. The hydrodynamic quantities are now given by discrete moments of the distribution functions

$$\begin{aligned} h(x,t) &= \sum_{i=0}^{N} f_i(x,t), \\ h(x,t)u(x,t) &= \sum_{i=1}^{N} c_i f_i(x,t), \end{aligned} \tag{4}$$

$$h(x,t)u(x,t)^2 + 0.5gh(x,t) = \sum_{i=0}^{N} c_i^2 f_i(x,t), \tag{5}$$

where $f_i(x,t) = f(x, c_i, t)$, and the LBGK equation is

$$\begin{aligned} f_i(x + c_i\Delta t, t) = f_i(x,t) - \frac{1}{\tau}(f_i(x,t) - q_i), \\ i = 0, 1, \ldots, N. \end{aligned} \tag{6}$$

Here $\{q_i, i = 0, 1, \ldots, N\}$ is the discrete local equilibrium distribution.

In fact all discrete velocities or LBGK models imply finding a discretization of the continuous equilibrium. From this viewpoint, the design of a proper discrete equilibrium plays a key role. The following four steps draw an outline to construct the cell–population equilibrium.

First, the Boltzmann–BGK equation is rewritten as

$$\begin{aligned} f(x + c\Delta t, c, t + \Delta t) =& f(x,c,t) - \frac{1}{\tau}(f(x,c,t) \\ & - q(x,c,t)), \end{aligned} \tag{7}$$

in which the particle velocity c is a continuous variable and $\tau = \lambda/\Delta t$ is the relaxation parameter.

Second, the non-equilibrium distribution is taken as the one-order Chapman–Enskog expansion form

$$f(x,c,t) = q(x,c,t) + \varepsilon f^{(1)}(x,c,t),$$

where

$$q(x,c,t) = \frac{h(x,t)}{\sqrt{2\pi}\sigma}\exp\{-\frac{(c - u(x,t))^2}{2\sigma^2}\} \tag{8}$$

is the local equilibrium, $\sigma^2 = \sigma(x,t)^2 = 0.5gh(x,t)$ and ε is the Knudsen number. Furthermore the one-order disturbance of f is assumed to have the form $f^{(1)} = q(x,c,t)\mu(x,c,t)$, i.e.

$$f(x,c,t) = q(x,c,t)(1 + \varepsilon\mu(x,c,t)), \tag{9}$$

with the collision conditions

$$\begin{aligned} \int_{-\infty}^{+\infty} \mu(x,c,t)q(x,c,t)\mathrm{d}c = 0, \\ \int_{-\infty}^{+\infty} c\mu(x,c,t)q(x,c,t)\mathrm{d}c = 0, \end{aligned} \tag{10}$$

and thus

$$\int_{-\infty}^{+\infty}\frac{1}{\tau}(q-f)\mathrm{d}c=-\frac{\varepsilon}{\tau}\int_{-\infty}^{+\infty}\mu q\mathrm{d}c=0,\ \int_{-\infty}^{+\infty}\frac{c}{\tau}(q-f)\mathrm{d}c=-\frac{\varepsilon}{\tau}\int_{-\infty}^{+\infty}c\mu q\mathrm{d}c=0. \tag{11}$$

Then the distribution function satisfies the following conservation laws:

$$\int_{-\infty}^{+\infty}f(x,c,t)\mathrm{d}c=\int_{-\infty}^{+\infty}q(x,c,t)\mathrm{d}c,\ \int_{-\infty}^{+\infty}cf(x,c,t)\mathrm{d}c=\int_{-\infty}^{+\infty}cq(x,c,t)\mathrm{d}c.$$

Let $\lambda=\varepsilon\hat{\lambda}$, where $\hat{\lambda}$ is of the same order as macroscopic time scale,[24] so $\tau=\varepsilon\hat{\tau}$, $\hat{\tau}=\hat{\lambda}/\Delta t$ and Eqs.(1) and (6) become

$$\frac{\partial f}{\partial t}+c\frac{\partial f}{\partial x}=\frac{1}{\varepsilon\hat{\lambda}}(q-f), \tag{12}$$

and

$$f(x+c\Delta t,c,t+\Delta t)=f(x,c,t)-\frac{1}{\varepsilon\hat{\tau}}(f(x,c,t)-q(x,c,t)). \tag{13}$$

respectively.

Third, let $D\subseteq R^1$ be a space domain and $X=\{x^1,x^2,\ldots,x^N\}\subseteq D$ be a discrete point set such that $x^1<x^2<\cdots<x^N$ with the space step $\Delta x=x^{i+1}-x^i$,$i=1,\ldots,N-1$. Denote by $C(x_0)$ a lattice cell with a centre x_0, i.e. $C(x_0)=[x_0-0.5\Delta x,x_0+0.5\Delta x]$, $\forall x_0\in\{x^i,i=1,\ldots,N\}$, then $D=\bigcup_{i=1}^{N}C(x^i)$. Note that $C(x_0)$ has $2k+1$ cell neighbours $\{C(x_{0i}),\ i=0,\pm1,\ldots,\pm k\}$, where $x_{0i}=x_0+i\Delta x$, $i=0,\pm1,\ldots,\pm k$. Sometimes we also write $C(x_{0i})=[x_i^{\mathrm{low}},x_i^{\mathrm{up}}]$ for symbolic simplification, here $x_i^{\mathrm{low}}=x_{0i}-0.5\Delta x$, $\quad x_i^{\mathrm{up}}=x_{0i}+0.5\Delta x$ and $x_{i+1}^{\mathrm{low}}=x_i^{\mathrm{up}}$, $i=0,\pm1,\ldots,\pm k$.

Theoretically, x is a continuous variable in the velocity distribution $f(x,c,t)$. However, a discrete scheme is necessary. In our discretization, the particles in $C(x_0)$ are considered to be at the cell centre x_0. It implies that only at x_0 the numerical information is available. Observing the change of the population at x_0 within a computational cycle $[t,t+\Delta t]$, we are easy to see that a particle with velocity c will reach x_0 to $x_0+c\Delta t$ at the terminal time $t+\Delta t$. As a consequence, a velocity cell $CV_i(\Delta t)=[c_i^{\mathrm{low}},c_i^{\mathrm{up}}]$ such that all particles at x_0 with velocity $c\in CV_i(\Delta t)$ will cross to the position cell $C(x_{0i})=[x_i^{\mathrm{low}},x_i^{\mathrm{up}}]$, the neighbour of $C(x_0)$, shown as Fig.1, where the low-bound $c_i^{\mathrm{low}}=(x_i^{\mathrm{low}}-x_0)/\Delta t$ and up-bound $c_i^{\mathrm{up}}=(x_i^{\mathrm{up}}-x_0)/\Delta t$. In this way, a one-to-one correspondence is constructed between the space cell $C(x_{0i})$ and the velocity cell $CV_i(\Delta t)$, $i=0,\pm1,\ldots,\pm k$. Notice that $h(x_0,t)=\int_{R^1}f(x_0,c,t)\mathrm{d}c$ is the total number of the particles in the cell $C(x_0)$ at time t. Then at $t+\Delta t$, the number of the particles transported from $C(x_0)$ to $C(x_{0i})$ is just

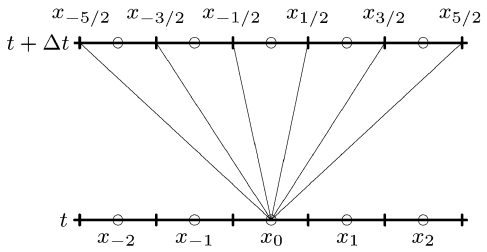


Fig.1. The particles in $C(x_0)$ will cross into its $2k+1$ neighbours.

$$h_i(x_0,t)=\int_{CV_i(\Delta t)}f(x_0,c,t)\mathrm{d}c,\quad i=0,\pm1,\ldots,\pm k, \tag{14}$$

and the transport momentum is

$$(hu)_i(x_0,t)=\int_{CV_i(\Delta t)}cf(x_0,c,t)\mathrm{d}c,\quad i=0,\pm1,\ldots,\pm k. \tag{15}$$

However, Eqs.(14) and (15) only consider the case of the particles transportation. More generally, the population $f(x_0+c\Delta t,c,t+\Delta t)$ in LBGK equation (13) includes the information of both the transportation and the collision at $t+\Delta t$. Hence the particle population cross into $C(x_{0i})$ from $C(x_0)$ at $t+\Delta t$ should be

$$h_i(x_0,t+\Delta t)=\int_{CV_i(\Delta t)}f(x_0+c\Delta t,c,t+\Delta t)\mathrm{d}c,\quad i=0,\pm1,\ldots,\pm k. \tag{16}$$

It gives a natural non-negative discretization of the continuous velocity distribution. Similarly we have a momentum approximation

$$(hu)_i(x_0, t+\Delta t) = \int_{CV_i(\Delta t)} cf(x_0 + c\Delta t, c, t+\Delta t)\mathrm{d}c,\ \ i = 0, \pm 1, \ldots, \pm k. \tag{17}$$

Due to the explicit expression of the non-equilibrium (9), Eqs.(16) and (17) also can be written as

$$h_i(x_0, t+\Delta t) = h_i(x_0, t) - \frac{\varepsilon}{\tau}\int_{CV_i(\Delta t)} q(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c, \tag{18}$$

$$(hu)_i(x_0, t+\Delta t) = (hu)_i(x_0, t) - \frac{\varepsilon}{\tau}\int_{CV_i(\Delta t)} cq(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c, \tag{19}$$

where $i = 0, \pm 1, \ldots, \pm k$.

The first term in the right of the equations describes particles transportation and the second term is particles collision. The zero and one order moments are easily obtained from the evolution equations (18)$\sim$(19) and the collision conditions (10):

$$\begin{aligned}\sum_{i=-k}^{k} h_i(x_0, t+\Delta t) &= \sum_{i=-k}^{k} h_i(x_0, t) - \frac{\varepsilon}{\tau}\sum_{i=-k}^{k}\int_{CV_i(\Delta t)} q(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c \\ &= \int_R f(x_0, c, t)\mathrm{d}c - \frac{\varepsilon}{\tau}\int_R q(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c \\ &= h(x_0, t),\end{aligned} \tag{20}$$

$$\begin{aligned}\sum_{i=-k}^{k} (hu)_i(x_0, t+\Delta t) &= \sum_{i=-k}^{k} (hu)_i(x_0, t) - \frac{\varepsilon}{\tau}\sum_{i=-k}^{k}\int_{CV_i(\Delta t)} cq(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c \\ &= \int_R cf(x_0, c, t)\mathrm{d}c - \frac{\varepsilon}{\tau}\int_R cq(x_0, c, t)\mu(x_0, c, t)\mathrm{d}c \\ &= h(x_0, t)u(x_0, t).\end{aligned} \tag{21}$$

By Chapman–Enskog expansion technique, the macro-equations (see Appendix for details)

$$\frac{\partial h(x,t)}{\partial t} + \frac{\partial (hu)(x,t)}{\partial x} = O(\Delta t), \tag{22}$$

$$\frac{\partial (hu)(x,t)}{\partial t} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = \frac{\partial}{\partial x}\left(\frac{\lambda}{2}gh^2\frac{\partial u}{\partial x}\right) + O(\Delta t), \tag{23}$$

are obtained. Where $\dfrac{\partial}{\partial x}\left(\dfrac{\lambda}{2}gh^2\dfrac{\partial u}{\partial x}\right)$ is a diffusive (viscous) term and as a byproduct, the following formula is useful in next section:

$$\int_{-\infty}^{+\infty} c^2 q\mu\mathrm{d}c = -\hat{\lambda}\frac{1}{2}gh^2\frac{\partial u}{\partial x}. \tag{24}$$

Especially, if $\varepsilon = 0$ (only transportation is considered), we have the 1D shallow water equation

$$\frac{\partial h(x,t)}{\partial t} + \frac{\partial (hu)(x,t)}{\partial x} = O(\Delta t), \tag{25}$$

$$\frac{\partial (hu)(x,t)}{\partial t} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = O(\Delta t). \tag{26}$$

2.2. Evolution formula

In our evolution scheme, the disturbance μ in the distribution (9) is taken as a $2n$-order polynomial

$$\mu = \beta_0 + \sum_{i=1}^{n}\beta_i(c-u)^{2i} + \sum_{i=1}^{n}\alpha_i(c-u)^{2i-1}. \tag{27}$$

By collision condition (10), the coefficients in Eq.(27) need to satisfy the following equations

$$\beta_0+\sum_{i=1}^{n}\beta_i\int_{-\infty}^{+\infty}(c-u)^{2i}\tilde{q}(x,c,t)\mathrm{d}c+\sum_{i=1}^{n}\alpha_i\int_{-\infty}^{+\infty}(c-u)^{2i-1}\tilde{q}(x,c,t)\mathrm{d}c=0, \tag{28}$$

$$\beta_0\int_{-\infty}^{+\infty}(c-u)\tilde{q}(x,c,t)\mathrm{d}c+\sum_{i=1}^{n}\beta_i\int_{-\infty}^{+\infty}(c-u)^{2i+1}\tilde{q}(x,c,t)\mathrm{d}c+\sum_{i=1}^{n}\alpha_i\int_{-\infty}^{+\infty}(c-u)^{2i}\tilde{q}(x,c,t)\mathrm{d}c=0, \tag{29}$$

here $\tilde{q}(x,c,t)=\dfrac{1}{\sqrt{2\pi}\sigma}\exp\{-\dfrac{(c-u(x,t))^2}{2\sigma^2}\}$. It is easy to obtain the relationship of the coefficients by a direct computation

$$\beta_0=-\sum_{i=1}^{n}\beta_i\sigma^{2i}m_{2i},\ \alpha_1=-\sum_{i=2}^{n}\alpha_i\sigma^{2(i-1)}m_{2i},$$

where $m_{2i}=\int_{-\infty}^{+\infty}s^{2i}\varphi(s)\mathrm{d}s=(2i-1)!!,\ \varphi(s)=\dfrac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{1}{2}s^2}$. Then the non-equilibrium distribution is

$$f(x,c,t)=q(x,c,t)\left\{1+\varepsilon\left[\sum_{i=1}^{n}\tilde{\beta}_i\left(\frac{(c-u)^{2i}}{\sigma^{2i}}-m_{2i}\right)+\sum_{i=2}^{n}\tilde{\alpha}_i\left(\left(\frac{c-u}{\sigma}\right)^{2i-1}-m_{2i}\left(\frac{c-u}{\sigma}\right)\right)\right]\right\}, \tag{30}$$

in which $\tilde{\beta}_i=\beta_i\sigma^{2i},\tilde{\alpha}_i=\alpha_i\sigma^{2i-1},i=1,2,\ldots,n$. We only consider the form of 2-order polynomial disturbance, i.e.

$$f(x,c,t)=q(x,c,t)\left[1+\varepsilon\tilde{\beta}\left(\left(\frac{c-u}{\sigma}\right)^2-1\right)\right],$$
$$(\text{note}\ \ m_2=1). \tag{31}$$

In this case, the coefficient $\tilde{\beta}=-\hat{\lambda}\dfrac{1}{4}gh\dfrac{\partial u}{\partial x}$ (by substituting Eq.(31) into Eq.(24)) and by use of Eq.(9), Eq.(13) becomes

$$f(x+c\Delta t,c,t+\Delta t)=q(x,c,t)(1+\varepsilon\mu(x,c,t))-\frac{1}{\tilde{\tau}}q(x,c,t)\mu(x,c,t). \tag{32}$$

Furthermore, substituting Eq.(31) into Eq.(32) we obtain

$$f(x+c\Delta t,c,t+\Delta t)=\frac{h}{\sigma}\varphi\left(\frac{c-u}{\sigma}\right)\left[1-\theta\left(\left(\frac{c-u}{\sigma}\right)^2-1\right)\right],\quad \theta=(\tau-1)\,\Delta t\frac{gh}{4}\frac{\partial u}{\partial x}. \tag{33}$$

Now due to Eq.(33), the evolution equations (16)$\sim$(17) have the following explicit expressions:

$$\begin{aligned}h_i(x_0,t+\Delta t)&=h(x_0,t)\int_{\frac{c_i^{\mathrm{low}}-u(z_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(z_0,t)}{\sigma}}\varphi(s)\left[1-\theta\left(s^2-1\right)\right]\mathrm{d}s\\&=h(x_0,t)\left\{(1+\theta)\int_{\frac{c_i^{\mathrm{low}}-u(z_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(z_0,t)}{\sigma}}\varphi(s)\mathrm{d}s-\theta\int_{\frac{c_i^{\mathrm{low}}-u(z_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(z_0,t)}{\sigma}}s^2\varphi(s)\mathrm{d}s\right\},\end{aligned} \tag{34}$$

$$\begin{aligned}(hu)_i(x_0,t+\Delta t)&=h(x_0,t)\int_{\frac{c_i^{\mathrm{low}}-u(x_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(x_0,t)}{\sigma}}(u+\sigma s)\varphi(s)\big(1-\theta\left(s^2-1\right)\big)\mathrm{d}s\\&=h_i(x_0,t+\Delta t)u(x_0,t)+h(x_0,t)\sigma\\&\times\left((1+\theta)\int_{\frac{c_i^{\mathrm{low}}-u(x_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(x_0,t)}{\sigma}}s\varphi(s)\mathrm{d}s-\theta\int_{\frac{c_i^{\mathrm{low}}-u(x_0,t)}{\sigma}}^{\frac{c_i^{\mathrm{up}}-u(x_0,t)}{\sigma}}s^3\varphi(s)\mathrm{d}s\right),\end{aligned} \tag{35}$$

where $i = 0, \pm 1, \ldots, \pm k$ and some auxiliary formulae are needed for these formulae:

$$\int_a^b s\varphi(s)\mathrm{d}s = \varphi(a) - \varphi(b),$$
$$\int_a^b s^2\varphi(s)\mathrm{d}s = a\varphi(a) - b\varphi(b) + \Phi(a) - \Phi(b),$$
$$\int_a^b s^3\varphi(s)\mathrm{d}s = a^2\varphi(a) - b^2\varphi(b) + 2(\Phi(a) - \Phi(b)).$$

To establish a non-negative evolution distribution $f(x+c\Delta t, c, t+\Delta t)$, we denote the support set parameter of the standard normal distribution $\varphi(x)$ by α, so $\varphi(x) \approx 0$ if $|x| > \alpha$. Then

$$q(x,c,t) = h(x,c,t)\varphi\left(\frac{c-u(x,t)}{\sigma(x,t)}\right)\Big/\sigma(x,t) \approx 0,$$

if $(c-u)/\sigma > \alpha$.
It implies neglecting the particles with velocity $c \notin [u-\alpha\sigma, u+\alpha\sigma]$. Now the condition $f(x+c\Delta t, c, t+\Delta t) \geq 0$ means $\varphi(s)(1-\theta(s^2-1)) \geq 0$, $s \in [-\alpha, \alpha]$ (see Eq.(32)) and we have

$$\left|(\tau-1)\Delta t\frac{gh}{4}u_x(s^2-1)\right| \leq 1\ , \quad s \in [-\alpha, \alpha],$$
$$\left|(\tau-1)\Delta t\frac{gh}{4}u_x(s^2-1)\right| \leq |\tau-1|\,\Delta t\frac{gh}{4}|u_x|(\alpha^2-1) \leq 1, \quad s \in [-\alpha, \alpha],$$
$$1 - \frac{4}{gh\,|u_x|\,(\alpha^2-1)\Delta t} \leq \tau \leq 1 + \frac{4}{gh\,|u_x|\,(\alpha^2-1)\Delta t}. \tag{36}$$

Combining Eq.(35) with $\tau > 0$, we obtain the range of the relaxation parameter τ

$$\max(1 - \frac{4}{gh\,|u_x|\,(\alpha^2-1)\Delta t}, 0) \leq \tau \leq 1 + \frac{4}{gh\,|u_x|\,(\alpha^2-1)\Delta t}. \tag{37}$$

The algorithm is a multi-speed evolution of LBGK equation: the particles in $C(x_0)$ will cross into its $2k+1$ neighbours $\{C(x_{0i}), i = 0, \pm 1, \ldots, \pm k\}$ (see Fig.1.). So for a given k and the lattice size Δx, these particles cannot be allowed to cross out of the set $\bigcup_{i=-k}^{k} C(x_{0i}) = [x_0 - (k+0.5)\Delta x, x_0 + (k+0.5)\Delta x]$ at the terminal time $t + \Delta t$. The fact introduces a velocity interval $[c_{-k}^{\mathrm{low}}, c_k^{\mathrm{up}}]$, where $c_{-k}^{\mathrm{low}} = -(k+0.5)\dfrac{\Delta x}{\Delta t} < 0$, $c_k^{\mathrm{up}} = (k+0.5)\dfrac{\Delta x}{\Delta t} > 0$ and $c_{-k}^{\mathrm{low}} \leq u(x_0,t) - \alpha\sigma(x_0,t) < u(x_0,t) + \alpha\sigma(x_0,t) \leq c_k^{\mathrm{up}}$, i.e. we only consider the particles with velocities $c \in [u(x_0,t) - \alpha\sigma(x_0,t), u(x_0,t) + \alpha\sigma(x_0,t)]$. Then it is easy to determine the time step Δt as follows:

$$\Delta t \leq \begin{cases} \dfrac{k\Delta x}{u+\alpha\sigma}, & u - \alpha\sigma > 0, \\ \min\left\{\dfrac{-k\Delta x}{u-\alpha\sigma}, \dfrac{k\Delta x}{u+\alpha\sigma}\right\}, & u - \alpha\sigma \leq 0 \leq u + \alpha\sigma, \\ \dfrac{-k\Delta x}{u-\alpha\sigma}, & u + \alpha\sigma < 0. \end{cases} \tag{38}$$

Finally, after a computational cycle, the hydrodynamic quantities at position x_0 are updated by

$$h^{\mathrm{new}}(x_0, t+\Delta t) = \sum_{i=-k}^{k} h_i(x_{0i}, t+\Delta t), \tag{39}$$

$$(hu)^{\mathrm{new}}(x_0, t+\Delta t) = \sum_{i=-k}^{k} (hu)_i(x_{0i}, t+\Delta t), \tag{40}$$

$$u^{\mathrm{new}}(x, t+\Delta t) = (hu)^{\mathrm{new}}(x_0, t+\Delta t)/h^{\mathrm{new}}(x_0, t+\Delta t), \tag{41}$$

for every grid point $x_0 \in \{x^1, x^2, \ldots, x^N\}$, where $\{x_{0i}, i = 0, \pm 1, \ldots, \pm k\}$ are x_0's $2k+1$ neighbours and the non-zero flux at x_{0i} cross into $C(x_0)$ at $t + \Delta t$, as shown in Fig.2.

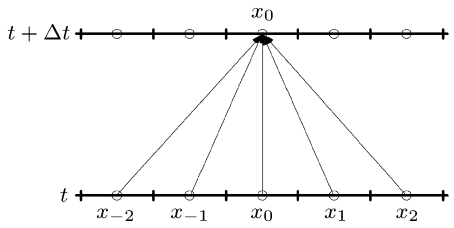


Fig.2. $2k+1$ neighbours of $C(x_0)$, for which the particles cross into $C(x_0)$.

2.3. Numerical examples

In this section, our lattice-cell BGK scheme is tested in 1D dam-break problem, where the homogeneous shallow-water equations are solved. The initial condition is

$$h(0,x)=\begin{cases} h_l, \text{ for } x\le 1000, \\ h_r, \text{ for } x>1000, \end{cases} \qquad u(0,x)=0,$$

$h_l > h_r$ is chosen to accord with the physical phenomenon of a dam-break from the left to the right. This test is allowed to isolate the behaviour of the scheme on a shock problem. The computational domain is symmetric around the point $x = 1000\,\mathrm{m}$. The total length L is 2000 m. Two different values for the space step, 10 m and 1 m have been used in order to show the effect of the mesh size. The time step is computed by using Eq.(37) and the nine-speed model is used in our work.

For the first test case, we prescribe $h_l = 100\,\mathrm{m}$ and $h_r = 50$ m. Figure 3(a) shows the water level h and the discharge velocity u for $\Delta x = 10\,\mathrm{m}$. The same result for $\Delta x = 1\,\mathrm{m}$ is shown in Fig.3(b). The computed solutions (the dot line) are compared with the exact one (solid line). This test shows the good shock capturing ability of the lattice-cell BGK scheme. However, when prescribe $h_l = 100\,\mathrm{m}$ and $h_r = 1\,\mathrm{m}$, a poorer result is shown in Fig.5(a) ($\Delta x = 10\,\mathrm{m}$). The result is improved after taking $\Delta x = 1\,\mathrm{m}$ but there still exist the slight fluctuations in Fig.5(b).

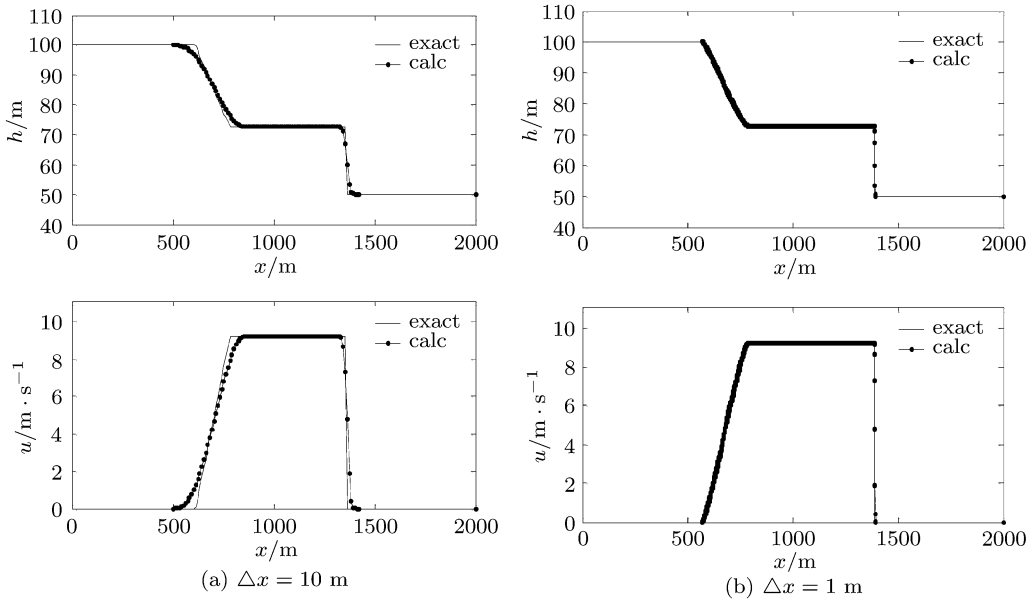
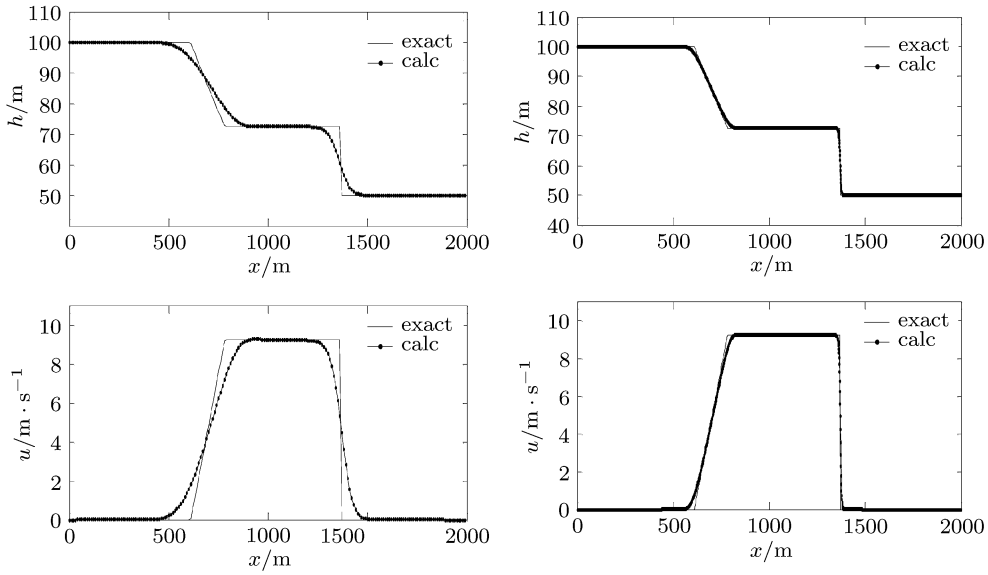


Fig.3. Dam-break: water level and discharge(100m vs 50m), the result in this paper compared with the exact one (right). Dot line: computed solutions. Solid line: exact solutions.

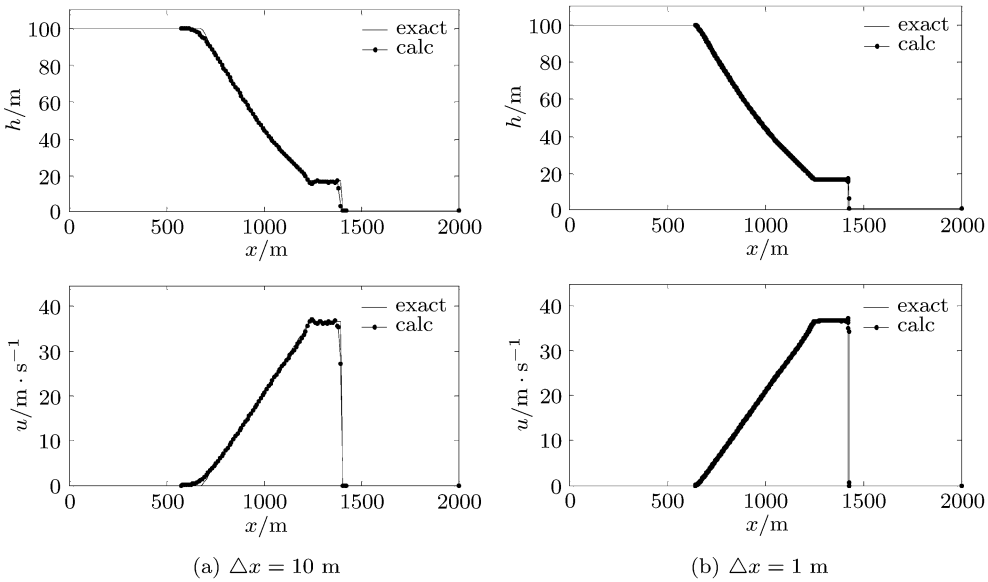
Compared with a usual lattice BGK method (3-speed, mentioned in Ref.[17], the results for $\Delta x = 10\,\mathrm{m}$ and $\Delta x = 1\,\mathrm{m}$ are shown in Figs.4(a) and 4(b) respectively), the lattice-cell BGK results agree with the exact solution better. When prescribe $h_l = 100\,\mathrm{m}$ and $h_r = 1$ m, the scheme mentioned in Ref.[16] is failed , it cannot solve such rush flow at all.

Remark An aggregate cell technique is used to deal with the still-flow part in the evolution process for a fewer computational cost. The details will be presented in another paper.



(a) $\triangle x = 10$ m (b) $\triangle x = 1$ m

Fig.4. Dam-break: water level and discharge(100m vs 50m), the result in Ref.[25] compared with the exact solution. Dot line: computed solutions. Solid line: exact solutions.



(a) $\triangle x = 10$ m (b) $\triangle x = 1$ m

Fig.5. Dam-break: water level and velocity(100m vs 1m). Dot line: computed solutions. Solid line: exact solutions.

3. Conclusion

In the LBM algorithms, constructing a discrete equilibrium is one of the central issues. Most of LBM schemes neglect the fact that both the equilibrium and the evolution population should be non-negative. However in our experience, an unstable numerical example always accompanies the negative evolution populations.[26] Another weakness is the assumption about a low Mach number which implies that the LBM is not effective to deal with some fluid models with larger velocity such as shock wave.

By applying the Chapman–Enskog distribution, two basic evolutionary steps of the LBM, the transportation and collision, are reduced to the transportation of the non-equilibrium distribution in our model. And then it is easy to design both the non-negative equilibrium and evolution population by selecting appropriate parameters. Furthermore, a multi-speed lattice Boltzmann (LB) scheme is also helpful to capture the shock wave.

A threshold value determines the range to main-

tain the non-negative evolutionary population. In our computational experience, the value is usually smaller than the one to make LB schemes numerically stable. The main reason is that LB schemes are tolerant to the negative evolutionary populations in some degree. In other words, it is possible that the scheme maintain the numerical stableness if situations where the negative populations appear in the evolutionary process is not too bad. This interesting issue is important and valuable to be further studied.

Appendix. Chapman–Enskog expansion and the shallow equation

To perform the Chapman–Enskog expansion we must expand the first-order Taylor equation[24,27]

$$f(x+c\Delta t,c,t+\Delta t)-f(x,c,t)=\Delta t\left(\frac{\partial}{\partial t}+c\frac{\partial}{\partial x}\right)f(x,c,t)+O(\Delta t), \tag{A1}$$

then take integrals on both sides of the equation:

$$h_i(x,t+\Delta t)-h_i(x,t)=\Delta t\left(\frac{\partial}{\partial t}\int_{CV_i(\Delta t)}f(x,c,t)\mathrm{d}c+\frac{\partial}{\partial x}\int_{CV_i(\Delta t)}cf(x,c,t)\mathrm{d}c\right)+O(\Delta t). \tag{A2}$$

From Eq.(18)

$$-\frac{\varepsilon}{\tau}\int_{CV_i(\Delta t)}q(x,c,t)\mu(x,c,t)\mathrm{d}c=\Delta t\left(\frac{\partial}{\partial t}\int_{CV_i(\Delta t)}f(x,c,t)\mathrm{d}c+\frac{\partial}{\partial x}\int_{CV_i(\Delta t)}cf(x,c,t)\mathrm{d}c\right)+O(\Delta t). \tag{A3}$$

Note $\tau=\varepsilon\hat{\tau}$, $\hat{\tau}=\hat{\lambda}/\Delta t$ so $\varepsilon/\tau=1/\hat{\tau}=\Delta t/\hat{\lambda}$, and from Eqs.(14) and (15) we have

$$\frac{\partial}{\partial t}h_i(x,t)+\frac{\partial}{\partial x}(hu)_i(x,t)=-\frac{1}{\hat{\lambda}}\int_{CV_i(\Delta t)}q(x,c,t)\mu(x,c,t)\mathrm{d}c+O(\Delta t),\ i=0,\pm1,\ldots,\pm k, \tag{A4}$$

where $\hat{\lambda}=\lambda/\varepsilon$. Similarly

$$(hu)_i(x,t+\Delta t)-(hu)_i(x,t)=\Delta t\left(\frac{\partial}{\partial t}\int_{CV_i(\Delta t)}cf(x,c,t)\mathrm{d}c+\frac{\partial}{\partial x}\int_{CV_i(\Delta t)}c^2f(x,c,t)\mathrm{d}c\right)+O(\Delta t), \tag{A5}$$

$$\frac{\partial}{\partial t}(hu)_i(x,t)+\frac{\partial}{\partial x}\int_{CV_i(\Delta t)}c^2f(x,c,t)\mathrm{d}c=-\frac{1}{\hat{\lambda}}\int_{CV_i(\Delta t)}cq(x,c,t)\mu(x,c,t)\mathrm{d}c+O(\Delta t). \tag{A6}$$

Summing to i on both sides of Eqs.(A4) and (A6), and applying the collision conditions (10), we obtain

$$\frac{\partial h(x,t)}{\partial t}+\frac{\partial(hu)(x,t)}{\partial x}=O(\Delta t), \tag{A7a}$$

$$\frac{\partial(hu)(x,t)}{\partial t}+\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}c^2f(x,c,t)\mathrm{d}c=O(\Delta t). \tag{A7b}$$

Now we need the expression of $\int_{-\infty}^{+\infty}c^2f(x,c,t)\mathrm{d}c$. Multiplying both sides of Eq.(9) by c^2 and taking integral, we obtain

$$\frac{\partial(hu)(x,t)}{\partial t}+\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}c^2q(x,c,t)\mathrm{d}c+\varepsilon\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}c^2q(x,c,t)\mu(x,c,t)\mathrm{d}c=O(\Delta t). \tag{A8}$$

From Eq.(3) we have

$$\frac{\partial(hu)(x,t)}{\partial t}+\frac{\partial}{\partial x}(hu^2+\frac{1}{2}gh^2)+\varepsilon\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}c^2q(x,c,t)\mu(x,c,t)\mathrm{d}c=O(\Delta t). \tag{A9}$$

The Chapman–Enskog expansion[9,20] seeks asymptotic solutions of Eq.(A9) in $\varepsilon \to 0$ by posing a multiple scales expansion of both f and t, but not x, in powers of ε.

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \varepsilon\frac{\partial}{\partial t_1}, \quad f = q + \varepsilon q\mu. \tag{A10}$$

We may think of t_0 and t_1 as advective and diffusive (viscous) respectively. From Eqs.(12) and (9) we have

$$\begin{aligned}&\left(\frac{\partial}{\partial t_0} + \varepsilon\frac{\partial}{\partial t_1}\right)(q + \varepsilon q\mu) + c\frac{\partial}{\partial x}(q + \varepsilon q\mu)\\ =&\frac{1}{\varepsilon\hat{\lambda}}(q - (q + \varepsilon q\mu)),\end{aligned} \tag{A11}$$

so

$$\left(\frac{\partial}{\partial t_0} + \varepsilon\frac{\partial}{\partial t_1} + c\frac{\partial}{\partial x}\right)(q + \varepsilon q\mu) = -\frac{1}{\hat{\lambda}}q\mu. \tag{A12}$$

Comparing coefficients of ε^0, ε and ε^2 on both sides of the equations, we can obtain the following equations:

$$\varepsilon^0: \quad \frac{\partial q}{\partial t_0} + c\frac{\partial q}{\partial x} = -\frac{1}{\hat{\lambda}}q\mu, \tag{A13a}$$

$$\varepsilon: \quad \frac{\partial q}{\partial t_1} + \frac{\partial(q\mu)}{\partial t_0} + c\frac{\partial(q\mu)}{\partial x} = 0, \tag{A13b}$$

$$\varepsilon^2: \quad \frac{\partial(q\mu)}{\partial t_1} = 0. \tag{A13c}$$

Taking the zero-order moment on both sides of Eqs.(A13a) and (A13b), we have

$$\frac{\partial h}{\partial t_0} + \frac{\partial(hu)}{\partial x} = 0, \quad \frac{\partial h}{\partial t_1} = 0. \tag{A14}$$

Then the continuous equation

$$\frac{\partial h}{\partial t} + \frac{\partial(hu)}{\partial x} = 0 \tag{A15}$$

can be rebuilt by these equations and the time relationship $\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \varepsilon\frac{\partial}{\partial t_1}$. Similarly, taking one-order moment on both sides of Eqs.(A13a) and (A13b) and noting Eq.(3), we have the relationships

$$\frac{\partial(hu)}{\partial t_0} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = 0,$$

$$\frac{\partial(hu)(x,t)}{\partial t_1} + \frac{\partial}{\partial x}\int_R c^2 q\mu \mathrm{d}c = 0.$$

Notice that Eq. (A13a) implies

$$\begin{aligned}\int_{-\infty}^{+\infty} c^2 q\mu \mathrm{d}c &= -\hat{\lambda}\left(\frac{\partial}{\partial t_0}\left(\int_{-\infty}^{+\infty} c^2 q\mathrm{d}c\right) + \frac{\partial}{\partial x}\left(\int_{-\infty}^{+\infty} c^3 q\mathrm{d}c\right)\right)\\ &= -\hat{\lambda}\left(\frac{\partial}{\partial t_0}(hu^2 + \frac{1}{2}gh^2) + \frac{\partial}{\partial x}(hu^3 + \frac{3}{2}gh^2u)\right)\\ &= -\hat{\lambda}\frac{1}{2}gh^2\frac{\partial u}{\partial x}\end{aligned} \tag{A16}$$

The third equation follows Eq.(3) and the fourth is derived as follows: from Eqs.(A14) and (A15) we have

$$\frac{\partial h}{\partial t_0} = -\frac{\partial(hu)}{\partial x}, \tag{A17a}$$

$$h\frac{\partial u}{\partial t_0} + u\frac{\partial h}{\partial t_0} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = 0, \tag{A17b}$$

by substituting equation (A17a) into equation (A17b), we can obtain

$$\begin{aligned}h\frac{\partial u}{\partial t_0} &= -u\frac{\partial h}{\partial t_0} - \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2)\\ &= u\frac{\partial(hu)}{\partial x} - \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2),\end{aligned}$$

and then

$$\frac{\partial}{\partial t_0}(hu^2 + \frac{1}{2}gh^2) + \frac{\partial}{\partial x}(hu^3 + \frac{3}{2}gh^2u) = u^2\frac{\partial h}{\partial t_0} + 2uh\frac{\partial u}{\partial t_0} + gh\frac{\partial h}{\partial t_0} + \frac{\partial}{\partial x}(hu^3 + \frac{3}{2}gh^2u)\frac{1}{2}gh\frac{\partial u}{\partial x}.$$

Now the momentum equation can be obtained by substituting Eq.(A16) into Eq.(A9)

$$\frac{\partial(hu)(x,t)}{\partial t} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = \frac{\partial}{\partial x}\left(\varepsilon\hat{\lambda}\frac{1}{2}gh^2\frac{\partial u}{\partial x}\right) + O(\Delta t).$$

Hence the macro-equations (A7a) and (A7b) can be written as follows:

$$\frac{\partial h(x,t)}{\partial t} + \frac{\partial (hu)(x,t)}{\partial x} = O(\Delta t), \tag{A18a}$$

$$\frac{\partial (hu)(x,t)}{\partial t} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = \frac{\partial}{\partial x}\left(\frac{\lambda}{2}gh^2\frac{\partial u}{\partial x}\right) + O(\Delta t). \tag{A18b}$$

Here, $\frac{\partial}{\partial x}\left(\frac{\lambda}{2}gh^2\frac{\partial u}{\partial x}\right)$ is a diffusive (viscous) term. Especially, let $\varepsilon = 0$, we obtain the 1D shallow water equation (only transportation is considered)

$$\frac{\partial h(x,t)}{\partial t} + \frac{\partial (hu)(x,t)}{\partial x} = O(\Delta t), \tag{A19a}$$

$$\frac{\partial (hu)(x,t)}{\partial t} + \frac{\partial}{\partial x}(hu^2 + \frac{1}{2}gh^2) = O(\Delta t). \tag{A19b}$$

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